5-1-2007

Vol. 6, No. 1 (Full Issue)

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Recommended Citation

Editors, JMASM (2007) "Vol. 6, No. 1 (Full Issue)," *Journal of Modern Applied Statistical Methods*: Vol. 6 : Iss. 1 , Article 36.

DOI: 10.22237/jmasm/1177994100

Available at: <http://digitalcommons.wayne.edu/jmasm/vol6/iss1/36>

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Invited Articles

Effects of Physical Activity on Psychological Change in Advanced Age: A Multivariate Meta-Analysis

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Loyola University Chicago

Betsy Jane Becker
Florida State University

Yael Netz
Wingate Institute, Israel

An example of multivariate meta-analysis is demonstrated by synthesizing the treatment effects of exercise of 15 groups on six mood state changes in elders measured by the Profile of Mood States (POMS) scale. Two different methods were used to analyze this multivariate dataset. The SAS codes for two set of the analyses were provided. Results showed that exercise has a modest and positive impact on elders mood change.

Key words: multivariate meta-analysis, mood state, POMS, Psychological change, exercise

Introduction

In this article, an application of meta-analysis to multivariate data is demonstrated. The eight primary studies included in the current meta-analysis are a subset of studies from a larger meta-analysis of the impact of exercise on psychological change in the elderly. The full list of studies on this topic, the search process, and

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study selection criteria can be found in Netz, Wu, Becker, and Tenenbaum (2005). This meta-analysis includes studies examining the treatment effects of exercise on mood change in the elderly, published between 1993 and 2001. Outcomes for participants in 15 treatment groups from these studies were measured by the Profile of Mood States (POMS; McNair, Lorr, & Droppleman, 1971), before and after exercise. Six identifiable mood states are measured in the POMS: Tension-Anxiety, Depression-Dejection, Anger-Hostility, Vigor-Activity, Fatigue-Inertia, and Confusion-Bewilderment, however, not all 15 groups provide measures of all six outcomes. (Below each scale is referred to using the first word of its label.) The numbers of mood states measured range from 4 to 6 in these groups. The 15 independent treatment groups in this meta-analysis produced 71 effect sizes.

Calculation of the Effect Size

The effect size in this synthesis is the standardized mean-change measure (Becker, 1988), which represents the magnitude of the

difference between the pretest and the posttest means for each outcome. It is defined as

$$g = \frac{\bar{Y}^{trt} - \bar{X}^{trt}}{S_X^{trt}}, \text{ where } \bar{Y}^{trt} \text{ denotes the posttest}$$

mean of the treatment group, $\bar{X}^{trt}$ denotes the pretest mean of the treatment group, and S_X^{trt} denotes the standard deviation of the pretest in the treatment group. The effect size g represents change from pretest to posttest in pretest-standard-deviation units. A g value of 1.0 for a treatment group indicates the participants' mean level of the outcome after exercise improved one standard deviation relative to their initial level.

All g s were corrected for bias due to small sample sizes. The unbiased effect size, denoted d , was obtained by correcting g via $d = (1 - \frac{3}{4n-5})g$, where n is the sample size for which g is computed. The variance of d is defined as $\text{var}(d) = \frac{4(1-r) + d^2}{2n}$, where r is the pretest-posttest correlation. Because r is not reported in any of the studies, it is assumed to be 0.7 in this meta-analysis.

The signs of effect sizes for all outcomes except vigor (which is scored positively) were reversed; therefore, all positive d values in the dataset indicate improved mood status.

Methodology

Several approaches to synthesizing multivariate data in meta-analysis are discussed and summarized in Becker (2000). Here, two methods are presented: One commonly used

approach creates independent subgroups for analysis; the other is more sophisticated, yet requires more assumptions. The latter approach uses generalized least squares (GLS) to take dependence among the outcomes into account while analyzing multivariate data (Raudenbush, Becker, & Kalaian, 1988). The two methods are used to calculate the mean effects of exercise (and associated standard errors) for each of the six mood states.

Method I: Creating Independent Subgroups

The 71 effect sizes were first categorized into six subgroups based on what mood state was measured. Effect sizes within each of the six sets of outcomes are independent, because each treatment group had at most one effect size for each mood state.

The mean effect size for each mood status can then be calculated separately. Each mean effect size is calculated by weighting each individual effect by its associated variance. The variance used for weighting was estimated based on the random-effects model, in which between-samples variation was accounted for, producing more conservative results. The variance of each effect was computed as $\text{var}(d) + S_\delta^2$, where $\text{var}(d)$ is defined above and S_δ^2 is a method-of-moments estimator of between-studies variation given in formula 18 of Shadish and Haddock (1994). More details on random-effects modeling can be found in Shadish and Haddock (1994, pp. 273-275).

Below is the SAS macro for calculating the mean effects and their standard errors for the six outcomes. The remarks in the right hand column document each of the steps.

%MACRO random(outcome);	<i>/*Start the macro;*/</i>
DATA &outcome;	
SET exercise.dat;	<i>/*Call in the data with the outcome</i>
IF outcome="&outcome"; RUN;	<i>of interest;*/</i>
DATA &outcome; SET &outcome;	<i>/*Calculate the sums of v (sv), d</i>
dd=d*d;	<i>(sd), and d² (sdd) for later</i>
PROC MEANS N SUM;	<i>calculation;*/</i>
VAR v d dd;	<i>/*v is variance of d; k is number of</i>
OUTPUT OUT=randeff N=k SUM=sv sd sdd;	<i>effect sizes;*/</i>
DATA randeff; SET randeff;	
svar=(sdd-sd*sd/k)/(k-1)-sv/k; RUN;	<i>/*Estimate between-group variation</i>
DATA RANDOM;	<i>(svar)based on random-effects</i>
IF _N_=1 then set randeff;	<i>model;*/</i>
SET &outcome;	
IF svar lt 0 then svar=0;	
vstar=v+svar;	<i>/*Calculate the new weight (vstar)</i>
wstar=1/vstar;	<i>that incorporates the between-group</i>
wdstar=wstar*d;	<i>variation;*/</i>
PROC MEANS NOPRINT N SUM;	
VAR wstar wdstar;	
OUTPUT OUT=sumup N=k	
SUM=swstar swdstar; RUN;	
DATA final; SET sumup;	
d_dot=swdstar/swstar;	<i>/*Calculate the mean effect(d_dot)</i>
se_d_dot=SQRT(1/swstar);	<i>and its standard error (se_d_dot);*/</i>
PROC PRINT DATA=final;	
VAR k d_dot se_d_dot; RUN;	
%MEND random;	<i>/*End of the macro;*/</i>
 %random(anger);%random(confus);	 <i>/*Run the macro for each outcome;*/</i>
%random(dep); %random(fatigue);	
%random(tens); %random(vigor);	

Method II: Accounting for Dependence among the Outcomes

To use the generalized least squares (GLS) method to model the dependence among outcomes and calculate the mean effects of exercise on each mood state, a vector $\mathbf{d}$ is created, containing all 71 effect sizes and a 71*71 variance-covariance matrix among the effects is obtained.

Let $\mathbf{d}_i$ represent the vector effect size for group i ($i=1$ to 15); d_{ij} in the vector represents the effect size from group i on measure j ($j=1$ to

6 for tension, depression, anger, vigor, fatigue, confusion). As noted earlier, not every study measured all six outcomes. Therefore, for example, the first group had only measures of tension ($j=1$), depression ($j=2$), anger ($j=3$), and vigor ($j=4$), and $\mathbf{d}_1=(d_{11}, d_{12}, d_{13}, d_{14})'$; The fifteenth group measured all six outcomes and $\mathbf{d}_{15}=(d_{(15)1}, d_{(15)2}, d_{(15)3}, d_{(15)4}, d_{(15)5}, d_{(15)6})'$.

The linear model that can be used to represent variation in effect sizes is:

$$\mathbf{d} = \mathbf{X} \times \boldsymbol{\delta} + \mathbf{e}$$

$$\begin{bmatrix} d_{11} \\ d_{12} \\ d_{13} \\ d_{14} \\ d_{21} \\ \vdots \\ d_{(15)6} \end{bmatrix}_{71 \times 1} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}_{71 \times 6} \times \begin{bmatrix} \delta_1 \\ \delta_2 \\ \delta_3 \\ \delta_4 \\ \delta_5 \\ \delta_6 \end{bmatrix}_{6 \times 1} + \begin{bmatrix} e_{11} \\ e_{12} \\ e_{13} \\ e_{14} \\ e_{21} \\ \vdots \\ e_{(15)6} \end{bmatrix}_{71 \times 1}$$

where the matrix $\mathbf{X}$ contains six columns to indicate which one of the six outcomes each effect size measured (e.g., a one in the first column means the effect was a measure of tension). The δ s, the regression coefficients for the dummy variables, represent the estimated mean effects, and e_{ij} is the corresponding residual for outcome j for group i .

The δ s can be estimated using GLS estimation, assuming the errors $\mathbf{e}$ have a mean vector of 0 and a known variance-covariance matrix Σ . The matrix Σ can be estimated by $\mathbf{S}$, which is the 71*71 variance-covariance matrix among the d_{ij} values, with the variance-covariance for each treatment group ($\mathbf{S}_i$) on the diagonal. Other elements in the matrix $\mathbf{S}$ are all 0 assuming the 15 treatment groups are independent of each other.

In each $\mathbf{S}_i$, the diagonal elements are the variances of each effect size, the $\text{var}(d_{ij})$ for $j = 1$ through 6 as defined above, plus the between studies variance. The off-diagonal elements in $\mathbf{S}_i$ are the covariances between pairs of effect sizes d_{ij} and $d_{ij'}$ for study i , each of which is defined as $S(d_{ij}, d_{ij'}) = r_{ijj'} S(d_{ij}) S(d_{ij'})$. The $S(d_{ij})$ and

$S(d_{ij'})$ are the square roots of $\text{var}(d_{ij})$ and $\text{var}(d_{ij'})$. The $r_{ijj'}$ are the correlations between outcomes j and j' , which unfortunately often are not reported and have to be assumed. In the current study, the correlations reported in the POMS manual (McNair et al., 1971) were used, which ranged from .13 between anger and vigor to .77 between tension and depression.

The mean effect for each outcome can be estimated by solving

$$\hat{\delta} = (\mathbf{X}'\mathbf{S}^{-1}\mathbf{X})^{-1} \mathbf{X}'\mathbf{S}^{-1}\mathbf{d}.$$

The variance-covariance matrix of the estimated mean effects is

$$\text{Var}(\hat{\delta}) = (\mathbf{X}'\mathbf{S}^{-1}\mathbf{X})^{-1}.$$

An easy way to obtain the estimates is to set up the values in $\mathbf{d}$, $\mathbf{X}$ and $\mathbf{S}$ in Excel, and then call them into SAS in the form of a vector ($\mathbf{d}$) and matrices ($\mathbf{X}$ and $\mathbf{S}$). That is, in the Excel spreadsheet the 71 effect sizes are in one column. Six more columns, each with 71 values, indicate the outcome(s) represented by each of the 71 effect sizes. Each column indexes one of the 6 outcomes, and each column contains a 1 in row r if the effect size in row r measured that specific outcome. The 71*71 variance-covariance matrix can be computed and saved in 71 columns, each with 71 values. The SAS IML code used to retrieve the data from Excel and to compute the estimates of mean effect for the outcomes and their standard errors are shown below.

DATA exercise.varcov; SET work.varcov; PROC IML; USE exercise.varcov; READ all var _num_ into S; STORE S; RUN;	<i>/*Save variance-covariance spreadsheet imported from Excel (work.varcov)as SAS dataset;*/ /*Save the data in the form of matrix S;*/</i>
PROC IML; USE exercise.data; READ all var {Danger Dconfuse Ddepress Dtension Dfatigue Dvigor} INTO X; READ all var {d} INTO d; STORE X d; RUN;	<i>/*Read in the six dummy coded outcomes in the SAS and form the (71*6) matrix X;*/ /*Read in the (71*1) effect size vector d;*/</i>
PROC IML; LOAD X d S; d_hat=inv(X*inv(S)*X)*X*inv(S)*d; se_d=SQRT(inv(X*inv(S)*X)); PRINT d_hat Vd; RUN;	<i>/*Estimate the means for each outcome (d_hat) and their standard errors (se_d);*/</i>

Results

The estimated mean effects of exercise on six mood states in the elderly are shown in Table 1. Under both methods, almost all mood states show significant improvement after the exercise intervention, except tension estimated using method I ($\bar{d}=0.12$) and vigor under both methods. Using method I, fatigue ($\bar{d}=0.30$), anger ($\bar{d}=0.29$), and depression ($\bar{d}=0.29$) improve the most; under method II, tension ($\bar{d}=0.28$), anger ($\bar{d}=0.27$), and depression ($\bar{d}=0.26$) improve the most.

The standard errors for outcomes based on method I are larger than those computed based on method II. This occurs in part because the intercorrelations among the outcomes allow estimates of each mean to borrow strength from other outcomes and thus precision is increased. Also, Table 1 shows the correlations among the group means. Although none of the entries is large, some are moderate in size suggesting that it would be wrong to treat the means as if they were independent, as one would if tests to compare means were conducted using method I.

Table 1. Results

Outcome	<i>k</i>	Method I		Method II						
		$\bar{d}$	<i>SE</i>	$\bar{d}$	<i>SE</i>	Correlations				
						C	D	T	F	V
Anger (A)	13	0.29*	0.076	0.27*	0.068	.34	.30	.28	.20	.02
Confusion (C)	12	0.15*	0.065	0.14*	0.053		.44	.40	.38	.08
Depression (D)	13	0.29*	0.084	0.26*	0.075			.35	.28	.07
Tension (T)	8	0.12	0.115	0.28*	0.065				.30	.06
Fatigue (F)	14	0.30*	0.072	0.13*	0.063					.09
Vigor (V)	11	0.20	0.243	0.17	0.204					

Note. The “*” indicates the mean effect size is significantly different from 0 at the .05 level

Conclusion

Exercise has a positive impact on elders' mood change, though all changes are modest (at most three tenths of a standard deviation). However, the magnitudes of the impact on different mood states are varied. Additional analyses would examine this variation among effect sizes, which can be quantified using *Q* statistics (Shadish & Haddock, 1994). Further investigation could focus on moderators such as type of exercise or participant age which might explain the variation in effects.

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Bimodality Revisited

Thomas R. Knapp
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Degree of bimodality is an important feature of a frequency distribution, because it could suggest heterogeneity, such as polarization or two underlying distributions combined into one. The literature contains several measures of bimodality. This article attempts to summarize most of those measures, with their attendant advantages and disadvantages.

Key words: Bimodality, kurtosis, moments, polarization

Introduction

The bimodality of a frequency distribution is of considerable interest in a number of disciplines. A Google search on ‘bimodality’ returns almost 300,000 entries. Applications of bimodality considerations are found in substantive investigations in fields as diverse as agriculture (e.g., Doehlert, et al., 2004), economics (e.g., Esteban & Ray, 1994), linguistics (e.g., Spivey, Grosjean, & Knoblich, 2005), medicine (e.g., Lim, Bakri, Morad, & Hamid, 2002; Grandi, et al., 2005), psychology (e.g., Lindner, 1997; Beach, Finchman, Amir, & Leonard, 2005), and sociology (e.g., DiMaggio, Evans, & Bryson, 1996; Greeley, 1997; Evans, Bryson, &

DiMaggio, 2001; Evans, 2003; Mouw and Sobel, 2001).

Esteban and Ray (1984) were concerned with the concept of societal polarization. They argued that one of the indicators of polarization is the bimodality of a frequency distribution for any variable that is an operationalization of an opinion construct such as attitude toward abortion. DiMaggio, Evans, and Bryson (1996), Greeley (1997), Mouw and Sobel (2001) studied the bimodality of several attitude variables--mostly Likert-type scales in the National Election Study (NES) and General Social Survey (GSS) data sets.

Purpose

The purpose of this article is to trace the methodological foundations of bimodality, some of the attempts that have been made to measure it, and some of the contributions to statistical inferences regarding it.

Historical Review

Karl Pearson

In his first of a series of articles on the mathematical theory of evolution, Pearson (1894) devised a procedure for determining whether or not a frequency distribution could be

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resolved into two normal distributions. The procedure involved six equations in six unknowns (the mean, standard deviation, and membership proportion for each of the two underlying normal distributions), which in turn led to a ninth-degree polynomial equation. If the given distribution had two peaks that were rather far apart it could be described as bimodal. He used as an example some data collected by Professor W.F.R. Weldon on 1000 crabs in Naples.

In a later article (1929) he showed that $b_2 - b_1$, where b_2 is the standardized fourth moment around the mean and b_1 is the square of the standardized third moment around the mean, must be greater than or equal to 1, with the equality holding for the two-point Bernoulli distribution, which is the most extreme case of bimodality.

Darlington to DeCarlo

Darlington (1970) claimed that b_2 (he called it k) is more a measure of unimodality vs. bimodality than a measure of peakedness vs. flatness as often discussed in statistics textbooks, i.e., it is a measure of the extent to which a distribution's z-scores cluster around +1 and -1, with the two-point Bernoulli distribution being the most bimodal, having a k of 1.

Chissom (1970) discussed various interpretations of the kurtosis statistic $\alpha_4 = b_2 - 3$, which is equal to 0 for the normal distribution. He pointed out that $\alpha_4 = -2$ for perfectly bimodal distributions.

In a brief note, Hildebrand (1971) expressed general agreement with Darlington, but gave examples of two bimodal distributions, for one of which $k-3$ was equal to -1.2 and for the other of which $k-3$ was equal to 3.

Moors (1986) agreed that k should be interpreted as the extent to which scores cluster around one s.d. to the right of the mean and one s.d. to the left of the mean.

Ruppert (1987) provided a long discussion of the various interpretations that have been made of b_2 , including peakedness and tail-thickness, and emphasized Hampel's (1974) influence function approach to the understanding of kurtosis.

Balandra and MacGillivray (1988) wrote a critical review of the literature on

kurtosis and favored the viewing of kurtosis as "a vague concept" (p. 116) regarding the location of a distribution's shoulders vis-a-vis its center and its tails.

In a more recent review of the literature on kurtosis, DeCarlo (1997) clarified the role of measures of kurtosis in tests for normality, tests for bimodality, and other matters, in the context of several previously-cited examples.

Reschenhofer and Schilling, Watkins, & Watkins

It has often been claimed that a mixture of two normal distributions is necessarily bimodal. Reschenhofer (2001) showed that to be true only if the two modes differ by two or more standard deviation units. Schilling, Watkins, and Watkins (2002) made the same claim for the special case of the distribution of adult heights when men and women are included in the same distribution. Those results are consistent with the arguments made by Darlington (1970) and Moors (1986) regarding the clustering of data at z-scores of +1 and -1 (a difference of two σ 's).

Choonpradub & McNeil

Choonpradub and McNeil (2005) were concerned that traditional box plots don't provide any indication of bimodality for the distributions such plots are meant to summarize. They recommended an enhancement (thickening the ends of the box denoting the quartiles) that might reflect bimodality.

Haldane to Frankland and Zumbo

The previously-cited authors were concerned primarily with the description of bimodality. Haldane (1952), however, suggested a fairly simple test for statistically significant bimodality, based upon the successive discrepancies of frequencies for adjacent categories in a sample frequency distribution. He used as an example the distribution of differences in hair color for 162 pairs of siblings.

Shenton & Bowman (1977) laid the groundwork for statistical inferences based upon the skewness coefficient $\sqrt{b_1}$, the kurtosis coefficient b_2 , their respective univariate sampling distributions, and their joint bivariate sampling distribution.

A truly bimodal distribution should have

a reasonably deep dip between the two modes. Hartigan and Hartigan (1985) developed a dip test that could be used to distinguish between unimodality and bimodality.

Tokeshi's (1992) test of the bimodality of a sample frequency distribution is a type of randomization (permutation) test that compares an actual sample distribution with all of the possible ways the total frequency could have been allocated to the various categories that comprise the variable of interest.

The estimation of the number and location of underlying modes for a sample frequency distribution was investigated by Minnotte (1997).

Frankland and Zumbo (2002) provided an SPSS program for distinguishing between a single underlying normal distribution and a bimodal composite of two underlying normal distributions.

Other Methodological Contributions

There is a set of miscellaneous formulas for the CLUSTER procedure in the SAS User's Guide. One of those formulas, derived by Warren Sarle (Personal Communication, 5/10/06), is a formula for the bimodality coefficient:

$$b = [(m_3^2 + 1)/(m_4 + [(3(n-1)^2)/((n-2)(n-3))])]$$

where m_3 is skewness and m_4 is kurtosis. Values of b greater than 0.555 (the value for a uniform population) may indicate bimodal or multimodal marginal distributions. The maximum of 1.0 (obtained for the Bernoulli distribution) is obtained for a population with only two distinct values. Very heavy-tailed distributions have small values of b regardless of the number of modes.

The notation is unconventional, because the m 's usually represent the unstandardized moments about the mean (so just substitute b_1 for m_3^2 and b_2 for m_4). Slight variations of it (for large n the term inside the square brackets is often deleted if 3 has not been subtracted from b_2 , or replaced by 3 if it has).

There is another statistic that is also called a bimodality coefficient; it is a function of the likelihood ratio for normal distributions vs. mixtures of normal distributions (see Ashman & Bird, 1994 for an application to astronomy).

In his technical article about L-moments, Hosking (1990) claimed that the ratio of two of them "could be interpreted as a measure of tendency to bimodality" (p. 111).

A Personal View of Bimodality

Bimodality should be thought of topologically. If you push down on the peak of a unimodal distribution the frequency curve gets flatter and flatter until it becomes a uniform distribution. If you keep pushing further the curve crawls upward to the left and to the right and ultimately ends up as a two-point distribution. How then to measure the degree of bimodality of an actual distribution? As Pearson (1929), Shenton and Bowman (1977), and others had pointed out, $b_2 - b_1$ must be greater than or equal to 1, so that $b_2 - b_1$ should be a reasonable measure of bimodality, because it takes on its smallest value (1), for the two-point Bernoulli distribution, and it takes on its largest value (conceptually infinite) for a distribution with a single tall peak.

That approach was taken in Knapp (1959) and in a subsequent unpublished paper Knapp (1970) in which an attempt was made to derive the sampling distribution of $b_2 - b_1$ for samples from a normal distribution. That attempt was only partially successful because only the first two moments could be derived mathematically (a Monte Carlo approach was used for the rest of the basis for statistical inference), and significant non-normality is not necessarily the same as significant bimodality.

Some Examples of Descriptive Comparisons

Consider the following hypothetical frequency distributions for a variable that ranges from 1 to 11 and for a sample size of 100 (see Figures 1 through 9).

X	f
1	6
2	10
3	11
4	10
5	9
6	8
7	9
8	10
9	11
10	10
11	6

Figure 1

X	f
1	1
2	7
3	9
4	11
5	10
6	8
7	9
8	11
9	12
10	13
11	9

Figure 2

X	f
1	2
2	8
3	10
4	11
5	12
6	14
7	12
8	11
9	10
10	8
11	2

Figure 3

X	f
1	1
2	3
3	6
4	12
5	18
6	20
7	18
8	12
9	6
10	3
11	1

Figure 4

X	f
1	1
2	2
3	4
4	6
5	12
6	16
7	21
8	23
9	14
10	1
11	0

Figure 5

X	f
1	3
2	3
3	4
4	6
5	12
6	44
7	12
8	6
9	4
10	3
11	3

Figure 6

X	f
1	2
2	3
3	3
4	3
5	3
6	4
7	5
8	11
9	21
10	41
11	4

Figure 7

X	f
1	13
2	11
3	10
4	9
5	7
6	1
7	8
8	9
9	9
10	11
11	12

Figure 8

X	f
1	10
2	10
3	10
4	10
5	10
6	10
7	10
8	10
9	10
10	10
11	0

Figure 9

Table 1. Results from Figures 1 through 9

Figure	b_1	b_2	rank*	$b_2 - b_1$	rank*	$(b_1+1)/b_2$	rank*
1	.000	1.757	2	1.757	2	.569	4
2	.021	1.786	4	1.765	3	.572	3
3	.000	2.046	5	2.046	6	.489	7
4	.000	2.804	6	2.804	8	.357	8
5	.549	3.113	7	2.564	7	.498	6
6	.000	4.043	8	4.043	9	.247	9
7	2.443	4.414	9	1.971	5	.780	1
8	.001	1.515	1	1.514	1	.660	2
9	.000	1.776	3	1.776	4	.563	5

Notes. * 1 = most bimodal; 9 = least bimodal

For each distribution, b_2 , $b_2 - b_1$, and $(b_1+1)/b_2$ were calculated (see Table 1). The relative agreement among the three measures of bimodality is fairly good except for Figure 7. That figure is clearly not bimodal, which would intuitively rule out $(b_1+1)/b_2$ as an indicator of its bimodality. b_2 alone would suggest that

Figure 7 is the least bimodal of the nine figures, but $b_2 - b_1$ would suggest that four of the other distributions (Figures 3, 4, 5, and 6) are less bimodal, with Figure 6 being the least. Therefore, $b_2 - b_1$ is the better indicator of bimodality because a flattening out in Figure 7 may be seen, followed by a second mode

popping up at the low end of the scale, if you push down hard enough on the mode at an abscissa value of 10. The appearance of two modes would take much longer with Figure 6 (Three modes would pop up there first--one at each end to go along with the one in the middle).

Statistical Inferences Using the Same Examples

In addition to its simplicity, Haldane's test appears to be the most defensible, because it is appropriate for both interval and ordinal scales. It has been applied to the distributions in Figures 1-9, with the relatively surprising result that none of those distributions is significantly bimodal at the .05 level (see Figure 10). It is

Surprising, because Figure 8, for example, really looks bimodal and the sample size is reasonably large (100). But, Figure 10 is an example of one that is; note the deeper trough between the two peaks.

Two real-data examples

Sullivan (2005) found that the frequency distribution of Type 1 rates for age at first birth (with number of previously childless women of childbearing age in the denominator) exhibited a bimodal pattern in the 90s, with peaks at both 20 and 30 years of age. Figure 11 is the Sullivan graph which illustrates that phenomenon for the years 1991, 1995, and 1999:

X	f
1	5
2	5
3	30
4	5
5	5
6	0
7	5
8	5
9	30
10	5
11	5

Figure 10

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Figure 11. Sullivan Graph

Another interesting recent example of bimodality is discussed in the paper by Roller (2005) regarding the results of a questionnaire sent to U.S. members of the International Reading Association that elicited responses to questions about President George W. Bush's "No Child Left Behind" (NCLB) program. In that

article, she said that several of the five-point frequency distributions were bimodal. Here is the example that she emphasized:

Item: "The educational benefits resulting from NCLB implementation in your school district will, on balance, outweigh any adverse impacts for students in the aggregate."

Table 2

Response	Frequency
Strongly Agree	115
Agree	396
Neither Agree Nor Disagree	285
Disagree	357
Strongly Disagree	219
Total	1372
No Response	178
Grand Total	1550

Roller (2005) called the attention of the reader to the modes at Agree and Disagree (see Table 2). b_2 for these data is 1.899; b_1 is .000 (to three decimal places--the distribution is very close to symmetric); $b_2 - b_1 = 1.899$; and $(b_1 + 1)/b_2 = .527$. Haldane's test supports the hypothesis of underlying bimodality. But the dip between those two modes at Neither Agree nor Disagree could be an artifact of a non-committal response rather than a valley between two peaks. (The large No Response percentage might be further evidence of such an artifact.)

There has been a considerable amount of empirical research regarding the middle category of a five-point Likert-type scale; see, for example, Guy & Norvell (1977) and Armstrong (1987). Mouw and Sobel (2001) argued that DiMaggio et al. (1996) should not have applied their measure of bimodality ($b_2 - 3$) to Likert-type scales, because it assumes interval-scale properties. The treating of ordinal scales as interval scales is one of the most controversial matters in statistical methodology. There appears to be no solution to the problem that would be acceptable to the warring factions.

Miscellany

Although all of the standard computer packages (SAS, SPSS, Minitab, Excel) include the calculation of one or more measures of skewness and kurtosis, the formulas used in those packages vary somewhat from one another. If you'd like to compute b_1 in Excel, for instance, you need to square SKEW and multiply that by $\{(n-1)^2/(n-2)^2\}$ in order to undo the sample adjustments. As well, in order to compute b_2 you need to add,

$$\{3(n-1)^2/(n-2)(n-3)\}$$

to KURT and multiply that by

$$\{(n-2)(n-3)/(n+1)(n-1)\}.$$

Baretto, Borges, & Guo (2003) pointed out that a typographical error in an article citing one of Tokeshi's (1992) formulas has led to several incorrect tests of the bimodality of distributions that are of interest to researchers concerned with the range-size of various animal species. (Even in their correct form his formulas are tricky, because they require very careful attention to summation operations and combinatorial notation.)

In an interesting article many years ago, Baker (1930) hinted that one should not get too excited about bimodality because a bimodal distribution can often be changed into a unimodal distribution by means of an algebraic transformation. He gave as an example a continuous bimodal fourth-degree polynomial distribution of X that could be converted into a continuous unimodal distribution by replacing X with e^X .

Conclusion

There are several measures of the bimodality of a frequency distribution. There are also several tests of the statistical significance of sample bimodality. Hopefully, this article has provided at least a partial summary of such procedures.

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Ordinal Versions of Coefficients Alpha and Theta for Likert Rating Scales

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Two new reliability indices, ordinal coefficient alpha and ordinal coefficient theta, are introduced. A simulation study was conducted in order to compare the new ordinal reliability estimates to each other and to coefficient alpha with Likert data. Results indicate that ordinal coefficients alpha and theta are consistently suitable estimates of the theoretical reliability, regardless of the magnitude of the theoretical reliability, the number of scale points, and the skewness of the scale point distributions. In contrast, coefficient alpha is in general a negatively biased estimate of reliability. The use of ordinal coefficients alpha and theta as alternatives to coefficient alpha when estimating the reliability based on Likert response items are recommended. The choice between the two ordinal coefficients depends on whether one is assuming a factor analysis model (ordinal coefficient alpha) or a principal components analysis model (ordinal coefficient theta).

Key words: Internal consistency, reliability, coefficient alpha, coefficient theta.

Introduction

Coefficient alpha is the most widely used index of reliability in the social sciences (Zumbo & Rupp, 2004). There is, however, ongoing debate about the use of alpha for Likert type rating response scales because alpha assumes that the item responses are continuous. Using Likert type

response scales, it has been demonstrated that the magnitude of coefficient alpha can be spuriously deflated with less than five scale points. However, reliability was found to level off beyond six points (Gelin, Beasley, & Zumbo, 2003). Likert type data are commonly utilized in psychological and educational settings to measure unobserved continuous variables. Yet, lack of clarity still prevails regarding the statistical impact of various numbers of response scale points on outcomes that are based on a continuous concept. Of course, a special case of coefficient alpha is KR-20, which is computed from binary data.

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One can compute estimates of reliability from correlation (or, more generally, covariance) matrices. For example, the Pearson correlation matrix is commonly used to compute coefficient alpha. An important assumption for the use of the Pearson correlation matrix is the assumption of continuity. If this assumption is violated, the

Pearson correlation matrix may be distorted (Rupp, Koh, & Zumbo, 2003). If the data are ordinal, the correlation matrix of choice is the polychoric correlation matrix, which estimates the linear relationship for two unobserved continuous variables given only observed ordinal data (Flora & Curran, 2004). Hence, for Likert type scales it may be useful to investigate reliability estimates based on the polychoric correlation matrix, thereby taking into account the ordinal nature of the data. A special case of the polychoric correlation matrix is the tetrachoric correlation matrix for binary data.

Rationale and theoretical framework

Coefficient alpha is used as a default for estimating the internal consistency based on the Pearson correlation matrix in widely available software packages such as SPSS and SAS; however, this is done ignoring the Likert response format of the items at hand. The purpose of this article was to introduce two new reliability indices, ordinal coefficient alpha and ordinal coefficient theta, and test their appropriateness as estimates of internal consistency for items with Likert response formats.

Considering only a Pearson correlation matrix and a factor analysis model, McDonald (1985, p. 217) describes how one can compute coefficient alpha from a factor analysis model. For a composite score based on p items coefficient alpha can be computed as

$$\alpha = \frac{p}{p-1} \left[\frac{p(\bar{f})^2 - \bar{f}^2}{p(\bar{f})^2 + \bar{u}^2} \right], \quad (1)$$

where $\bar{f}$ is the average of the p factor loadings, $\bar{f}^2$ is the average of the squares of the p factor loadings, and $\bar{u}^2$ is the average of the p uniquenesses.

Armor (1974) introduced a reliability estimate, coefficient theta, which was developed to account for multidimensionality in a scale and is based on a principal components model. Coefficient theta for the single factor solution is computed with the following equation (Armor, p. 28):

$$\Theta = [p/(p-1)] * [1 - (1/\lambda_1)], \quad (2)$$

where the only new symbol λ_1 denotes the largest eigenvalue from the principal component analysis of the correlation matrix of the items involved in the composite.

Ordinal coefficient alpha and ordinal coefficient theta are computed by applying equations (1) or (2), respectively, to the polychoric correlation matrix. These reliability estimates are ordinal in the sense that they take into account the ordinal nature of the Likert response data.

In the following, a computer simulation study is reported that investigated the population estimation bias of ordinal coefficients alpha and theta for response scales ranging from two to seven points, with symmetric as well as skewed Likert response distributions, and theoretical reliabilities of .4, .6, .8, and .9. Next, ordinal coefficients alpha and theta were demonstrated with real data. The article closes with discussion of the findings and recommendations.

Methodology

Simulation study

Simulation data were generated to reflect the conditions of theoretical alpha (.4, .6, .8, and .9) as well as skewness conditions of zero and -2 of the item responses. The fundamental equations of factor analysis were used to create a population covariance matrix; this covariance matrix was then used to generate normally distributed item responses. That is, item response data were generated using a factor analysis model. As indicated by Jöreskog (1971) and Henrysson and Wedman (1972), the decomposition of an observed score X into a true score and an error score in classical test theory can be generalized to a factor analytic model with one common factor. The formula $X = T + E$ can be defined as

$$X_i = f_i \xi + u_i \quad i=1, 2, \dots, p, \quad (3)$$

where X_i denotes the observed scores, f_i denotes the factor loadings, ξ the common factor that can also be regarded as true score, u_i , uniqueness of variables, denotes the error

scores, and i indexes the items running from one to p . In a factor model, the reliability of the observed score can be obtained by summing all true score variances and covariances in the matrix and then by dividing this sum by the total variance (Reuterberg & Gustafsson, 1992). Novick and Lewis (1967) showed that coefficient alpha yields an unbiased estimate of reliability when the loadings of each variable on the common factor are equal. The formula for the reliability of a composite score is

$$\rho_{xx} = \frac{\left(\sum_{i=1}^p f_i \right)^2}{\left(\sum_{i=1}^p f_i \right)^2 + \sum_{i=1}^p \text{var}(e)_{ii}}, \quad (4)$$

where $\text{var}(e)_{ii}$ denotes the error variance in a factor analytical model and all the other symbols are defined above. To obtain the population reliabilities of .4, .6, .8, and .9, factor loadings of .213, .311, .471, and .625, respectively, were computed using the above formula. Therefore, in summary 14 items with continuous (normally distributed) distributions were generated using one common factor model with equal factor loadings across the 14 items. Fourteen items were chosen because it is a typical scale length in health and educational research (Slocum, 2005).

These (underlying) item response distributions were then transformed into Likert responses by applying the thresholds (for the symmetric as well as skewed item responses) as provided in the Appendix. The number of response options was simulated to range from 2 to 7; by including 2 response options, one is also able to investigate how the new reliability estimates perform in the presence of binary data.

As noted above, the unidimensionality and equal factor loadings provide a strict condition where empirical alpha should equal theoretical alpha. It was confirmed that the simulation methodology worked correctly because the theoretical alpha was obtained when analyzing the continuous data. It should be noted that, given the simulation design, there was no

interest in the sample-to-sample variability in the estimates but rather the focus was on accuracy (bias) of the estimates. Therefore, population analogues of the empirical reliability estimates were computed with a sample size of 10,000 simulees in each cell of our simulation design.

The following steps were followed for the analysis. The data were simulated and coefficient alpha was obtained using SPSS. The simulated data were then read into PRELIS. In order to compute ordinal coefficient alpha the polychoric correlation matrix was factor analysed using the MINRES procedure. The resulting factor loadings and uniquenesses were then used to compute ordinal coefficient alpha. In addition, the eigenvalues of the polychoric correlation matrix among the items were computed from the principal components analysis and used to compute ordinal theta.

Results

The reliability estimates for the simulated data are displayed in Tables 1 to 4, for theoretical reliability of 0.4 to 0.9, respectively. As can be seen from these tables, coefficient alpha is consistently a negatively biased estimate of the theoretical reliability. Note that in the case of equal factor loadings and unidimensionality coefficient alpha should equal the reliability; that is, it is not a lower bound. The negative bias of alpha was even more evident under the condition of negative skewness; for example, in the case of theoretical reliability of .6 and 3 response options alpha underestimates the theoretical reliability by .175. These results highlight that coefficient alpha, likewise KR-20 for binary data, gives one a downwardly biased estimate of the theoretical reliability with Likert data. With regard to the number of scale points our finding is a replication of the finding of Gelin, Beasley, and Zumbo (2003) that showed that alpha computed from Likert item response data approaches its theoretical value as the number of scale points increases, and levels off at about 6 scale points.

Table 1. Reliability Estimates for Theoretical Alpha of .4 (all factor loadings are .213)

# of response options	Skewness					
	0			-2		
	Alpha	Ordinal Alpha	Ordinal Theta	Alpha	Ordinal Alpha	Ordinal Theta
2	.288	.393	.395	.211	.389	.391
3	.328	.401	.400	.233	.383	.387
4	.356	.399	.400	.258	.379	.382
5	.377	.406	.408	.255	.384	.387
6	.378	.398	.400	.291	.382	.387
7	.386	.401	.404	.303	.391	.391

Table 2. Reliability Estimates for Theoretical Alpha of .6 (all factor loadings are .311)

# of response options	Skewness					
	0			-2		
	Alpha	Ordinal Alpha	Ordinal Theta	Alpha	Ordinal Alpha	Ordinal Theta
2	.488	.608	.609	.379	.596	.596
3	.527	.609	.609	.425	.603	.603
4	.561	.608	.609	.421	.598	.600
5	.576	.607	.609	.452	.597	.598
6	.587	.609	.609	.459	.599	.600
7	.589	.606	.607	.477	.598	.598

Table 3. Reliability Estimates for Theoretical Alpha of .8 (all factor loadings are .471)

# of response options	Skewness					
	0			-2		
	Alpha	Ordinal Alpha	Ordinal Theta	Alpha	Ordinal Alpha	Ordinal Theta
2	.702	.802	.802	.629	.806	.806
3	.732	.799	.799	.655	.798	.798
4	.762	.800	.800	.668	.803	.804
5	.773	.798	.798	.689	.800	.800
6	.783	.801	.801	.709	.803	.804
7	.785	.798	.798	.725	.804	.804

Table 4. Reliability Estimates for Theoretical Alpha of .9 (all factor loadings are .625)

	Skewness					
# of response options	0			-2		
	Alpha	Ordinal Alpha	Ordinal Theta	Alpha	Ordinal Alpha	Ordinal Theta
2	.826	.897	.897	.778	.899	.899
3	.849	.899	.899	.806	.899	.899
4	.872	.897	.897	.810	.898	.898
5	.882	.897	.897	.830	.899	.899
6	.886	.898	.898	.840	.900	.900
7	.891	.898	.898	.852	.900	.900

In contrast to coefficient alpha, ordinal coefficients alpha and theta were consistently found to be suitable estimates of reliability regardless of the magnitude of the theoretical reliability and number of scale points. In addition, it should be noted that the skewness of the item response distribution affects coefficient alpha, whereas ordinal coefficients alpha and theta remain unaffected by skewness. Specifically, ordinal coefficients alpha and theta are still suitable in the presence of skewed data; however, coefficient alpha becomes more biased with skewness. A comparison between the two ordinal estimates shows that they are almost exactly identical. In the following, ordinal coefficients alpha and theta are compared to coefficient alpha in the context of real data.

Real data examples

The real data examples are based on two samples. The data of the first sample was collected between 1995-1996 by Professor Ed Diener and his collaborators worldwide with College students from 42 nations. The following scales were used. The Satisfaction with Life Scale (SWLS) (Diener, Emmons, Larsen, & Griffin, 1985) is a 5-item instrument designed to measure global cognitive judgments of one's life using a 7-point Likert-type scale ranging from 1

(strongly disagree) to 7 (strongly agree). Diener's Affect Balance Scale (Veenhoven, 2004) is an 8-item instrument designed to measure positive and negative affect (each being one dimension with four items; this was supported in the present study by a principal component analysis of the polychoric correlation matrix) using a 7-point Likert-type response scale ranging from 1 (never) to 7 (always). The Positive and Negative Affect Schedule (PANAS) (Watson, Clark, & Tellegen, 1988) consists of two 10-item scales with a 5-point Likert type response scale, ranging from 1 (very slightly) to 5 (extremely). In the present study only the Positive Affect Schedule (PAS) was used. Sample sizes for these questionnaires ranged between 6958 and 7014.

The data of the second sample was collected in 1993 by the first author at a Canadian university. The Eysenck Personality Questionnaire (EPQ) (Eysenck & Eysenck, 1975) was administered to 922 students. This questionnaire consists of four subscales with a binary response scale with 0 (no) and 1 (yes). For the present study only the neuroticism (23 items) and extraversion (21 items) subscales were used.

Coefficient alpha was computed for the (sub)scales using SPSS. The data were entered into PRELIS to obtain the polychoric correlation matrix to compute ordinal coefficients alpha and theta as described above. The items of the SWLS exhibited a skewness ranging from -.56 to .18, with an average skewness of -.27. The positive items of the affect scale exhibited a skewness ranging from -.06 to .53, with an average skewness of .17. The negative items of the affect scale exhibited a skewness ranging from .90 to 1.27, with an average skewness of 1.04. The items of the PAS exhibited a skewness ranging from -.39 to .05, with an average skewness of -.21. The items of the extraversion scale exhibited a skewness ranging from -3.27 to .56, with an average skewness of -1.02. The items of the neuroticism scale exhibited a skewness of -1.88 to .89, with an average skewness of -.32.

The reliability estimates, coefficient alpha and ordinal coefficients alpha and theta,

for the scales are provided in Table 5. Table 5 shows that ordinal coefficients alpha and theta display a larger reliability estimate than coefficient alpha for all scales. However, for the four scales with the 5- and 7-point Likert type response scales, the difference between coefficient alpha and ordinal coefficients alpha and theta is small. In contrast, for the scales with the binary response format the difference between coefficient alpha and ordinal coefficients alpha and theta is more prominent. This is in accordance with the findings of the simulation study, which showed that with increased number of response options, coefficient alpha and the ordinal estimates become closer. Based on the findings from the simulation study, where ordinal coefficients alpha and theta were consistently demonstrated to be more precise estimates, this finding can be interpreted as showing that ordinal coefficients alpha and theta are closer to the theoretical alpha of the scales.

Table 5. Reliability Estimates for Real Data with the SWLS, Positive and Negative Affect, PAS, Extraversion and Neuroticism Scales

Scale	Alpha	Ordinal Alpha	Ordinal Theta
SWLS	.814	.835	.836
Positive Affect	.709	.735	.738
Negative Affect	.667	.684	.686
PAS	.824	.845	.846
Extraversion	.819	.908	.916
Neuroticism	.830	.905	.910

Conclusion

In summary, it was found that coefficient alpha computed from Likert response data results in a negatively biased estimate of the theoretical reliability. Because it is a special case of coefficient alpha, KR-20 also shows this bias when used with binary response data. It should be noted that coefficient alpha (and KR-20) are correlation-based statistics and hence assume continuous data. What is noteworthy about the coefficient alpha findings is that the measurement model used in the simulation involves all of the assumptions of coefficient alpha, so that alpha would equal the conceptual/theoretical reliability. However, it was found that coefficient alpha is rather drastically affected by Likert data – e.g., imagine a 14 item scale comprised of a 3-point Likert response format with a skewness of -2 ; the resulting coefficient is .66 when the theoretical reliability is .80.

Ordinal coefficients alpha and theta, on the other hand, were found to be suitable alternatives to coefficient alpha when a researcher is confronted with having to compute a reliability estimate with Likert response data. It should be noted that with advances in statistical software, these ordinal coefficients are easy to calculate using the newly developed and freely available software FACTOR (Lorenzo-Seva & Ferrando, in press) or with widely available software such as PRELIS that provide polychoric correlation matrices. Depending on how they are computed, polychoric correlation matrices can be non positive-definite – i.e., pairwise estimation of the elements of a polychoric correlation matrix is problematic because it can lead to non positive-definite correlation matrices; as opposed to estimating all the correlations in the matrix simultaneously.

The matter of how to estimate polychoric correlation matrices to avoid non positive-definiteness is an open area of research that needs further study but in the meantime a solution to this potential problem, when a non positive-definite matrix is found, is to use software, e.g., EQS, that estimates the polychoric correlations in a manner that reduces the concern for non positive-definite matrices.

In the present study, ordinal coefficients alpha and theta performed equally well. A direction for future research would be to compare ordinal coefficients alpha and theta in the presence of multidimensional items because theta was originally developed to account for multidimensionality in an item set.

Based on the present study, the following recommendations are presented:

1. Use either ordinal coefficient alpha or ordinal coefficient theta to correct for the negative bias in coefficient alpha, and of course KR-20, due to Likert or binary response data.
2. In terms of which of these two ordinal reliability coefficients to use, the decision should be based on whether one is assuming a factor analysis model (ordinal coefficient alpha) or a principal components model (ordinal coefficient theta). For a distinction between principal components analysis and factor analysis the reader is referred to Fabrigar, Wegener, MacCallum, & Strahan (1999) or Zumbo (2007).

It should be noted that the strategy of using the polychoric correlation could be applied to any reliability estimate that can be computed from a correlation matrix. For example, although it is not described herein, one would have an ordinal version of the McDonald's coefficient omega, yet another reliability estimate, by applying the equation described by McDonald (1985, p. 217), or of Revelle's reliability coefficient beta (Zinbarg, Revelle, Yovel, & Li, 2005). Future research should explore these other coefficients as well.

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Appendix: Thresholds for Symmetric and Skewed Likert Responses

Thresholds for symmetric scale point distribution:

1. Two-point scale: (Lowest thru 0=1) (ELSE=2)
2. Three-point scale: (Lowest thru -1=1) (-.9999 thru 1=2) (ELSE=3)
3. Four-point scale: (Lowest thru -1.5=1) (-1.4999 thru 0=2) (0.0001 thru 1.5=3) (ELSE=4)
4. Five-point scale: (Lowest thru -1.8=1) (-1.7999 thru -0.6=2) (-0.5999 thru 0.6000=3) (0.6001 thru 1.8=4) (ELSE=5)
5. Six-point scale: (Lowest thru -2=1) (-1.9999 thru -1.0=2) (-0.9999 thru 0=3) (0.0001 thru 1=4) (1.0001 thru 2=5) (ELSE=6)
6. Seven-point scale: (Lowest thru -2.14286=1) (-2.14285 thru -1.28571=2) (-1.28570 thru -0.42857=3) (-0.42857 thru 0.428571=4) (0.428572 thru 1.28571=5) (1.28571 thru 2.14286=6) (else =7)

Thresholds for scale point distribution with skewness of -2:

1. Two-point scale: (Lowest thru -1.06251930227=1) (ELSE=2)
2. Three-point scale: (Lowest thru 0.9002=3) (0.9003 thru 1.29883663264=2) (ELSE=1)
3. Four-point scale: (Lowest thru 0.8508=4) (0.8509 thru 1.086=3) (1.087 thru 1.2816 =2) (ELSE=1)
4. Five-point scale: (Lowest thru 0.6808=5) (0.6809 thru 1.036=4) (1.037 thru 1.2816 =3) (1.2817 thru 1.6546=2) (ELSE=1)
5. Six-point scale (Lowest thru 0.5008=6) (0.5009 thru 1.036=5) (1.037 thru 1.0816 =4) (1.0817 thru 1.4546=3) (1.4547 thru 1.8002=2) (ELSE=1)
6. Seven-point scale: (Lowest thru 0.4008=7) (0.4009 thru 0.8360=6) (0.8361 thru 1.1816 =5) (1.1817 thru 1.4546=4) (1.4547 thru 1.8002=3) (1.8003 thru 2.1002=2) (ELSE=1)

On Flexible Tests of Independence and Homoscedasticity

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Consider the nonparametric regression model $Y = m(X) + \tau(X)\varepsilon$, where X and ε are independent random variables, ε has a mean of zero and variance σ^2 , τ is some unknown function used to model heteroscedasticity, and $m(X)$ is an unknown function reflecting some conditional measure of location associated with Y , given X . Detecting dependence, by testing the hypothesis that $m(X)$ does not vary with X , has the potential of being more sensitive to a wider range of associations compared to using Pearson's correlation. This note has two goals. The first is to point out situations where a certain variation of an extant test of this hypothesis fails to control the probability of a Type I error, but another variation avoids this problem. The successful variation provides a new test of $H_0 : \tau(X) \equiv 1$, the hypothesis that the error term is homoscedastic, which has the potential of higher power versus a method recently studied by Wilcox (2006). The second goal is to report some simulation results on how this method performs.

Key words: Heteroscedasticity, smoothers, wild bootstrap, Winsorized correlations.

Introduction

Consider the nonparametric regression model $Y = m(X) + \tau(X)\varepsilon$, where X and ε are independent random variables, ε has a mean of zero and variance σ^2 , τ is some unknown

Pearson's correlation between X and Y . A concern about this approach is that it limits the function used to model heteroscedasticity, and $m(X)$ is an unknown function reflecting some conditional measure of location associated with Y , given X . Typically, it is assumed that $m(X) = \beta_0 + \beta_1 X$, where β_0 and β_1 are the unknown slope and intercept, and of course a common approach toward establishing an association is testing $H_0 : \rho = 0$, where ρ is types of associations between X and Y that can be detected. For example, there are many types of curvilinear associations between X and Y for which ρ will be close to zero, which in turn can mean relatively low power when

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testing $H_0 : \rho = 0$. Also, heteroscedasticity can affect power when using the usual Student's T test of this hypothesis (e.g., Wilcox, 2003), roughly because the wrong standard error is being used. In some cases, heteroscedasticity might increase power, but the reverse can happen as well. Perhaps more importantly, when Student's T rejects, there is uncertainty whether the main reason is due to heteroscedasticity or because $m(X)$ varies with X .

A test of $H_0 : \rho = 0$ that allows heteroscedasticity is given in Wilcox (2003, section 7.3.2), but again, curvilinear associations might be missed. Of course, if it is assumed that curvature can be represented by a particular parametric model, curvilinear associations can be addressed. For example, it might be assumed that $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \varepsilon$.

However, experience with smoothers (e.g., Hastie & Tibshirani, 1990) suggest that it is not always evident which parametric model provides a good reflection of the data.

Using a special case of a wild bootstrap method derived by Stute, Manteiga and Quindimil (1998), it is possible to test

$$H_0 : m(X) = \theta, \quad (1)$$

where θ is some unknown measure of location. That is, the hypothesis is that the regression line is a straight, horizontal line having intercept θ . Wilcox (2001) reported simulation results indicating that good control over the probability of a Type I error is achieved when θ is taken to be the population mean of the Y values, μ_y . A seemingly natural way of robustifying this method is to replace the mean with some robust estimator, and a 20% trimmed mean was suggested by (Wilcox, 2003). One goal here is to describe situations where using a 20% trimmed mean, control over the probability of a Type I error is very poor, but when using the usual mean, satisfactory control is maintained. (Using the median of the Y values can also result in poor control over the probability of a Type I error.)

Wilcox (2006) suggested a flexible method for testing

$$H_0 : \tau = 1, \quad (2)$$

the hypothesis that the error term is homoscedastic. The success of the wild bootstrap test of (1) suggests an alternative approach to testing (2). The second goal in this paper is to report simulation results on this alternative approach and to describe situations where it has more power than the approach studied by Wilcox (2006).

Description of the Methods

Testing (1)

The wild bootstrap test of (1) is applied as follows. Let $(X_1, Y_1), \dots, (X_n, Y_n)$ be a random sample of n points from some unknown bivariate distribution. Let $\bar{Y}$ be the usual sample mean based on the Y values. Fix j and set $I_i = 1$ if $X_i \leq X_j$, otherwise $I_i = 0$, and let

$$R_j = \frac{1}{\sqrt{n}} \sum I_i r_i, \quad (3)$$

where $r_i = Y_i - \bar{Y}$. The test statistic is the maximum absolute value of all the R_j values:

$$D = \max |R_j|, \quad (4)$$

where the maximum is over all j . The critical value is computed as follows. Generate n observations from a uniform distribution and label the results $U_1, \dots, U_n$. For $i = 1, \dots, n$, set $V_i = \sqrt{12}(U_i - .5)$, $r_i^* = r_i V_i$, and $Y_i^* = \bar{Y} + r_i^*$. Then based on the n pairs of points $(X_1, Y_1^*), \dots, (X_n, Y_n^*)$, compute the test statistic as described in the previous paragraph and label it D^* . Repeat this process B times and label the resulting (bootstrap) test statistics $D_1^*, \dots, D_B^*$. Finally, put these B values in ascending order, which are labeled $D_{(1)}^* \leq \dots \leq D_{(B)}^*$. Then, the α level critical value is $D_{(u)}^*$, where $u = (1 - \alpha)B$ rounded to the nearest integer. That is, reject if $D \geq D_{(u)}^*$.

The corresponding p-value is the proportion of D_b^* values, among the B bootstrap samples, for which $D < D_b^*$.

Let $Y_{(1)} \leq \dots \leq Y_{(n)}$ be the Y_i values written in ascending order and let g be equal to $.2n$ rounded to the nearest integer. Then the 20% trimmed mean of the Y values is

$$\bar{Y}_t = \frac{1}{n-2g} \sum_{i=g+1}^{n-g} Y_{(i)}.$$

An alternative test of (1) is obtained simply by replacing the usual sample mean, $\bar{Y}$, with $\bar{Y}_t$.

Testing (2).

Now a test of (2) is described that is based on a simple modification of the method in Wilcox (2006). Let $m(X)$ be the conditional median of Y , given X . The first step is to approximate $m(X)$ using what is called a running interval smoother, which is applied follows. Let f , called a span, be some constant to be chosen and let M be the median of the values $X_1, \dots, X_n$. The median absolute deviation (MAD) measure of dispersion is the median of the values $|X_1 - M|, \dots, |X_n - M|$. The point X is said to be close to X_i if

$$|X_i - X| \leq f \frac{MAD}{.6745}.$$

Under normality, $MAD/.6745$ estimates the standard deviation, in which case X is close to X_i if X is within f standard deviations of X_i . Let

$$N(X_i) = \{j : |X_j - X_i| \leq f \times MADN\},$$

where for convenience, $MADN$ is $MAD/.6745$. That is, $N(X_i)$ indexes the set of all X_j values that are close to X_i . Then $m(X_i)$ is taken to be the median of the Y_j values such that

$j \in N(X_i)$. Generally, a good choice for the span is $f = .8$ (Wilcox, 2005), and this value is used here exclusively. Let $v_i = |Y_i - m(X_i)|$ ($i = 1, \dots, n$) be the absolute residuals. When (2) is true (there is homoscedasticity), the regression line between X and v should be a straight, horizontal line, which can be tested with the method.

Wilcox (2006) suggested two alternative methods for testing (2). Let β be the slope of the regression line between the X_i and v_i values. Then, a test of (2) corresponds to testing

$$H_0 : \beta = 0. \quad (5)$$

Alternatively, if ρ is some correlation between X_i and v_i , then $H_0 : \rho = 0$ should be true. A natural strategy is to use least squares regression or Pearson's correlation, but this was found to be unsatisfactory. What was found to perform well in simulations was a test of (5) using the Theil (1950) and Sen (1968) regression estimator in conjunction with a percentile bootstrap method, or an approach based on a so-called Winsorized correlation coefficient.

Consider first the regression method. The goal is to test the hypothesis that the (population) regression line between v and X is horizontal. To elaborate on the Theil-Sen estimator, for any $i < i'$, for which $X_i \neq X_{i'}$, let

$$S_{ii'} = \frac{v_i - v_{i'}}{X_i - X_{i'}}.$$

The Theil-Sen estimate of the slope is $\hat{\beta}_{ts}$, the median of all the slopes represented by $S_{ii'}$. Let β_{ts} be the population slope estimated by $\hat{\beta}_{ts}$. To test $H_0 : \beta_{ts} = 0$, it currently seems that a basic percentile bootstrap method performs relatively well. In particular, a bootstrap sample is obtained by randomly sampling, with replacement, n pairs of points from $(v_1, X_1), \dots, (v_n, X_n)$. Let $\hat{\beta}^*$ be the Theil-Sen

estimate of β_{ts} based on this bootstrap sample. Repeat this bootstrap process B times yielding $\hat{\beta}_1^*, \dots, \hat{\beta}_B^*$. Let $\hat{\beta}_{(1)}^* \leq \dots \leq \hat{\beta}_{(B)}^*$ be the bootstrap estimates written in ascending order. Let $l = \alpha/2$, rounded to the nearest integer, and $u = B - l$. Then,

$$(\hat{\beta}_{(l+1)}^*, \hat{\beta}_{(u)}^*)$$

is an approximate $1 - \alpha$ confidence interval for β_{ts} . Let $\hat{p}$ be the proportion of bootstrap estimates less than zero. Then, a p-value is $2\min(\hat{p}, 1 - \hat{p})$.

As for the Winsorized correlation approach, set $Y_{i1} = v_i$ and $Y_{i2} = X_i$ ($i = 1, \dots, n$). Next, Winsorize the Y values. That is, for fixed j , let $Y_{(1)j} \leq \dots \leq Y_{(n)j}$ be the n values written in ascending order, and let

$$\begin{aligned} W_{ij} &= Y_{(g+1)j} \text{ if } Y_{ij} \leq Y_{(g+1)j} \\ W_{ij} &= Y_{ij} \text{ if } Y_{(g+1)j} < Y_{ij} < Y_{(n-g)j} \\ W_{ij} &= Y_{(n-g)j} \text{ if } Y_{ij} \geq Y_{(n-g)j} \end{aligned}$$

where $g = [\gamma n]$, γ ($0 \leq \gamma < .5$) is the amount of Winsorizing to be done and $[.]$ is the greatest integer function. Here, $\gamma = .2$ is used. Then the estimate of ρ_w , the sample Winsorized correlation between R and X , is just Pearson's correlation based on the Winsorized values. That is, estimate ρ_w with

$$r_w = \frac{\sum (W_{i1} - \bar{W}_1)(W_{i2} - \bar{W}_2)}{\sqrt{\sum (W_{i1} - \bar{W}_1)^2 \sum (W_{i2} - \bar{W}_2)^2}}$$

To test $H_0 : \rho_w = 0$, compute

$$T_w = r_w \sqrt{\frac{n-2}{1-r_w^2}},$$

and reject if $|T_w| \geq t_{1-\alpha/2}$, the $1 - \alpha/2$ quantile of Student's t distribution with $\nu = h - 2$ degrees of freedom, where $h = n - 2g$.

A Simulation Study

Wilcox (2006) studied the small-sample properties of the method using simulations where both the X and Y values were generated from one of four g-and-h distributions (Hoaglin, 1985), one of which was normal. If Z has a standard normal distribution, then

$$W = \frac{\exp(gZ) - 1}{g} \exp(hZ^2/2) \quad \text{if } g > 0$$

$$W = \exp(hZ^2/2) \quad \text{if } g = 0$$

has a g-and-h distribution where g and h are parameters that determine the first four moments. The four distributions used were the standard normal ($g=h=0.0$), a symmetric heavy-tailed distribution ($h=0.2, g=0.0$), an asymmetric distribution with relatively light tails ($h=0.0, g=0.2$), and an asymmetric distribution with heavy tails ($g=h=0.2$). Table 1 shows the skewness (κ_1) and kurtosis (κ_2) for each distribution considered. Additional properties of the g-and-h distribution are summarized by Hoaglin (1985).

Table 1. Some Properties of the g-and-h Distribution.

g	h	K_1	K_2
0.00	0.00	0.00	3.00
0.00	0.2	0.00	21.46
0.2	0.0	0.61	3.68
0.2	0.2	2.81	155.98

Although skewed distributions were considered, it turns out that when Y has other skewed distributions, not considered by Wilcox (2001), control over the probability of a Type I error is poor when using a 20% trimmed mean, but control remains good when using the mean instead. Suppose, for example, Y has a chi-squared distribution with 1 degree of freedom. Then, when X has a standard normal distribution and $n=30$, the actual Type I error probability is approximately .54 when testing at the .05 level (based on simulations with 1,000 replications). In contrast, when using the mean of Y , the Type I error probability is approximately .034. Problems remain with 3 degrees of freedom but they become negligible when the degrees of freedom are increased to 5. If Y has a lognormal distribution, the Type I error probability is .25 and .035 using a 20% trimmed mean and mean, respectively. So, it is evident that when Y has a sufficiently skewed distribution, using a 20% trimmed mean can be disastrous.

Now consider the problem of testing (2) with the wild bootstrap method. First consider the exact same conditions considered by Wilcox (2001), where observations were generated with either $m(X)=X$ or $m(X)=X^2$. Table 2 shows the estimated probability of a Type I error when testing at the .05 level with $n=30$. Again the estimates are based on 1,000 replications with $B=500$. (From Robey and Barcikowski, 1992, 1,000 replications is sufficient from a power point of view. More specifically, if the hypothesis that the actual Type I error rate is .05 is tested and if one wants power to be .9 when testing at the .05 level and the true α value differs from .05 by .025, then 976 replications are required.)

Table 2. Type I Error Rates, $n=30$, $\alpha=.05$

X		$\mathcal{E}$		$m(X)=X$	$m(X)=X^2$
g	h	g	h		
0.0	0.0	0.0	0.0	.036	.038
0.0	0.0	0.0	0.2	.040	.032
0.0	0.0	0.2	0.0	.046	.028
0.0	0.0	0.2	0.2	.041	.028
0.0	0.2	0.0	0.0	.039	.042
0.0	0.2	0.0	0.2	.039	.034
0.0	0.2	0.2	0.0	.043	.038
0.0	0.2	0.2	0.2	.043	.032
0.2	0.0	0.0	0.0	.040	.041
0.2	0.0	0.0	0.2	.037	.025
0.2	0.0	0.2	0.0	.044	.038
0.2	0.0	0.2	0.2	.033	.027
0.2	0.2	0.0	0.0	.034	.039
0.2	0.2	0.0	0.2	.033	.035
0.2	0.2	0.2	0.0	.043	.036
0.2	0.2	0.2	0.2	.040	.034

As indicated in Table 2, among all situations considered, the estimated probability of a Type I error ranged between .027 and .044. From Wilcox (2006), when using the Theil-Sen estimator, the estimates ranged between .030 and .067. As for the method based on the Winsorized correlation, the estimates ranged between .021 and .050. Because generating observations from a chi-squared distribution with 1 degree of freedom, or a lognormal distribution, caused problems when using the wild bootstrap method with a 20% trimmed mean, these two distributions were also

considered when using the wild bootstrap to test (2). The estimated probability of a Type I error for these two cases were .037 and .036, respectively.

A practical issue is how the power of the method compares to the power of the methods studied by Wilcox (2006). Checks revealed that the method can have more or less power depending on the nature of the heteroscedasticity. For example, if $Y = X^2 + |.2X|\varepsilon$, with both X and ε having standard normal distributions, the wild bootstrap method has power .34, versus .09 and .04 when using the Winsorized correlation or the Theil-Sen estimator, respectively. But if $Y = X^2 + |X + 1|\varepsilon$, the estimated power for these three methods is .39, .51 and .35. Currently, it is unclear how best to characterize the situations where the wild bootstrap method will have more or less power. All that can be said is that given some data, the choice of method can make a practical difference.

Conclusion

For a wide range of situations, inferences based on a 20% trimmed mean, rather than a mean, can have considerable practical value in terms of both Type I errors and power (Wilcox, 2003, 2005). But, it is evident that when testing (1) with a wild bootstrap, using a 20% trimmed mean can be disastrous. Perhaps there is some modification of the wild bootstrap that both corrects this problem and has some practical advantage over using means, but this remains to be seen.

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Regular Articles

Application of a New Procedure for Power Analysis and Comparison of the Adjusted Univariate and Multivariate Tests in Repeated Measures Designs

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A relationship between the multivariate and univariate noncentrality parameters in repeated measures designs was developed for the purpose of assessing the relative power of the univariate and multivariate approaches. An application is provided examining the use of repeated measures designs to evaluate student achievement in a K-12 school system.

Key words: Repeated measures designs, adjusted degrees of freedom test, noncentrality parameter, sphericity.

Introduction

Repeated measures designs are used frequently by social and behavioral science researchers (Maxwell & Delaney, 2004; Keselman, H. J., Huberty, Lix, Olejnik, Cribbie, Donahue, Kowalchuk, Lowman, Petoskey, Keselman, J. C., & Levin, 1998). A major advantage of repeated measures designs is that subjects serve as their own controls, thus variability among the subjects due to individual differences is removed, and test results are more powerful. Various procedures can be used to do variance analysis in repeated measures designs. In

addition to the traditional approaches, univariate and multivariate analyses, some methods such as Improved General Approximate method (Huynh, 1978), multivariate Welch (1951)/James (1951)-type test (*WJ* test), mixed model approach (Littell, Milliken, Stroup, & Wolfinger, 1996), and empirical Bayes method (Boik, 1997) have also been studied and recommended. Guidelines for choosing an analysis strategy are generally based on whether the design is balanced or not (Keselman, 1998; Keselman, Algina, & Kowalchuk, 2002). If group sizes are equal and there is no missing data, univariate and multivariate methods are frequently used by researchers and are recommended as appropriate statistical methods (Kirk, 1995; Morrison, 1990; Maxwell & Delaney, 2004).

Both of the univariate and multivariate methods require the data satisfy certain assumptions: independent observations, multivariate normality, and homogeneous variance/covariance across groups. In addition to the above assumptions, the univariate analysis has the additional assumption of sphericity (Huynh & Feldt, 1970; Rouanet & Lépine, 1970). Sphericity refers to differences between any pair of repeated measures are equally variable. If sphericity is met, the univariate analysis has greater power than the multivariate analysis (due to a clear degrees of freedom advantage in the denominator), and it allows the

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use of fewer subjects than the multivariate analysis for equal power (Morrison, 1990). Unfortunately, the assumption of sphericity is not often met in the behavioral and social research (Davidson, 1972; McCall & Appelbaum, 1973; Rogan, Keselman, & Mendoza, 1979; Keselman, Huberty *et al.*, 1998). If sphericity is not satisfied, the univariate analysis produces biased tests of significance (Box, 1954), and an adjusted degrees of freedom test, such as Greenhouse & Geisser (1959) or Huynh & Feldt (1976) test is suggested. The adjusted univariate analyses modify the *df* of the traditional *F* statistic using a sample estimate of the sphericity parameter epsilon (ϵ). The ϵ is a measure of the degree of violation of the sphericity assumption, with perfect conformity to sphericity producing a ϵ of 1.0 (Huynh & Feldt, 1970).

Because the empirical evidence indicates that if the design is balanced, both the adjusted univariate and the multivariate approaches give the necessary control of Type I error (Davidson, 1972; Maxwell & Arvey, 1982; Muller & Barton, 1989; Keselman, J., Lix, & Keselman, H., 1996), power becomes a critical factor in the selection between the adjusted univariate analysis and the multivariate analysis. Prospective power analysis will help researchers to determine an appropriate sample size to obtain the desired level of power to detect the meaningful differences that are hypothesized. Selecting an insufficient sample size will increase the risk of failing to detect an important difference when it may exist (Type II error). Conversely, selecting an excessive sample size may produce a statistically significant result, but one with limited meaningfulness due to small differences.

Sample size also affects the relative power of the adjusted univariate and multivariate tests. Without sphericity, multivariate tests may be more powerful than the adjusted univariate tests (Davidson, 1972). However, if sample sizes are small, the adjusted univariate analysis may still be more powerful than the multivariate analysis, because the estimators of the covariance parameters lack precision, and as a result, the power of the multivariate analysis is low (Boik, 1981). As sample size increases, the power of the

multivariate test improves and can be greater than the power of the adjusted univariate test (Boik, 1997).

Power analysis and minimum sample size calculations are needed for choosing the most suitable method under different conditions. Using the expansions of Fujikoshi (1973), Sugiura (1973), or Vander Merwe and Crowther (1984), power of the multivariate tests can be computed. Muller and Peterson (1984) provided power approximations of the multivariate tests. For the adjusted univariate tests, Muller and Barton (1989, 1991) provided power approximations based on the expected value approximations for the epsilon (ϵ) estimator. Vonesh and Schork (1986) presented a statistical methodology for determining the minimum sample size for the within-subjects repeated-measures design.

They developed a formulae for calculating the multivariate noncentrality parameter, subject to constraint $\Delta = |\mu_j - \mu_k|$, which represents a minimal difference between any pair of treatment means. Rochon (1991) extend the procedures of Vonesh and Schork to the between-subjects repeated-measures design when there are only two treatment groups under consideration. All of the above researches provide strong basis for the purpose of the current paper, that is, to develop a relationship between the multivariate and univariate noncentrality parameters for assessing the relative power of the univariate and multivariate approaches in repeated measures designs. A major goal of this article is to compare the statistical power of the univariate and multivariate procedures and provide a method for selecting an appropriate sample size, given a desired effect size and level of power, when researchers are developing a study.

Theoretical Foundations and Statistics

The Model and Hypothesis

The usual general linear model with *g* between-subject groups and one within-subject repeated measures factor having *p* levels can be written as follows:

$$Y = XM + E \quad (1)$$

Where Y is an $N \times p$ matrix from N subjects; X is an $N \times g$ between-subject design matrix; M is an $g \times p$ parameters matrix; and E is an $N \times p$ matrix of random errors. The rows of E are assumed to be independently and identically distributed as $N_p(0, \Sigma)$, where Σ is a $p \times p$ positive definite covariance matrix.

The general linear multivariate model hypothesis has the usual form:

$$H_0: \Theta = CMU = \Theta_0 \quad (2)$$

where C is an $a \times g$ between-subject contrasts; M is an $g \times p$ parameters matrix; U is an $p \times b$ within-subject contrasts; and Θ is an $a \times b$ secondary parameters matrix. Without loss of generality, assume $\Theta_0 = 0$. Define $\Sigma_* = U' \Sigma U$, which is a covariance matrix of $\text{row}_i(EU)'$. Also define $\omega = (\Theta - \Theta_0)' [C(X'X)^{-1}C']^{-1} (\Theta - \Theta_0)$, which is an unscaled noncentrality matrix. Then, the scaled noncentrality matrix (Ω) and its trace (δ_m) are given by $\Omega = \omega \Sigma_*^{-1}$ and $\delta_m = \text{tr}(\Omega)$ respectively. Using two theorems (Theorem 2, p30; and Theorem 3, p31) from Magnus and Neudecker (1988), the general form of the noncentrality parameter for the F -distribution can be written as:

$$\delta_m = \frac{(\text{vec } M')'(C' \otimes U) \left[\left[C(X'X)^{-1}C' \right]^{-1} \otimes \Sigma_*^{-1} \right] (C \otimes U)(\text{vec } M')}{(C \otimes U)(\text{vec } M')} \quad (3)$$

The hypothesis in (2) can be tested using the multivariate test. If using the Hotelling-Lawley trace statistic, the noncentrality parameter has the form (Muller & Peterson, 1984; Muller, LaVange, Ramey, & Ramey, 1992):

$$\begin{aligned} \delta_{\text{HLT}} &= (ab) \cdot F_A(\text{HLT}) \\ &= \frac{\text{HLT}_A / S}{1/\text{df}_d(\text{HLT})} \end{aligned} \quad (4)$$

where $a = g - 1$, $b = p - 1$, $S = \min(a, b)$, and $\text{df}_d(\text{HLT}) = S[(N - g) - b - 1] + 2$.

The hypotheses in (2) also can be tested using the adjusted univariate test. Additionally,

for repeated measures designs, the univariate analysis is a simply by-product of the multivariate analysis (Wang, 1983). A Univariate noncentrality parameter can be derived from (3) and be expressed as:

$$\delta_u = b\epsilon \frac{\text{tr}(\omega)}{\text{tr}(\Sigma_*)} = \left(\frac{\text{tr}(\Sigma_*)}{\text{tr}(\Sigma_*^2)} \right) \cdot \text{tr}(\omega) \quad (5)$$

where

$$\epsilon = \frac{\text{tr}^2(\Sigma_*)}{b \cdot \text{tr}(\Sigma_*^2)} \quad (\text{Box, 1954}).$$

The sphericity parameter ϵ ($1/b \leq \epsilon \leq 1$) reflects a discrepancy from sphericity. If sphericity is not met ($\epsilon \neq 1$), $T^2_{\text{univariate}} \approx F(ab\epsilon, b(N-g)\epsilon, \delta_u)$. The Greenhouse & Geisser test uses the maximum likelihood estimator (MLE) $\hat{\epsilon}$ to adjust the degrees of freedom of the univariate test.

Lower Bounds of Noncentrality Parameters

The noncentral F -distribution can be used for power and sample size calculations. The power associated with the F -test is a monotonically increasing function of the noncentrality parameter. In this subsection, minimizing of the noncentrality parameters, developing the lower bounds of the multivariate and univariate noncentrality parameters using the same constraints, and establishing a relationship between them are described.

As shown and demonstrated in the Appendix, for fixed $\epsilon > 0$, subject to the constraint

$$\Delta = \frac{|c'Md|}{\sqrt{c'c}\sqrt{d'd}} \quad \text{and} \quad \bar{\theta} = \frac{\text{tr}(\Sigma_*)}{b} \quad (6)$$

the lower bounds of multivariate and univariate noncentrality parameters can be expressed as:

$$\delta_m^* = \frac{N\Delta^2}{d'\Sigma d} \quad \text{and} \quad \delta_u^* = \frac{\epsilon N\Delta^2}{\bar{\theta}} \quad (7)$$

where c and d are arbitrary vectors of contrast coefficients. $\delta_m \geq \delta_m^*$, and $\delta_u \geq \delta_u^*$. The value of $\bar{\theta}$ is represented as:

$$\bar{\theta} = \frac{tr(\Sigma^*)}{b} = \frac{\sum_{i=1}^b \lambda_i}{b} \quad (8)$$

which is the mean eigenvalue of the error matrix Σ^* .

From (7) and (8), the relationship between the lower bounds of multivariate and univariate noncentrality parameters can be expressed as:

$$\delta_u^* = \epsilon^* \delta_m^* \quad (9)$$

where $\epsilon^* = \epsilon\phi$, $\phi = \frac{\sigma_0^2}{\bar{\theta}}$, and ϕ represents the bias ratio.

As shown by Boik (1981), $\sigma_0^2 = d'\Sigma d$ is the experimental error of contrast among the p -repeated measures, and $\bar{\theta}$ is the average experimental error of any set of $b = p - 1$ orthonormal contrasts. Further, when the sphericity assumption is met ($\epsilon = 1.0$), ϕ will always equal unity (Boik, 1981). For fixed ϵ , the bias ratio has a range of values, $\phi_{\min} < \phi < \phi_{\max}$. The upper and lower limits of ϕ are given by Boik (1981):

$$\phi_{\max} = 1 + B, \text{ when } 1/b \leq \epsilon \leq 1,$$

$$\phi_{\min} = \begin{cases} 1 - B & \text{when } \frac{b-1}{b} \leq \epsilon \leq 1.0 \\ 0 & \text{when } \frac{1}{b} \leq \epsilon \leq \frac{b-1}{b} \end{cases} \quad (10)$$

where $B = \left[\frac{(b-1)(1-\epsilon)}{\epsilon} \right]^{1/2}$. If $\epsilon = 1$, then $B = 0$, and $\phi_{\min} = \phi_{\max} = 1$.

Because $\epsilon^* = \epsilon\phi$ and $\phi_{\min} < \phi < \phi_{\max}$, the maximum and minimum values of multiplier ϵ^* can be obtained as:

$$\epsilon_{\max}^* = \epsilon(1 + B) = \epsilon + \sqrt{(b-1)(1-\epsilon)\epsilon} \quad (11)$$

and

$$\epsilon_{\min}^* = \epsilon(1 - B) = \epsilon - \sqrt{(b-1)(1-\epsilon)\epsilon} \quad (12)$$

$\epsilon_{\max}^*$ varies between a minimum of 1, when $\epsilon = 1/b$ or $\epsilon = 1$; and a maximum of $\frac{1}{2}(1 + \sqrt{b})$, when $\epsilon = \frac{1}{2}(1 + \sqrt{\frac{1}{b}})$. $\epsilon_{\min}^*$ varies between a minimum of 0, when $\epsilon = (b-1)/b$; and a maximum of 1, when $\epsilon = 1$. For example, let

$\epsilon = \frac{1}{2}(1 + \sqrt{\frac{1}{b}})$ and $(b-1)/b < \epsilon \leq 1$, then

$$\epsilon_{\max}^* = \frac{1}{2}(1 + \sqrt{b}), \text{ and } \epsilon_{\min}^* = \frac{1}{2} \left[1 - (b-2)\sqrt{\frac{1}{b}} \right]. \text{ Let}$$

$\epsilon = \frac{1}{2}(1 + \sqrt{\frac{1}{b}})$, but if ϵ is in the interval of $[1/b, (b-1)/b]$, then $\epsilon_{\max}^* = \frac{1}{2}(1 + \sqrt{b})$, but

$\epsilon_{\min}^* = 0$, because of the restrictive nature of the bias ratio $\phi_{\min} = 0$, when $1/b \leq \epsilon \leq (b-1)/b$.

Best and Worst Case Scenarios for the Univariate Test

An examination of (9), (11), and (12) allows the determination of best and worst case scenarios for the lower bound of univariate noncentrality parameter (δ_u^*) by substituting the maximum and minimum values of ϵ^* in (9). The best case scenario for δ_u^* is

$$\delta_u^*_{best} = \left[\varepsilon + \sqrt{(b-1)(1-\varepsilon)\varepsilon} \right] \cdot \delta_m^* \quad (13)$$

Because

$$1 \leq \varepsilon_{\max}^* = \left[\varepsilon + \sqrt{(b-1)(1-\varepsilon)\varepsilon} \right] \leq \frac{1}{2}(1 + \sqrt{b})$$

this suggests the best case scenario for the univariate case, which means the minimum power of the univariate test will generally exceed the minimum power of the multivariate test.

However, substituting $\varepsilon_{\min}^*$ in (9) yields the worst case scenario:

$$\delta_u^*_{worst} = \left[\varepsilon - \sqrt{(b-1)(1-\varepsilon)\varepsilon} \right] \cdot \delta_m^* \quad (14)$$

Because

$$0 \leq \varepsilon_{\min}^* = \left[\varepsilon - \sqrt{(b-1)(1-\varepsilon)\varepsilon} \right] \leq 1,$$

this suggests the worst case scenario for the univariate case, which means the minimum power of the univariate test will be generally lower than the minimum power of the multivariate test.

Univariate versus Multivariate

Power Analysis and Minimum Sample Size Calculation

For computing the minimum necessary sample size to obtain a desired level of power in the multivariate case, Vonesh and Schork (1986) presented a statistic method, and Rochon (1991) extended it to the between-subjects repeated-measures design. If let Σ to be a positive covariance matrix, which means $\rho_{jk} \geq 0$ for $j < k$; and let $\sigma_{\max}^2$ represents the largest variance, then the lower bound of δ_m can be approximated:

$$\delta_m^* = \frac{N\Delta^2}{2\sigma_{\max}^2(1-\rho_{\min})} \leq \delta_m \quad (15)$$

where $\rho_{\min} = \min_t \{\rho_t\}$. This would guarantee power greater than the normal level. Using the above approximation, the minimum sample size for the multivariate case can be determined by utilizing

$$1 - \beta_m = P[F(df_n, df_d; \delta_m) > F_\alpha(df_n, df_d)] \quad (16)$$

To determine sample sizes in the univariate case when the assumption of sphericity is untenable, the following is used

$$1 - \beta_u = P \left[F(ab\varepsilon, b(N-g)\varepsilon; \delta_u) > F_\alpha(ab\varepsilon, b(N-g)\varepsilon) \right] \quad (17)$$

where δ_u and ε are given in (5).

In order to determine the minimum sample sizes in the univariate case, applying (13) and (14), the upper (best case) and lower (worst case) limits of the δ_u^* can be obtained, if ε and δ_m^* are known. δ_m^* can be approximated by (15). In general, however, it will not be known.

In the present context, suppose $\varepsilon = \frac{1}{2}(1 + \sqrt{\frac{1}{b}})$, then if ε is in the interval $[(b-1)/b, 1]$, the upper (best case scenario) limit of the δ_u^* can be

obtained as $\delta_u^* = \frac{1}{2}(1 + \sqrt{b})\delta_m^*$; and the lower

(worst case) limit of the δ_u^* can be obtained as

$$\delta_u^* = \frac{1}{2} \left[1 - (b-2)\sqrt{\frac{1}{b}} \right] \delta_m^*.$$

This enables determination of the upper and lower limits of the δ_u^* for simulation study of the best and the worst case scenarios for the univariate case.

Simulation Procedure

The simulation was conducted in SAS/IML and SAS program is available from the author on request. The process of minimum sample size determination, or statistical power

analysis, involves the following four components: Type I error (α), power ($1-\beta$), effect size Δ or standardized effect size Δ_* , and the minimum correlation $\rho_{\min}$. Desired statistical power is set to be 0.80 in this study. The 80% level of power is based on Cohen's well-informed conjecture that the rate of Type II error should be about fourfold that of Type I error (Cohen, 1992). Detailed procedures were given as the following steps:

1) Specify the desired power ($1 - \beta$) to be 0.8, and $\alpha = 0.05$. Set all possible combinations of the following values: $p = 3, 4$; $g = 2, 3, 4$; $\rho_{\min} = .1, .2, \dots, .9$ by .1; and $\Delta_* = .2, .3, \dots, 1.5$ by .1.

2) The necessary sample size (N_m) was computed for all the above combinations using the multivariate procedure.

3) Using the upper limit of the δ_u^* ($\delta_u^* = \frac{1}{2}(1 + \sqrt{b})\delta_m^*$) to calculate the necessary sample size (N_u) for the best case scenario of the univariate procedure.

4) Using the lower limit of the δ_u^* ($\delta_u^* = \frac{1}{2}\left[1 - (b-2)\sqrt{\frac{1}{b}}\right]\delta_m^*$) to calculate the necessary sample size (N_l) for the worst case scenario of the univariate procedure.

Monte Carlo

Table 1 contains a selection of the results from the univariate and multivariate simulations. A comparison of the minimum sample size estimates between the multivariate procedure and the univariate procedure for the best and the worst case scenarios indicates some clear trends.

First, when the effect size is small, for example, $\Delta_* \leq 0.4$, and if minimum correlation is also small, then the minimum sample sizes of

the multivariate procedure (N_m) are much larger than the univariate procedure for the best case scenario (N_u). This trend indicates that when the above conditions hold, researchers need to consider using the univariate procedure, especially when sample sizes anticipated for the study may be small. This result is consistent with Boik's (1997) conclusion that if sample sizes are small, the adjusted univariate analysis may still be more powerful than the multivariate analysis. When the design becomes more complex, this trend is more obvious, because the minimum sample sizes generally increase as the number of groups and repeated trials increases (due to space considerations, results of other combinations of groups and trials are not included in the table).

Second, when the effect size is large, for example, $\Delta_* \geq 0.8$, the multivariate procedure could generally be recommended due to small minimum sample sizes. Simulation results indicate that there is small degree of divergence of the minimum sample sizes between the multivariate procedure (N_m) and the univariate procedure for the best case scenario (N_u).

Third, when the effect size is moderate, for example, $0.4 < \Delta_* < 0.8$, the minimum correlation ($\rho_{\min}$) will provide valuable information in selecting between the univariate and multivariate procedures. If $\rho_{\min}$ is large, for example, $\rho_{\min} \geq .80$, then the univariate procedure is recommended; otherwise, researchers need to consider using the multivariate procedure.

Upon inspection of this table, a pattern was also found for the relationship between the minimum sample size and the effect size. For fixed power, the minimum sample size generally decreases as the effect size increases. Thus, if sample size is fixed, larger treatment differences will provide greater power. The same pattern can be observed for the relationship between the minimum sample size and the minimum correlation.

Table 1. Necessary sample size estimates by groups, trials, standardized effect size (Δ^*), and minimum correlation ($\rho_{\min}$) for desired power = .80 at $\alpha = .05$

Groups	trials	Δ^*	$\rho_{\min}$	N_m	N_u	N_l
2	3	0.2	0.1	227	9	> 500
2	3	0.2	0.2	202	9	> 500
2	3	0.2	0.3	177	9	> 500
2	3	0.2	0.4	152	9	> 500
2	3	0.2	0.5	127	9	> 500
2	3	0.2	0.6	103	8	> 500
2	3	0.2	0.7	78	8	> 500
2	3	0.2	0.8	53	8	> 500
2	3	0.2	0.9	28	7	> 500
2	3	0.3	0.1	103	8	> 500
2	3	0.3	0.2	92	8	> 500
2	3	0.3	0.3	81	8	> 500
2	3	0.3	0.4	70	8	> 500
2	3	0.3	0.5	59	8	> 500
2	3	0.3	0.6	48	7	> 500
2	3	0.3	0.7	37	7	> 500
2	3	0.3	0.8	26	7	> 500
2	3	0.3	0.9	15	6	> 500
2	3	0.4	0.1	59	8	> 500
2	3	0.4	0.2	53	8	> 500
2	3	0.4	0.3	47	8	> 500
2	3	0.4	0.4	41	7	> 500
2	3	0.4	0.5	35	7	> 500
2	3	0.4	0.6	28	7	> 500
2	3	0.4	0.7	22	6	> 500
2	3	0.4	0.8	16	6	> 500
2	3	0.4	0.9	10	5	> 500
2	3	0.5	0.1	39	7	> 500
2	3	0.5	0.2	35	7	> 500
2	3	0.5	0.3	31	7	> 500
2	3	0.5	0.4	27	7	> 500
2	3	0.5	0.5	24	6	> 500
2	3	0.5	0.6	20	6	> 500
2	3	0.5	0.7	16	6	> 500
2	3	0.5	0.8	12	5	> 500
2	3	0.5	0.9	8	5	26
2	3	0.6	0.1	28	7	> 500
2	3	0.6	0.2	26	7	> 500
2	3	0.6	0.3	23	6	> 500
2	3	0.6	0.4	20	6	> 500
2	3	0.6	0.5	18	6	> 500

2	3	0.6	0.6	15	6	> 500
2	3	0.6	0.7	12	5	> 500
2	3	0.6	0.8	10	5	> 500
2	3	0.6	0.9	7	5	8
2	3	0.7	0.1	22	6	> 500
2	3	0.7	0.2	20	6	> 500
2	3	0.7	0.3	18	6	> 500
2	3	0.7	0.4	16	6	> 500
2	3	0.7	0.5	14	5	> 500
2	3	0.7	0.6	12	5	> 500
2	3	0.7	0.7	10	5	> 500
2	3	0.7	0.8	8	5	37
2	3	0.7	0.9	6	5	6
2	3	0.8	0.1	18	6	> 500
2	3	0.8	0.2	16	6	> 500
2	3	0.8	0.3	15	5	> 500
2	3	0.8	0.4	13	5	> 500
2	3	0.8	0.5	12	5	> 500
2	3	0.8	0.6	10	5	> 500
2	3	0.8	0.7	9	5	63
2	3	0.8	0.8	7	5	11
2	3	0.8	0.9	6	5	5
2	3	0.9	0.1	15	6	> 500
2	3	0.9	0.2	14	5	> 500
2	3	0.9	0.3	13	5	> 500
2	3	0.9	0.4	11	5	> 500
2	3	0.9	0.5	10	5	> 500
2	3	0.9	0.6	9	5	> 500
2	3	0.9	0.7	8	5	14
2	3	0.9	0.8	7	5	6
2	3	0.9	0.9	6	5	5
2	3	1.0	0.1	13	5	> 500
2	3	1.0	0.2	12	5	> 500
2	3	1.0	0.3	11	5	> 500
2	3	1.0	0.4	10	5	> 500
2	3	1.0	0.5	9	5	> 500
2	3	1.0	0.6	8	5	26
2	3	1.0	0.7	7	5	10
2	3	1.0	0.8	6	5	6
2	3	1.0	0.9	6	5	5
2	3	1.1	0.1	11	5	> 500
2	3	1.1	0.2	11	5	> 500
2	3	1.1	0.3	10	5	> 500
2	3	1.1	0.4	9	5	> 500
2	3	1.1	0.5	8	5	49
2	3	1.1	0.6	8	5	9
2	3	1.1	0.7	7	5	7
2	3	1.1	0.8	6	5	5
2	3	1.1	0.9	5	5	5

2	3	1.2	0.1	10	5	> 500
2	3	1.2	0.2	10	5	> 500
2	3	1.2	0.3	9	5	> 500
2	3	1.2	0.4	8	5	63
2	3	1.2	0.5	8	5	10
2	3	1.2	0.6	7	5	8
2	3	1.2	0.7	6	5	6
2	3	1.2	0.8	6	5	5
2	3	1.2	0.9	5	5	5
2	3	1.3	0.1	9	5	> 500
2	3	1.3	0.2	9	5	100
2	3	1.3	0.3	8	5	52
2	3	1.3	0.4	8	5	11
2	3	1.3	0.5	7	5	9
2	3	1.3	0.6	7	5	6
2	3	1.3	0.7	6	5	5
2	3	1.3	0.8	6	5	5
2	3	1.3	0.9	5	5	5
2	3	1.4	0.1	9	5	37
2	3	1.4	0.2	8	5	37
2	3	1.4	0.3	8	5	11
2	3	1.4	0.4	7	5	11
2	3	1.4	0.5	7	5	7
2	3	1.4	0.6	6	5	6
2	3	1.4	0.7	6	5	5
2	3	1.4	0.8	6	5	5
2	3	1.4	0.9	5	5	5
2	3	1.5	0.1	8	5	26
2	3	1.5	0.2	8	5	11
2	3	1.5	0.3	7	5	11
2	3	1.5	0.4	7	5	7
2	3	1.5	0.5	7	5	6
2	3	1.5	0.6	6	5	5
2	3	1.5	0.7	6	5	5
2	3	1.5	0.8	5	5	5
2	3	1.5	0.9	5	5	5

Notes: * Due to space considerations, not all of the simulation results are included in the table, but they are available from the author on request.

¹ N_m represents the necessary sample size computed using the multivariate procedure.

² N_u represents the necessary sample size computed for the “best case scenario” of the univariate procedure.

³ N_l represents the necessary sample size computed for the “worst case scenario” of the univariate procedure.

A Case Study: Examination of Student Achievement Models

The most effective method to evaluate student achievement is to monitor change in performance between two or more points, or more specifically a repeated measures design. Recent “No Child Left Behind” (NCLB) legislation has contributed to a proliferation of growth models advocated as best methods to examine student achievement. A major concern with the use of most of these growth models is they assume large samples. However, within most traditional educational settings, sample sizes are relatively small. The use of the more traditional repeated measures designs, univariate or multivariate, may be more appropriate than hierarchical linear models or latent growth analyses.

Case Study

A recent and growing concern in K-12 education has been the preparation of students to be successful in college. To address this issue, numerous studies have been completed that examine a student’s high school record of achievement. However, education is a linear system, with students in theory, starting at grade one and progressing through the system to grade twelve. Additionally, in large school districts, a significant amount of concern is directed at the preparation of student’s prior to high school. This case study examines three elementary schools and the difference in performance of students as they progress through this K-12 school system.

Each elementary school has grades kindergarten through fifth grade. Students were administered standardized reading tests in fifth, seventh (while at a middle school within the same district), and tenth grade. The primary research question, does elementary school you attended makes a difference in determining your starting point (10th grade) at the local high school? Table 2 provides a means and standard deviations of scaled scores for students from

each of the three elementary schools. The small sample sizes reflect the issue of mobility of students, and in particular from School A, where annually 30 percent of students are identified as highly mobile.

A total of four analyses were completed: (1) School A versus School B, (2) School A versus School C, (3) School B versus School C, and (4) School A, School B, and School C. Table 3 provides the multivariate and univariate results in addition to retrospective and prospective power estimation values. The result demonstrated the importance of the univariate procedure with large effect sizes and a limited number of observations. Additionally, it is expected that standardized tests will have a strong correlation from year to year, which also contributes to the strength of the univariate procedure.

The case study was done as a study of convenience with data that represented the most common type of educational data used to complete school evaluations. In practice, analyses will be completed at the classroom, grade or school level in efforts to evaluate the impact of instructional practices or new educational interventions. The present case study does an excellent job of replicating the sample size and type of outcome variables (standardized test) that will be employed and demonstrated, in practice, why greater consideration needs to be given to use of the univariate method in repeated measures designs.

Table 2. Case Study: School Test Scores

School	N	Score 1	Score 2	Score 3
A	12	614.3(37.6)	653.5(34.6)	685.2(29.5)
B	27	666.1(35.1)	680.6(26.1)	713.0(27.6)
C	25	653.4(34.3)	678.8(27.9)	704.8(29.7)

Table 3. Power Results for Univariate and Multivariate Comparisons

Comparison Schools	N	Retrospective Power			Univ_F	Mult_F	N	Prospective Power				
		Delta	GG_PWR	M_PWR				Delta	PM	PU	LU	UU
A vs. B	39	2.74	0.88	0.23	7.51(.0015)	5.67(.0072)	60	0.5	0.81	0.81	0.53	0.90
A vs. C	37	1.99	0.60	0.14	3.95(.0291)	2.82(.0738)	75	0.5	0.81	0.81	0.53	0.90
B vs. C	52	1.40	0.36	0.17	1.95(>.05)	1.79(>.05)	78	0.5	0.81	0.81	0.53	0.90
A vs. B vs. C	64	2.94	0.82	0.13	4.31(.0037)	3.46(0.114)	117	0.5	0.80	0.80	0.49	0.89
N = sample size Delta = effect size GG_PWR = Univariate Power M_PWR = Multivariate Power Univ_F = Univariate F-test and alpha Mult_F = Hotelling-Lawley Trace F-test and Alpha								N = sample Size Delta = Effect size PM = Prospective Multivariate Power PU = Prospective Univariate Power LU = Lower Bound Univariate Power UU = Upper Bound Univariate Power				

Conclusion

The relationship between δ_u^* and δ_m^* , which was developed in this study, provides a theoretical foundation for calculation of prospective power estimates for the univariate case in repeated measures designs. The relationship $\delta_u^* = \epsilon^* \delta_m^*$ can be employed to compute the univariate noncentrality parameter when the multivariate noncentrality parameter has been computed. This permits calculation of minimum sample size estimates and power analysis for the univariate procedure; and it provides a basis to address the question of which procedure to propose, univariate or multivariate, when designing a study which involves repeated measures.

Some researchers have compared the benefits of using either a multivariate or univariate procedure. Barcikowski and Robey (1984) and Stevens (2002) suggested that when conducting an exploratory analysis, both the adjusted univariate and multivariate procedures should be employed because each analysis could possibly reveal different treatment effects. O'Brien and Kaiser (1985) reported after a thorough review of the literature, under no conditions is one procedure uniformly more powerful. Results from this study indicate that generally, a researcher can use the multivariate procedure in most cases, as it does provide adequate power protection. However, the univariate procedure clearly provides greater

protection under some specific conditions, indicated as best case scenarios, and therefore can be recommended for these conditions.

Maxwell and Delaney (1990) provided an empirical guideline that if the sample size (N) is less than $p + 10$ (p representing the number of repeated trials), the univariate procedure is recommended; otherwise, if $N \geq p + 10$, the multivariate procedure is recommended. In the 2nd edition, Maxwell & Delaney (2004) modified the empirical guideline, and it is that the multivariate approach probably should be used if (1) $p \leq 4$, $\epsilon \leq .90$, and $n \geq p + 15$, or if (2) $5 \leq p \leq 8$, $\epsilon \leq .85$, and $n \geq p + 20$. Results from this study indicate that the suggested guideline by Maxwell and Delaney works well, but only when the effect size and the minimal correlation are large.

In closing, this study effectively validates many of the recommendations of Boik, Maxwell & Delaney, and others; additionally, it expands the window where univariate repeated measures designs should be employed.

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Appendix A

Proof of Rationale for Lower Bounds of Noncentrality Parameters

In (3), for matrix C ($g-1 \times g$), $C C' = I_{g-1}$; and for matrix U ($p-1 \times p$), $U U' = I_{p-1}$. Define vectors of contrast coefficients c ($g \times 1$) and d ($p \times 1$) as $a' C = c$ and $b' U = d$, where a is a vector ($g-1 \times 1$) and b is a vector ($p-1 \times 1$). Thus, $a' C M U b = c' M d = \Delta$. Because Δ is a scalar, it can be expressed as the form: $b'(U' M' C') a = \Delta$. Using the vec operator, we obtain:

$$\text{vec}[b'(U' M' C') a] = (a' C \otimes b' U') \text{vec} M'$$

Applying the constraints in (6), and using (1f.1.3) of Rao (1973, p. 60) to (3), the lower bound of δ_m is obtained by evaluating:

$$\min_{a,b} \left\{ \inf_{[a' C \otimes b' U'] \text{vec} M'} \delta_m \right\} = \frac{n \Delta^2}{d' \Sigma d} = \delta_m^*$$

For the lower bound of δ_u , subject to the same constraint as used in the multivariate case, the minimum of $\text{tr}(\omega)$ is $n \Delta^2$, then replacing $\text{tr}(\omega)$ with $n \Delta^2$, the lower bound of δ_u is obtained as:

$$\delta_u^* = b \varepsilon \cdot \frac{n \Delta^2}{\text{tr}(\Sigma_*)} = \frac{\varepsilon n \Delta^2}{\bar{\theta}},$$

where

$$\bar{\theta} = \frac{\text{tr}(\Sigma_*)}{b}.$$

Appendix B
SAS Programming Notation and Code for
Monte Carlo Procedures

```
options ls= 121 ps= 40 nodate pageno= 1;
data temp1;
set ade.adv_multi_data_set2;
if gender = "M" then gender1= 1;
if gender= "F" then gender1= 2;
if readss1= . or readss2= . or readss3= . then
delete;
*if leanob1 in(7203014 7203010);* 7203013);
if leanob1 in(7203014 7203010 7203013);
/* combinations: 7203014 with (7203010*/
run;

proc glm;
class leanob1;
model readss1 readss2 readss3 = leanob1;
repeated trials 3;
means leanob1;
run;

proc sort data= temp1; by gender1; run;

%macro powerint(pdelta=, power=, alpha= );
proc iml;
use work.temp1;
read all var {leanob1} into xx3;
gender1= unique(xx3[,1]);
read all var {leanob1 readss1 readss2 readss3}
into xx;
groups= unique(xx[,1]);

pdelta= &pdelta;
power= &power;
alpha= &alpha;

/*****
/*      Generate Basic Values for Repeated
Measures Analysis      */
/*
*****/
n1= nrow(xx);
study_n= n1;
t= ncol(xx);
p= ncol(xx)-1;
x= xx[, 2:t];
b= p-1;
g= ncol(groups);
dd= ncol(leano);
```

```
a= g-1;
m= (p - 1)*ncol(groups);
sum= x(+,|);
mean1= sum/n1;
d_Mean= mean1;
xpx= t(x)*x - t(sum)*sum/n1;
s= diag(1/sqrt(vecdiag(xpx)));
corrmatrix= corr(x);
covmatrix= xpx/(n1-1);

/*****
/*      Generate Contrast Matrices for RM-Design:
Group Matrix      */
/*****

cmatrix1= vecdiag(i(g));
cmatrix2= J(g,g-1,0);
do h= 1 to g;
do i= 1 to a while (i < h);
cmatrix2[h,i]= -1;
cmatrix2[i,i]= g - i;
end;
end;
cmatrix1= t(cmatrix1);
cmatrix2= t(cmatrix2);

/*****
/*      Generate Orthonormalized Contrast Matrices
*/
/*****

u_i1= j(p,p-1,0);
do k= 1 to p;
do l= 1 to b while (l < k);
u_i1[k,l]= -1;
u_i1[l,l]= p - l;
end;
end;

u_i1=
u_i1/shape(sqrt(u_i1[##,]),nrow(u_i1),ncol(u_i1
));

/*****
```

```

/* The next piece is the iterative do-loop to
make this program a generalized form.
Generating */
/* the necessary within matrix components
regardless of the number of groups or subjects
within a group */

do i=1 to ncol(groups);
  do rm=1 to p;
    subset=
subset||remove(xx[,rm+1],loc(choose(xx[,1]=gro
ups[i],0,1)))`;
  end;
n= nrow(subset);
  nn= nn/nrow(subset);
  sum= subset[+,];
  mean= mean//sum/n;
  xpx= subset`*subset - sum`*sum/n;
  s= xpx/(n-1);
  s_st= s_st/(n-1)*u_i1`s*u_i1;
  x_pop= diag(nn);
  free subset;
end;

/*****/
/* Generate Comparison Matrices to Compute
Sigma_st and use these matrices and the
information ob- */
/* tained using the do-loop to generate the
pooled sigma_st matrix */
/*****/

if p= 2 then
  do;
    a1= shape({1}, p-1, m);
    pool1= a1*s_st;
    sigma_st= pool1/(n1-g);
  end;
else if p= 3 then
  do;
    a1= shape({1 0}, p-1, m);
    a2= shape({0 1}, p-1, m);
    pool1= a1*s_st; pool2= a2*s_st;
    sigma_st= (pool1[1,]/pool2[2,])/(n1-g);
  end;
else if p=4 then
  do;
    a1= shape({1 0 0}, p-1, m);
    a2= shape({0 1 0}, p-1, m);
    a3= shape({0 0 1}, p-1, m);

```

```

    pool1= a1*s_st; pool2= a2*s_st; pool3=
a3*s_st;
    sigma_st=
(pool1[1,]/pool2[2,]/pool3[3,])/(n1-g);
  end;

/*****/
/* Complete the necessary computations for the
within groups and one-between one-within */
/* groups repeated measures designs for the
multivariate and univariate cases */
/*****/

sigma= u_i1`*covmat*u_i1;
m_sigma= sigma_st*(n1-g);
eval1= eigval(sigma_st);
epsilon= (sum(eval1)*sum(eval1))/((p-
1)*eval1`*eval1);
theta1= cmatrix1*mean*u_i1;
delta1=
theta1`*inv(cmatrix1*inv(x_pop)*cmatrix1`)*th
eta1;
theta= cmatrix2*mean*u_i1;
delta_st=
theta`*inv(cmatrix2*inv(x_pop)*cmatrix2`)*thet
a;
delta= sqrt(trace(delta_st))/sqrt(trace(sigma_st));
hlt= trace(delta_st*inv(m_sigma));
hlt1= trace(delta1*inv(m_sigma));
s= a><b;
m_within= (hlt1/b)/(1/(n1-p-g+2));
m_inter= ((hlt/s)/(a*b))/(1/(s*(n1-g-b-1)+2));
f_within= trace(delta1)/trace(sigma_st);
f_inter=
(trace(delta_st)/(a*b))/(trace(sigma_st)/(b));
rho= min(corrmat);
m_ndf= (p-1)*(g-1);
m_ddf= s*((n-g) - (p-1)-1 + 2);
m_ncp= (m_ddf/s)*hlt;
if m_ncp >= 50 then m_ncp= 50;
m_fcrit= finv(1-alpha, m_ndf, m_ddf);
m_pwr= 1 - probf(m_fcrit, m_ndf, m_ddf,
m_ncp);
gg_ndf= (p-1)*(g-1)*epsilon;
gg_ddf= (p-1)*(n-g)*epsilon;
gg_ncp=
b*epsilon*trace(delta_st)/trace(sigma_st);
gg_fcrit= finv(1-alpha, gg_ndf, gg_ddf);
gg_pwr= 1 - probf(gg_fcrit, gg_ndf, gg_ddf,
gg_ncp);

```



```

do n2= 12 to 1000 by 3 until (rm_pwr > power);
rm_ndf= (p-1)*(g-1);
rm_ddf= s*(n2-(p-1)-1) + 2;
rm_ncp= ((n2/g)*(delta**2)/2)/(2*(1-rho));
rm_fcrit= finv(1-alpha, rm_ndf, rm_ddf);
rm_pwr= 1 - probf(rm_fcrit, rm_ndf, rm_ddf,
rm_ncp);
end;

lb_eps= 1/(p-1);
do eps1_str= lb_eps to 0.999 by .001 until
(rgg_pwr >= rm_pwr);
rgg_ndf= (p-1)*(g-1)*eps1_str;
rgg_ddf= (p-1)*(n2-g)*eps1_str;
rgg_ncp= rm_ncp*eps1_str;
rg_fcrit= finv(1-alpha, rgg_ndf, rgg_ddf);
rgg_pwr= 1 - probf(rg_fcrit, rgg_ndf, rgg_ddf,
rgg_ncp);
end;

do n3= 12 to 1000 by 3 until (pm_pwr > power);
pm_ndf= (p-1)*(g-1);
pm_ddf= s*(n3-(p-1)-1) + 2;
pm_ncp= ((n3/g)*(pdelta**2)/2)/(2*(1-rho));
pm_fcrit= finv(1-alpha, pm_ndf, pm_ddf);
pm_pwr= 1-probf(pm_fcrit, pm_ndf, pm_ddf,
pm_ncp);
end;

total_n= n3;
grp_size= total_n/g;
do eps_star= lb_eps to 1.0 by .001 until
(pgg_pwr >= pm_pwr);
pgg_ndf= (p-1)*(g-1)*eps_star;
pgg_ddf= (p-1)*(n3-g)*eps_star;
pgg_ncp= pm_ncp*eps_star;
pg_fcrit= finv(1-alpha, pgg_ndf, pgg_ddf);
pgg_pwr= 1 - probf(pg_fcrit, pgg_ndf, pgg_ddf,
pgg_ncp);
if (pm_pwr > power) & (pgg_pwr >= pm_pwr)
then do;
end;
end;

/* Generate E_Max and E_Min for Bias Ratio */

B= P - 1;
Q= P + 1;
E1= 1/B;
E2= (B - 1)/B;
E3= 1/2*(1 + SQRT(1/B));

```

```

E_MAX= 1/2*(1 + SQRT(B));
E_MIN= 1/2*(1 - (B - 2)*SQRT(1/B));
IF E_MIN < .00 THEN E_MIN= .00;

/* GENERATE THE UNIVARIATE UPPER
BOUND ESTIMATE */

U_NDF= (p-1)*(g-1)*EPSILON;
U_DDF= (p-1)*(n3-g)*EPSILON;
U_NCP= PM_NCP*e_max;
U_FCRIT= FINV(1-ALPHA, U_NDF,
U_DDF);
*U_FCRIT= 7.85;
UU_PWR= 1 - PROBF(U_FCRIT, U_NDF,
U_DDF, U_NCP);

/* GENERATE THE UNIVARIATE LOWER
BOUND ESTIMATE */
U_NDF= (p-1)*(g-1)*EPSILON;
U_DDF= (n-1)*(n3-g)*EPSILON;
U_NCP= PM_NCP*e_min;
U_FCRIT= FINV(1-ALPHA, U_NDF,
U_DDF);
LU_PWR= 1 - PROBF(U_FCRIT, U_NDF,
U_DDF, U_NCP);
print
'*****';
print ' ';
print ' Power Analysis Results
';
print ' ';
print 'Retrospective: ' Study_n delta rho
gg_pwr m_pwr epsilon eps1_str ' ';
print ' ' f_within f_inter m_within
m_inter ' ';
print ' ';
print ' Prospective: ' total_n grp_size
pdelta epsilon pm_pwr pgg_pwr lu_pwr uu_pwr
' ';
print ' ';
print
'*****';
%mend powerint;
%powerint(pdelta= .50, power= .80, alpha= .05);
quit;

```

Analyses of Unbalanced Groups-Versus-Individual Research Designs Using Three Alternative Approximate Degrees of Freedom Tests: Test Development and Type I Error Rates

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Three approximate degrees of freedom quasi-F tests of treatment effectiveness were developed for use in research designs when one treatment is individually delivered and the other is delivered to individuals nested in groups of unequal size. Imbalance in the data was studied from the prospective of subject attrition. The results indicated the test that best controls the Type I error rate depends on the number of groups in the group-administered treatment but does not depend on the subject attrition rates included in the study.

Key words: Groups versus-individuals, approximate degrees of freedom, unbalanced designs, Type I error rate

Introduction

In the simplest groups-versus-individuals research design, two treatments are compared, one of which is administered to J groups. The j th group ($j = 1, \dots, J$) has n_j participants, for a total of $N_G = \sum_{j=1}^J n_j$ such participants. The other treatment is administered individually to N_I participants. For example, psychotherapy researchers investigating the efficacy of group therapy often use a wait-list control group (Burlingame, Kircher, & Taylor, 1994). The therapy is provided to participants in groups because the researcher believes group processes will enhance the effectiveness of the therapy. Group processes do not affect the participants in

the wait-list control group because they do not receive a treatment. In comparative studies, the effectiveness of an active treatment delivered to groups is compared to the effectiveness of an active treatment delivered individually. For example, Bates, Thompson, and Flanagan (1999) compared the effectiveness of a mood induction procedure administered to groups to the effectiveness of the same procedure administered to individuals. Using a more complex groups-versus-individuals research design, Boling and Robinson (1999) investigated the effects of three types of study environment on a measure of knowledge following a distance-learning lecture. The three types of study environment included a printed study guide accessed by individuals, an interactive multi-media study guide accessed by individuals, and a printed study guide accessed by cooperative study groups.

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Burlingame, Kircher, and Taylor (1994) reported that independent samples t tests, ANOVAs, and ANCOVAs were the most commonly used methods for analyzing data in group psychotherapy research. It is well known that the independent samples t test requires scores be independently distributed both between and within treatments—an assumption that is most likely violated in the groups-versus-individual research design. This lack of

independence is indicated by a non-zero intraclass correlation coefficient for participants who receive the group-administered treatment. Myers, Dicecco, and Lorch (1981), using simulated data, showed that the Type I error rates for independent samples t test is greater than nominal alpha when the intraclass correlation is positive. Burlingame, Kircher, and Honts (1994) reported similar results.

The Myers, Dicecco, & Lorch (1981) Quasi-F Test Statistic

Myers et al. (1981) developed a quasi-F statistic that takes into account the lack of independence of data collected from the participants in the same group in a groups-versus-individuals research design. The Myers et al. test statistic is based on the two models for the data. The model for the i th ($i = 1, \dots, N_I$) participant within the individually administered treatment (T_I) is

$$Y_{i/T_I} = \mu_I + \varepsilon_{i/T_I} \quad (1)$$

and the model for the i th participant ($i = 1, \dots, n_j$) within the j th group ($j = 1, \dots, J$) within the group-administered treatment (T_G) is

$$Y_{i/j/T_G} = \mu_G + \alpha_{j/T_G} + \varepsilon_{i/j/T_G}. \quad (2)$$

Myers et al. assumed that $\varepsilon_{i/T_I} \sim N(0, \sigma_{S/T_I}^2)$, $\alpha_{j/T_G} \sim N(0, \tau^2)$, and $\varepsilon_{i/j/T_G} \sim N(0, \sigma_{S/G/T_G}^2)$. The assumption about the α_{j/T_G} implies that the groups in the group-administered treatment are considered to be representative of an infinitely large number of groups. Therefore, the Myers et al. method permits generalization of the result to this larger number of groups. In addition, Myers et al. assumed that the groups within the group-administered treatments were balanced ($n_1 = \dots = n_J$).

Formulated as an approximate degrees of freedom (APDF) t statistic, the Myers et al. test statistic is

$$t_{APDF} = \frac{\bar{Y}_I - \bar{Y}_G}{\sqrt{a_1 MS_{S/T_I} + a_2 MS_{G/T_G}}}$$

where a_1 is $(1/N_I)$ and a_2 is $(1/N_G)$. The mean

$$\bar{Y}_I = \frac{1}{N_I} \sum_{i=1}^{N_I} Y_{i/T_I}$$

is the mean of the criterion scores for the participants in the individually administered treatment (T_I),

$$MS_{S/T_I} = \frac{\sum_{i=1}^{N_I} (Y_{i/T_I} - \bar{Y}_I)^2}{N_I - 1}$$

is the variance for participants who received the individually-administered treatment,

$$\bar{Y}_G = \frac{1}{N_G} \sum_{j=1}^J \sum_{i=1}^{n_j} Y_{i/j/T_G}$$

is the mean of the criterion scores of participants who received the group-administered treatment, and

$$MS_{G/T_G} = \frac{\sum_{j=1}^J n_j (\bar{Y}_{j/T_G} - \bar{Y}_G)^2}{J - 1}$$

is the between-group mean square for these participants. It can be shown that the squared denominator of the t statistic estimates the sampling variance of the numerator given the assumptions made by Myers et al. about the random effect and residuals. The estimated Satterthwaite (1941) approximate degrees of freedom are

$$\hat{f}_2 = \frac{(a_1 MS_{S/T_I} + a_2 MS_{G/T_G})^2}{\frac{(a_1 MS_{S/T_I})^2}{N_I - 1} + \frac{(a_2 MS_{G/T_G})^2}{J - 1}}.$$

An Alternative Approximation for the Degrees of Freedom

The Satterthwaite (1941) approximation of the distribution of the linear combination of mean squares in the denominator of the t statistic is based on the assumptions that MS_{S/T_I} and MS_{G/T_G} are independent random variables that are distributed as multiples of chi-square distributions. The distribution of the sum is approximated as chi-square with degrees of freedom estimated by equating the first two moments of the sample and the approximating chi-square distribution.

The discussion in Satterthwaite (1941) implied that this approximation of the distribution of the denominator improves as $J-1$ or N_I-1 increases and as

$$\frac{(N_I - 1)(n\tau^2 + \sigma_{S/G/T_G}^2)}{(J - 1)\sigma_{S/T_I}^2} \quad (3)$$

becomes closer to 1.0. When there are two groups in the group-administered treatment level, J is as small as possible and the ratio of equation (3) is typically larger than 1.0 and increases as the number of participants in the two groups increases and as the intraclass correlation increases. Scarino and Davenport (1986) studied the Type I error rate of the Welch APDF t test and found it could be seriously inflated when (a) there is a negative relationship between the sampling variances of the means and the degrees of freedom for the estimated sampling variances and (b) the smaller of the two degrees of freedom is small. Wehry and Algina (2003) applied the work of Scarino and Davenport to the Myers et al. (1981) quasi-F test and showed that when J equals two or three and $\tau > 0$, the Satterthwaite approximation of the denominator degrees of freedom also resulted in a quasi-F test that does not control the Type I error rate at nominal alpha.

Scarino and Davenport (1986) developed a four-moment approximation of the degrees of freedom for use with the Welch t when the ratio of the sampling variances is large and the corresponding ratio of degrees of freedom is small. Wehry and Algina (2003) adapted the four-moment approximation for use with the groups-versus-individual research design. The four-moment approximation to the degrees of freedom is

$$\hat{f}_4 = \frac{\left\{ \frac{u^2}{m_1} + \frac{1}{m_2} \right\}^3}{\left(\frac{u^3}{m_1^2} + \frac{1}{m_2^2} \right)^2} \quad (4)$$

where $u = a_2 MS_{G/T_G} / a_1 MS_{S/T_I}$, $m_1 = J - 1$, and $m_2 = N_I - 1$. Like the Satterthwaite approximation employed by Myers et al. (1981), the four-moment degrees of freedom is based on the assumption of a balanced design.

Scarino and Davenport (1986) reported that the four-moment APDF test is conservative under some conditions and suggested using an average of the two-moment and four-moment approximations of the degrees of freedom. Wehry and Algina (2003) conducted a study of the APDF quasi-F test with the two-moment, four-moment, and an arithmetic average of the two- and four-moment approximations of the degrees of freedom using both analytical results and simulated data. They concluded that when the group-administered treatment is delivered to two groups, the four-moment APDF quasi-F test should be used and when the group-administered treatment is delivered to three or more groups, the average-moment APDF quasi-F test should be used. However, the two-moment APDF quasi-F test is only slightly liberal in conditions involving more than three groups.

Quasi-F Statistics For Use When Data Are Not Balanced Across Groups In The Group-Administered Treatment Level

The purpose of the present study is to extend the work of Myers et al. (1981) and Wehry and Algina (2003) to include groups-versus-individuals research designs that are not

balanced across either treatment levels (i.e., $N_I \neq N_G$) or the groups in the group-administered treatment level (i.e., $n_j \neq n_{j'}$ for at least one pair of j and j'). Usually in experimental research an equal number of participants are randomly assigned to each treatment level; however, N_I and N_G , as well as the n_j can be affected by attrition of participants. Burlingame, Kircher, and Taylor (1994) found 18% subject attrition was the median reported attrition rate of subjects in a survey of psychotherapy literature. Clarke (1998) suggested that the attrition rate in wait-list control groups could even be higher than that of the active treatment level.

Imbalance can also result from studying naturally occurring groups such as family units and classrooms. Methods that accommodate imbalance across groups in the group-administered treatment level have not been developed. A possible solution to the imbalance across groups in the group-administered treatment level is to randomly eliminate participants until balance is achieved. However, eliminating data results in a loss of statistical power.

APDF Quasi-F Test for Unbalanced Data

As is well known, if the variances of $\bar{Y}_I$ and $\bar{Y}_G$ were known, the hypothesis $H_0: \mu_I - \mu_G = 0$ could be tested by

$$\chi^2 = \frac{(\bar{Y}_I - \bar{Y}_G)^2}{\text{Var}(\bar{Y}_I - \bar{Y}_G)}. \quad (5)$$

Because observations are independent across treatment levels, substituting the variances of $\bar{Y}_I$ and $\bar{Y}_G$ into equation (5) results in

$$\chi^2 = \frac{(\bar{Y}_I - \bar{Y}_G)^2}{\frac{\sigma_{S:I}^2}{N_I} + \frac{\tau^2 \sum_{j=1}^J n_j^2}{N_G^2} + \frac{\sigma_{S:G/T_G}^2}{N_G}}. \quad (6)$$

However, the variances are not known, and, in order to develop a test statistic that can be used

in practice, two steps must be completed: Develop estimators of the variance components in equation (6) and approximate the distribution of the resulting test statistic. Approximating the distribution of the denominator by a chi-square distribution and the distribution of the test statistic by an F distribution is a common practice in statistics.

Variance Component Estimates

There are numerous methods for estimating the variance components. Perhaps the most commonly used method is the method of moments, also called the ANOVA estimation of variance components (Milliken & Johnson, 1992). Meyers et al. (1981) used the method of moments variance component estimators in formulating the quasi-F test statistic. The method of moments procedure is based on equating the expected values of the sums of squares to their respective observed values.

Other estimation methods include maximum likelihood (ML), restricted maximum likelihood (REML), minimum norm quadratic unbiased (MINQUE), and minimum variance quadratic unbiased (MIVQUE) estimators. ML estimators are values of the parameter space that maximize the likelihood function. In REML, the likelihood equations are partitioned into two parts, one part that is free of fixed effects. REML maximizes the part that has no fixed effects. MINQUE and MIVQUE are iterative and the researcher must provide initial values of the components. All methods produce the same results when the design is balanced (Milliken & Johnson, 1992; Swallow & Monahan, 1984).

Swallow and Monahan (1984) conducted a Monte Carlo study of ANOVA, ML, REML, MIVQUE and MINQUE methods of estimating the variance components of a one-way unbalanced, random effects design. All simulated data were normal, and the variables manipulated were the degree of imbalance, the number of groups, and the ratio of $\tau^2 / \sigma_{S:I/G/T_G}^2$.

In terms of bias of the estimates, the results indicated, except in cases of extreme patterns of imbalance, $n_j = (1, 1, 1, 1, 13, \text{and } 13)$ and $n_j = (1, 1, 1, 1, 1, 1, 19, \text{and } 19)$, ANOVA, REML, and MINQUE estimators showed little difference. However, the results indicated that

ML methods were the best estimators of τ^2 when $\tau^2/\sigma_{S/G/T_G}^2 \leq .5$ because of the small bias and the low mean square error of the estimate. When $\tau^2/\sigma_{S/G/T_G}^2$ is large, Swallow and Monahan indicated there may be a substantial downward bias and that ML methods have no superiority over the other methods. There was little difference among the methods studied when estimating $\sigma_{S/G/T_G}^2$. Milliken and Johnson (1992) suggested that ANOVA estimates should have good properties for nearly balanced data, and Swallow and Monahan concluded that unless the data are severely unbalanced and $\tau/\sigma_G^2 > 1$, ANOVA estimates are adequate.

The results of the Swallow and Monahan (1984) study and the recommendations of Milliken and Johnson (1992) suggested that ANOVA estimates of the variance components are likely to be adequate for the groups-versus-individuals research design. Data as extreme as that simulated in the Swallow and Monahan study seems likely to be rare in group research; therefore, method of moments estimators of the variance components are used for the quasi-F test for comparing the effectiveness of two treatment levels when data are unbalanced.

The expected values for the mean squares for groups (henceforth when the term groups is used, it will refer to the groups within the group-administered treatments) are

$$EMS_{G/T_G} = \sigma_{S/G/T_G}^2 + n_o \tau^2, \quad (7)$$

where

$$n_o = \frac{1}{J-1} \left(N_G - \frac{\sum_{j=1}^J n_j^2}{N_G} \right)$$

(Snedecor & Cochran, 1956). The other two expected values are

$$EMS_{S/G/T_G} = \sigma_{S/G/T_G}^2 \quad (8)$$

and

$$EMS_{S/T_I} = \sigma_{S/T_I}^2.$$

The mean squares are equated with their respective expected values of equations (7), (8), and (9) are the resulting equations are solved for the ANOVA variance component estimates. The variance component estimates are then substituted into equation (6) to obtain the quasi-F test statistic for comparing weighted treatment level means.

The Quasi-F Test Statistic

Using the estimated variance components the quasi-F test statistic is

$$\hat{F}_{quasi} = \frac{(\bar{Y}_I - \bar{Y}_G)^2}{\left\{ \frac{MS_{S/T_I}}{N_I} + \frac{(MS_{G/T_G} - MS_{S/G/T_G}) \sum_{j=1}^J n_j^2 / n_o}{N_G^2} + \frac{MS_{S/G/T_G}}{N_G} \right\}}, \quad (9)$$

which simplifies to

$$\hat{F}_{quasi} = \frac{(\bar{Y}_I - \bar{Y}_G)^2}{\left\{ \frac{MS_{S/T_I}}{N_I} + \frac{MS_{G/T_G} \sum_{j=1}^J n_j^2}{n_o N_G^2} + \frac{MS_{S/G/T_G} \left(n_o N_G - \sum_{j=1}^J n_j^2 \right)}{n_o N_G^2} \right\}}.$$

The denominator of the quasi-F statistic is a synthetic mean square in the form of

$$MS = a_1 MS_{S/T_I} + a_2 MS_{G/T_G} + a_3 MS_{S/G/T_G}, \quad (10)$$

where

$$a_1 = \frac{1}{N_I},$$

$$a_2 = \frac{\sum_{j=1}^J n_j^2}{n_o N_G^2},$$

and

$$a_3 = \left(\frac{n_o N_G - \sum_{j=1}^J n_j^2}{n_o N_G^2} \right).$$

Approximating Chi-Square Distribution

The model for the group-administered treatment is a random effects ANOVA model [see equation (2)]. For a design that is balanced across classes, Searle (1992) showed the mean squares between and within classes are independent and are distributed as multiples of chi-square distributions. When the data are not balanced across classes, the mean squares within and between are still independent; however, the mean square between classes is not distributed as a multiple of a chi-square distribution. Nevertheless, Burdick, and Graybill (1988) indicated as long as τ is not too large, approximating the mean square between as a multiple of a chi-square distribution does not result in a large error.

Two-Moment Approximation of the Degrees of Freedom

The Satterthwaite (1941) approximation for the degrees of freedom for the linear combination in equation (10) is

$$\hat{f}_2 = \frac{(a_1 MS_{S/T_I} + a_2 MS_{S/G/T_G} + a_3 MS_{S/G/T_G})^2}{\frac{(a_1 MS_{S/T_I})^2}{N_I - 1} + \frac{(a_2 MS_{S/G/T_G})^2}{J - 1} + \frac{(a_3 MS_{S/G/T_G})^2}{N_G - J}}.$$

It should be noted that $a_3 \leq 0$, with equality holding only when $n_o = n$. Therefore, when

data are not balanced across groups in the group-administered treatment level, it is possible for the denominator of the quasi-F statistic to be less than or equal to zero when the estimate of τ^2 is substantially smaller than zero. In these cases, as suggested by Searle (1992), it is reasonable to assume τ^2 is zero and replace the quasi-F statistic by the Welch t -test where

$$t_{W_{APDF}} = \frac{(\bar{Y}_I - \bar{Y}_G)}{\sqrt{\frac{MS_{S/T_I}}{N_I} + \frac{MS_{S/T_G}}{N_G}}}$$

and

$$MS_{S/T_G} = \frac{\sum_{j=1}^J \sum_{i=1}^{n_j} (Y_{i/j/T_G} - \bar{Y}_G)^2}{(N_G - 1)}$$

with two-moment degrees of freedom

$$\hat{df} = \frac{\left(\frac{MS_{S/T_I}}{N_I} + \frac{MS_{S/T_G}}{N_G} \right)^2}{\frac{(MS_{S/T_I})^2}{N_I^2 (N_I - 1)} + \frac{(MS_{S/T_G})^2}{N_G^2 (N_G - 1)}}$$

(Welch, 1938).

Modified Four-Moment Approximation of the Degrees of Freedom

Because the coefficients of the variance component terms in the synthetic error term for unbalanced data are not all positive and because of the occurrence of conditions in which the ratio of the degrees of freedom is less than one when the ratio of the corresponding sampling variances is greater than one, the two-moment quasi-F test may not control the Type I error rate at the nominal level. The four-moment approximation was developed by Scariano and Davenport (1986) for a synthetic mean square that is the sum of two positive terms. Rather than expanding the four-moment approach to three terms including one that is negative, a simpler approach that combines the two-moment and four-moment approximations was used in this study.

In order to compute the modified four-moment approximation, the degrees of freedom for $a_2MS_{G/T_G} + a_3MS_{S/G/T_G}$ are first approximated using the two-moment approach. As noted previously, Searle (1992) showed MS_{G/T_G} and $MS_{S/G/T_G}$ are independent when data are unbalanced, Burdick and Graybill (1988) indicated as long as τ^2 is not too large MS_{G/T_G} can be approximated as a multiple of chi-square distribution, and Swallow and Monahan (1984) showed that method of moments estimation works well in one-way, random effects, unbalanced ANOVA designs as long as $\tau^2/\sigma_{S/G/T_G}^2 \leq 1$. The two-moment degrees of freedom for

$$MS_{error_{T_G}} = a_2MS_{G/T_G} + a_3MS_{S/G/T_G}$$

are

$$\hat{f}_{2_G} = \frac{(MS_{error_{T_G}})^2}{\left[\frac{(a_2MS_{G/T_G})^2}{(J-1)} + \frac{(a_3MS_{S/G/T_G})^2}{(N_G - J)} \right]}.$$

This value of $\hat{f}_{2_G}$ along with $MS_{error_{T_G}}$ and the estimate of the individual treatment level variance, MS_{S/T_I} , are used in the four-moment approximation of equation (4). In the modified four-moment approximation,

$u = MS_{error_{T_G}}/a_1MS_{S/T_I}$, $m_1 = \hat{f}_{2_G}$, and $m_2 = (N_I - 1)$. When $MS_{error_{T_G}} \leq 0$, the quasi-F statistic is replaced by the Welch t -test.

Modified Averaged Degrees of Freedom Approximation of the Degrees of Freedom

Scariano and Davenport (1986) reported that, with completely balanced data, the four-moment quasi-F test is conservative under some conditions. Therefore, an arithmetic average of the two-moment and the modified four-moment approximations was also included in the present study. When $MS_{error_{T_G}} \leq 0$, data were analyzed using the Welch t test; otherwise, the two-moment approximation and the modified four-

moment approximation to the degrees of freedom were arithmetically averaged resulting in an averaged degrees of freedom quasi-F test.

Example 1

Participants were randomly assigned to two conditions and completed three trials of the prisoner's dilemma. The data are the number of competitive choices across the three trials. In one condition, participants completed the three trials independently. In the second condition, participants worked in teams and discussed how to respond to each trial. However, participants within a team responded individually. For participants in the individual treatment the relevant results are $N_I = 32$, $\bar{Y}_I = .469$, $MS_{S/T_I} = .773$. For participants in the group-administered treatment, the results are $N_G = 48$, $J = 15$, $\sum_{j=1}^J n_j^2 = 141$, $\bar{Y}_G = .905$, $MS_{G/T_G} = 1.896$, and $MS_{S/G/T_G} = .833$. The calculated t statistic is -1.86. The degrees of freedom are $\hat{f}_2 = 56.37$, $\hat{f}_4 = 56.04$, and $\hat{f}_a = 54.70$. For all three degrees of freedom, $(Prob > |t|) = .068$. Because the theory predicts more competitive response following group discussion, the results are in support of the theory.

Example 2

In an evaluation of a pre-school literacy program, the evaluators were interested in whether reading achievement was different in single-classroom sites and multiple-classroom sites. The available data are mean end-of year reading achievement for each of the classrooms. For single-classroom sites the relevant results are $N_I = 38$, $\bar{Y}_I = 88.85$, $MS_{S/T_I} = 57.84$. For participants in the multiple-classroom sites, the results are $N_G = 63$, $J = 29$, $\sum_{j=1}^J n_j^2 = 216$, $\bar{Y}_G = 87.52$, $MS_{G/T_G} = 69.09$, and $MS_{S/G/T_G} = 22.22$. The calculated t statistic is

0.71. The degrees of freedom are $\hat{f}_2 = 30.87$, $\hat{f}_4 = 17.76$, and $\hat{f}_a = 24.31$. For all three degrees of freedom, $(Prob > |t|) = .76$. The results do not support the belief that mean reading achievement is different in single-classroom and multiple classroom sites.

Methodology

Variables Manipulated in the Monte Carlo Study

The design of the Monte Carlo study had five between-subjects factors and one within-subjects factor. There were a total of 2700 conditions. The design included the three approaches to the approximation of the error term degrees of freedom as levels of the within-subjects factor. The number of groups, planned size of the groups, level of the intraclass correlation, ratio of the group to individual treatment level variances, and the rate of subject attrition were the five between-subjects factors. There were five levels of the number of groups, $J = 2, 3, 4, 5$, and 6; five levels of planned group size, $n = 4, 8, 12, 16$, and 20 subjects nested in the groups; three levels of intraclass correlation, $\tau^2 / (\tau^2 + \sigma_{S/G/T_G}^2) = .0, .2$, and $.4$; three levels of the ratio of group to individual treatment level variances, $(\tau^2 + \sigma_{S/G/T_G}^2) / \sigma_{S/I}^2 = 0.75, 1.00$, and 1.25 ; and four combinations of individual and group treatment level attrition rates, $.15$ and $.15$, $.15$ and $.25$, $.25$ and $.15$, and $.25$ and $.25$.

Data Generation

The simulation in the study was carried out using the random number generation functions of SAS, Release 6.12. Scores for simulated participants in the individually administered treatment level were generated using the equation

$$Y_{i/I} = \mu_I + \varepsilon_{i/I}$$

where μ_I was arbitrarily set at 100 and the $\varepsilon_{i/I}$ s were pseudorandom standard normal deviates generated using RANNOR. The

variable Y_{i/T_I} was set to the missing data indicator if $U_{i/T_I} < p_{T_I}$ where p_{T_I} is the individually administered treatment level attrition rate and U_{i/T_I} was a pseudorandom uniform deviate generated using RANUNI. However, N_I was not permitted to be smaller than two.

Scores for simulated participants in the group-administered treatment level were generated using the equation

$$Y_{i/j/T_G} = \mu_G + \alpha_{j/T_G} + \varepsilon_{i/j/T_G}$$

where μ_G was arbitrarily set at 100, α_{j/T_G} was a pseudorandom normal deviate with mean zero and variance τ^2 , and $\varepsilon_{i/j/T_G}$ was a pseudorandom normal deviate with mean zero and variance $\sigma_{S/G/T_G}^2$. The variable $Y_{i/j/T_G}$ was set to a missing value indicator if $U_{i/j/T_G} < p_{T_G}$, where p_{T_G} is the group-administered treatment level attrition rate and $U_{i/j/T_G}$ was a pseudorandom uniform deviate generated using RANUNI. However, in all cases n_j was not permitted to be smaller than two.

Each of the conditions was replicated 10,000 times, and the Type I errors of the three tests were counted over the replications of each condition. All tests were conducted at $\alpha = .05$.

Results

A Number of Groups (5) $\times$ Planned Group Size (5) $\times$ Intraclass Correlation (3) $\times$ Ratio of Variance (3) $\times$ Attrition Rate (4) $\times$ Degrees of Freedom Approximation (3), with repeated measures on the last factor, ANOVA was used to analyze the Type I error rate data. Because there was only one data point for each combination of the six factors, the five-way interaction of the first five factors was used as the error term for between-replications effects and the six-way interaction was used as the error term for all within-replications effects. For each effect omega squared was used to express the size of the effect as a proportion of the total variance. An effect was considered important if

it was significant at $\alpha = .05$ and accounted for more than 1% of the total variance in the Type I error rate. Table 1 presents the omega squares for all significant effects. The sum of the omega squares for all of the important effects was 0.929. All factors except subject attrition rate were involved in an effect that met our criterion for an important influence on the Type I error rate.

Averaged over all factors, other than number of groups in the group-administered treatment, the average Type I error rate of the two-moment test was greater than that for the averaged degrees of freedom test. Also the average Type I error rate of the averaged degrees of freedom test was greater than that for the modified four-moment test. When there were two groups only the modified four-moment test controlled the Type I error rate near nominal alpha; however, the modified four-moment test resulted in a conservative quasi-F test with three or more groups. In all conditions involving two groups, increasing the planned size of the groups, the ratio of treatment level variances, or the intraclass correlation increased the Type I error rate. Under conditions involving three or more groups, increasing the intraclass correlation increased the Type I error rate of all three tests and increasing the ratio of treatment level variances and the planned size of the groups increased the Type I error rate of the two-moment and averaged degrees of freedom tests. As the number of groups increased the effect of increasing the ICC or the planned size of the groups declined. However, under conditions of three groups or more groups, increasing the ratio of the treatment level variances and the planned size of the groups decreased the Type I error rate of the modified four-moment quasi-F test.

Table 2 contains the minimum and maximum Type I error rate averaged over subject attrition by number of groups, approximate degrees of freedom approach, and intraclass correlation. Minima and maxima were computed over planned size of groups and ratio of treatment level variances. In Table 2 bold and italicized figures indicate the degrees of freedom approach that resulted in better control of Type I error rate for a particular number of groups and ICC. When both bold figures and italicized

figures are presented, the italicized figures indicate the degrees of freedom approximation that tended to result in a higher Type I error rate. Tests are considered unacceptable if the maximum Type I error rate is above .075, the upper limit of Bradley's (1978) liberal criterion for a robust test or if the minimum Type I error rate is below .025 the lower limit of Bradley's (1978) liberal criterion.

Inspection of Table 2 indicates that when there are two groups, the modified four-moment test should be used at the risk of a conservative test when the ICC is near zero. The averaged degrees of freedom test may be more attractive with a low ICC, but the fact that it has a strong liberal tendency when the ICC is 0.20 raises the question of how the two tests function for ICCs between 0.00 and 0.20. Supplementary results are shown in Table 3 for ICCs of 0.05, 0.10, and 0.15. In the simulations conducted to obtain these results, all other conditions were the same as in the original study. The findings that the averaged degree of freedom test has a liberal tendency for an ICC of 0.10 and that the conservative tendency of the modified four-moment test is less marked with an ICC of 0.05 than with an ICC of 0.00 suggest the modified four-moment test should be used when there are two groups in the group-administered treatment.

When there are three groups, the results in Tables 2 and 3 suggest the averaged degree of freedom test should be used at the risk of a slightly conservative test when the ICC is near zero. Then the two-moment test may be more attractive. However, it is not clear how valid an estimated ICC will be in selecting between the two tests. Given the very mild conservative tendency for the averaged degrees of freedom test, it is recommended when there are three groups.

When there are four or more groups either the two-moment test or the averaged degrees of freedom test might be used. The former can be somewhat liberal, with the tendency increasing as the ICC increased, but decreasing as the number of groups increased. The averaged degrees of freedom test can be somewhat conservative, with the tendency decreasing as the ICC increased and as the number of groups decreased.

Table 1. Mean Square Components and $\hat{\omega}_j^2$ for the Important Effects ($\hat{\omega}_j^2 > .01$)

Source of MS	$\hat{\omega}_j^2$
Between Replications Effects	
Number of Groups – g	0.239
Planned Size of Groups - n	0.024
Intraclass Correlation - icc	0.073
$g \times n$	0.056
$g \times icc$	0.079
Within-Replication Effects	
Approximation – t	0.390
$t \times g$	0.020
$t \times n$	0.031
$t \times \text{ratio of treatment level variance}$	0.017

Table 2. Minimum and Maximum Average Type I Error Rate by Number of Groups, Test, and ICC

Number of Groups	Test	ICC		
		0.00	0.20	0.40
2	$\hat{f}_2$	.0470, .0759	.0532, .1118	.0571, .1204
	$\hat{f}_{ave}$	.0390, .0572	.0459, .0907	.0496, .1005
	$\hat{f}_4$	.0338, .0401	.0412, .0580	.0437, .0663
3	$\hat{f}_2$	.0471, .0589	.0514, .0770	.0537, .0776
	$\hat{f}_{ave}$	.0411, .0488	.0450, .0634	.0476, .0637
	$\hat{f}_4$	.0299, .0362	.0322, .0404	.0319, .0403
4	$\hat{f}_2$	.0488, .0560	.0506, .0631	.0520, .0637
	$\hat{f}_{ave}$	.0422, .0481	.0459, .0528	.0458, .0539
	$\hat{f}_4$	.0281, .0400	.0283, .0393	.0298, .0390
5	$\hat{f}_2$	.0473, .0533	.0513, .0585	.0491, .0603
	$\hat{f}_{ave}$	.0436, .0467	.0469, .0499	.0451, .0509
	$\hat{f}_4$	.0282, .0417	.0303, .0411	.0326, .0410
6	$\hat{f}_2$	.0480, .0557	.0488, .0568	.0507, .0557
	$\hat{f}_{ave}$	.0442, .0491	.0451, .0500	.0464, .0505
	$\hat{f}_4$	.0299, .0436	.0317, .0423	.0326, .0405

Table 3. Minimum and Maximum Average Type I Error Rate by Number of Groups, Test, and ICC: Supplemental Conditions

Number of Groups	Test	ICC		
		0.05	0.10	0.15
2	$\hat{f}_2$	.0482, .0908	.0489, .0990	.0508, .1066
	$\hat{f}_{ave}$	.0396, .0705	.0404, .0784	.0430, .0870
	$\hat{f}_4$	.0352, .0481	.0360, .0513	.0383, .0562
3	$\hat{f}_2$	.0492, .0660	.0472, .0711	.0495, .0733
	$\hat{f}_{ave}$	.0418, .0538	.0416, .0585	.0436, .0604
	$\hat{f}_4$	.0296, .0377	.0310, .0373	.0307, .0389

Conclusion

Myers et al. (1981) presented a two-moment, quasi-F test for use when one treatment is delivered to individuals and one is delivered to groups of participants and the data are balanced for the groups in the group-administered treatment. Wehry and Algina (2003) extended that quasi-F test to include a four-moment and an averaged degrees of freedom quasi-F test for use when data are balanced across the group-administered treatment level.

In this study, the two-moment approach developed by Myers et al. (1981) and the four-moment and averaged degrees of freedom approaches developed by Wehry and Algina (2003) were extended to include groups versus individual research designs in which data are not necessarily balanced across treatment levels or across groups in the group-administered treatment level. In addition, Type I error rates of the resulting tests were estimated. The results indicated the modified four-moment test should be used when the group-administered treatment is delivered to two groups and the averaged degrees of freedom approach should be used when the group-administered treatment is delivered to three groups. When there are four or more groups, either test could be used—the averaged degrees of freedom test has a slightly conservative tendency and the two-moment test has a slightly liberal tendency. When there are four or five groups the Type I error rate for the averaged degrees of freedom test is between .040 and .055. The Type I error for two-moment test can be larger than .06. When there are six groups, the averaged degrees of freedom test controls the Type I error rate between .044 and .051; the two-moment test controls it between .048 and .057.

Although, it is recommended to use the four-moment test when there are two groups, researchers should be very cautious about using a group-versus-individuals design with only a few groups. For a balanced design, Wehry and Algina (2003) showed that power is likely to be very low when there are just two groups and there is no reason for the design to be more powerful when the design is unbalanced. More generally, Myers et al. (1981) have shown that the number of groups can have a larger effect on

power than the number of participants per groups and therefore recommended designs with as large a number of groups as possible.

At least four lines of additional research are attractive. Comparison of the three approximate degrees of freedom tests to mixed model tests using Satterthwaite or Kenward-Rogers degrees of freedom might be investigated. One difference between the current approaches and the mixed-model approach is the estimate of the mean for the group-administered treatment. In the present approach the estimated mean is computed by weighting the group means by the group sample sizes. In the mixed model approach, the mean for the group-administered treatment would be estimated by generalized least squares and would have a sampling variance that is not larger than the sampling variance of the mean used in the present approach. This may make the mixed model approach more powerful. However, Wehry and Algina (2003) found that with balanced designs, the mixed model approach had poor control of the Type I error rate in some situations and this problem may generalize to unbalanced designs.

The performance of the three tests when data are not normal is important. Micceri (1987) reported that a wide variety of psychometric distributions may not be normal and that random-effects ANOVA tests may not be robust to departures from normality, especially when conditions involve unbalanced designs or small sample sizes. Developing robust versions of the tests is important. Finally extension of the tests to more than two groups and to multivariate designs would be useful.

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Type I Error Rates of the Kenward-Roger Adjusted Degree of Freedom F -test for a Split-Plot Design with Missing Values

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The Type I error rate of the Kenward-Roger (KR) test, implemented by PROC MIXED in SAS, was assessed through a simulation study for a one between- and one within-subjects factor split-plot design with ignorable missing values and covariance heterogeneity. The KR test controlled the Type I error well under all of the simulation factors, with all estimated Type I error rates between .040 and .075. The best control was for testing the between-subjects main effect (error rates between .041 and .057) and the worst control was for the between-by-within interaction (.040 to .075). The simulated factors had very small effects on the Type I error rates, with simple effects in two-way tables no larger than .01.

Key words: Missing values, Kenward-Roger F -test, robustness, mixed models, split-plot design.

Introduction

According to Keselman et al. (1998), one of the most commonly used designs in educational and psychological research is the split-plot design, a design which includes both between-subjects and within-subjects factors. Responses on the within-subjects factor are obtained by repeatedly measuring each participant in the study. The repeated measures might be obtained at different points in time or under different treatments. Unfortunately, data collected in split-plot designs can be incomplete for a variety of reasons. Consider participants who drop out of a longitudinal study because of illness or death, refuse to answer questions on a survey because of its length or the sensitivity of the questions, or are unable to answer questions on a performance assessment test because of time constraints or lack of ability. Each results in missing values.

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Little and Rubin (2002, p. 12) and Rubin

(1976) defined three types of missing data mechanisms. The missing data mechanisms, ordered from most restrictive to least restrictive in terms of assumptions made about the process that leads to the missing data, are missing completely at random (MCAR), missing at random (MAR), and not missing at random (NMAR). Generally, the NMAR missing data condition constitutes any missing data condition that is not MCAR or MAR. Let $f(r_i | y_i, X_i, \psi)$ denote the distribution of the missing data indicators for participant i , where r_i is a $K \times 1$ vector whose elements are zero for missing and one for observed in the corresponding elements of the $K \times 1$ vector of repeated variables y_i , X_i is the design matrix for the factors, and ψ contains the parameters for the relationship of r_i to y_i and X_i .

Data are MCAR if $f(r_i | y_i, X_i, \psi) = f(r_i | X_i, \psi)$, that is, if the distribution of the missing data indicators does not depend on the repeated measures. The y_i vector can be partitioned as $y_i = [y'_{io} \ y'_{im}]'$ where y_{io} contains the repeated measures variables on which participant i has observed scores and y_{im} contains the repeated measures variables on which participant i has missing scores. If $f(r_i | y_i, X_i, \psi) = f(r_i | y_{io}, X_i, \psi)$, that is, the missing data indicator does not depend on the variables of which participant i

has missing scores, then the data are MAR.

The distribution of y_i can be written as $f(y_i | X_i, \theta)$, where θ contains the main effect and interaction parameters as well as the parameters for the covariance matrix for the repeated measures. A general method for consistent maximum likelihood (ML) estimation of θ is obtained by including both the observed scores on the repeated measures and the missing data indicators, as well as θ and ψ , in the likelihood. However, Rubin (1976) showed that if the missing data mechanism is MCAR or MAR and if the parameters ψ and θ are disjoint, ML estimators of the θ parameters are consistent when the missing data indicators and ψ are excluded from the data analysis.

Excluding the missing data indicators and ψ is referred to as ignoring the missing data mechanism. Thus, the MCAR or MAR missing data mechanisms are ignorable for purposes of ML estimation. If the data are MCAR, both listwise deletion and ML ignoring the missing data mechanism will produce consistent estimators, but the ML estimators will be more accurate because they use all of the available data. Rubin (1976) also showed that the MCAR missing data mechanism is ignorable for sampling distribution based inference procedures such as hypothesis tests and confidence intervals. So, if the data are MCAR, either listwise deletion or ML ignoring the missing data mechanism can be used for inference, but ML will result in more powerful tests and narrower confidence intervals because it does not delete the observed data for participants with some missing values.

When ML estimation is used, whether the MAR missing data mechanism is ignorable for sampling distribution based inference depends on how the sampling covariance matrix is calculated. The MAR missing data mechanism is ignorable for sampling distribution based inferences on the means if the sampling covariance matrix is estimated from the observed information matrix for the means and the covariance parameter estimates, but not if the matrix is estimated from the portion of the observed information matrix that pertains only to the means (Kenward & Molenberghs, 1998).

The MAR mechanism may not be ignorable for sampling distribution based inferences if the sampling covariance matrix is estimated from the expected information matrix. If the expected information matrix is used, it must take into account the actual sampling process implied by the MAR mechanism (Kenward & Molenberghs, 1998). Kenward and Molenberghs (1998) referred to using this type of expected information matrix as using the unconditional sampling framework; whereas using the information matrix that ignores this sampling process is referred to as using the naïve sampling framework.

If the missing data mechanism is NMAR, the missing data mechanism is non-ignorable for purposes of ML estimation, and the pattern of missing values must be taken into account to obtain consistent ML estimates. This can be accomplished by using a selection model that incorporates a model for the missing values indicator or by using a pattern mixture model, which stratifies the data on the basis of the pattern of missing values (Albert & Follmann, 2000; Algina & Keselman, 2004a, 2004b; Diggle & Kenward, 1994; Fitzmaurice, Laird, & Shneyer, 2001; Kenward, 1998; Little, 1995; Troxel, 1998). Little (1995) provided details about these two approaches.

Unfortunately, traditional methods for analyzing data from a split-plot design such as ANOVA, adjusted degrees of freedom ANOVA, and MANOVA use listwise deletion and therefore are not likely to yield valid inferences except when the missing data mechanism is MCAR, an often unrealistic assumption in applied settings. Furthermore, these tests also assume that the covariance matrices ($\Sigma_j, j = 1, \dots, J$) are homogenous across the J levels of the between-subjects factor, another often-unrealistic assumption. The tests will often fail to control the Type I error when the homogeneity assumption is violated (Keselman & Keselman, 1990; Keselman, Keselman, & Lix, 1995; Keselman, Lix, & Keselman, 1996). For further details about these tests, see Greenhouse-Geisser (1959), Huynh and Feldt (1976), Huynh and Feldt (1970), Keselman and Keselman (1993), Mendoza (1980), and Looney and Stanley (1989).

As a response to the unsatisfactory results created by violating the homogeneity of covariance assumption required by the standard F -tests, the multivariate Welch-James (WJ) test, which does not require the sphericity assumption or the homogeneity of covariance assumption, has been proposed for use in split-plot designs (Algina & Keselman, 1997, 1998; Keselman, Algina, Wilcox, & Kowalchuk, 2000; Keselman, Carriere, & Lix, 1993). The WJ test tends to control the Type I error rates for the within-subjects main effect and the between- by within-subjects interaction whether or not the dispersion matrices are heterogeneous. However, the WJ test also utilizes listwise deletion when there are missing values and would be expected to yield valid inferences only when the missing data are MCAR.

The Kenward-Roger (KR) adjusted degrees of freedom F -test is similar to the WJ test, but uses all available data in parameter estimation when there are missing values. Because parameter estimation is carried out by ML, the estimated parameters are consistent when data are MCAR or MAR. Additionally, the KR test is computed through a mixed-effects linear model so multisample sphericity is not required and heterogeneity of covariance can be modeled. Furthermore, the KR test uses a more accurate estimator of the sampling covariance matrix than the standard mixed model F -test.

When the mixed-effects linear model is used to analyze data, likelihood ratio, score, or Wald hypothesis tests can be used. Wald tests seem to be the most common. For example, when PROC MIXED in SAS is used, the default procedure for tests on the fixed effects is the Wald test. Let $\mathbf{L}$ be a $r \times JK$ contrast matrix of full row rank and let $\boldsymbol{\mu} = [\boldsymbol{\mu}'_1 \quad \boldsymbol{\mu}'_2 \quad \cdots \quad \boldsymbol{\mu}'_J]'$. Each $\boldsymbol{\mu}_j$ is a $K \times 1$ vector of population means for the K levels of the within-subjects factor in the split-plot design. The main effect and interaction hypotheses about the between- and within-subjects factors can be expressed as

$$H_0: \mathbf{L}\boldsymbol{\mu} = \mathbf{0} \quad (1)$$

where $\mathbf{0}$ is a $r \times 1$ vector with all elements equal to zero. Let $\boldsymbol{\Sigma}_j$ denote the $K \times K$ population covariance matrix of the repeated measures for

the j^{th} level of the between-subjects factor, $\mathbf{S}_j$ the $K \times K$ restricted ML (REML) estimate of the covariance matrix and $\boldsymbol{\Sigma}_{ij}$ and $\mathbf{S}_{ij}$ the $K_i \times K_i$ sections ($i = 1, 2, \dots, n_j$) of the population and sample covariance matrices, respectively that pertain to the dependent variables on which the i^{th} participant in the j^{th} group has observed scores. In addition let $\mathbf{A}_i$ denote a $K_i \times K$ indicator matrix obtained by eliminating the k^{th} ($k = 1, 2, \dots, K$) row from the $K \times K$ identity matrix if the data for the i^{th} participant is missing on the k^{th} level of the within-subjects factor. The PROC MIXED default test statistic for testing the null hypothesis is

$$F = \frac{\bar{\mathbf{y}}' \mathbf{L}' (\mathbf{L} \hat{\mathbf{M}}^{-1} \mathbf{L}')^{-1} \mathbf{L} \bar{\mathbf{y}}}{r} \quad (2)$$

where $\bar{\mathbf{y}} = [\bar{\mathbf{y}}'_1 \quad \bar{\mathbf{y}}'_2 \quad \cdots \quad \bar{\mathbf{y}}'_J]'$ is the ML estimate of $\boldsymbol{\mu}$, $r = \text{rank}(\mathbf{L})$, and $\hat{\mathbf{M}}$ is a block diagonal matrix in which the j^{th} block is $\sum_i \mathbf{A}'_i \mathbf{S}_{ij}^{-1} \mathbf{A}_i$. The vector

$$\bar{\mathbf{y}}_j = \left(\sum_i \mathbf{A}'_i \mathbf{S}_{ij}^{-1} \mathbf{A}_i \right)^{-1} \left(\sum_i \mathbf{A}'_i \mathbf{S}_{ij}^{-1} \mathbf{y}_i \right).$$

The matrix $\hat{\mathbf{M}}^{-1}$ is the estimated sampling covariance matrix of the mean vector $\bar{\mathbf{y}}$ and is based on the expected information matrix calculated under the naïve sampling framework. Even when data are MCAR or there are no missing data, using $\hat{\mathbf{M}}^{-1}$ has two drawbacks:

1. $\hat{\mathbf{M}}^{-1}$ tends to be too small because it fails to take into account the uncertainty in $\bar{\mathbf{y}}$ introduced by substituting $\mathbf{S}_{ij}$ for $\boldsymbol{\Sigma}_{ij}$ when $\bar{\mathbf{y}}$ is obtained (Kackar & Harville, 1984).

2. $\hat{\mathbf{M}}^{-1}$ is a biased estimate of $\mathbf{M}^{-1}$ (Prasad & Rao, 1990; Booth & Hobert 1998). Harville and Jeske (1992) developed a better estimator of $\mathbf{M}^{-1}$, denoted by $\hat{\mathbf{m}}^@$. Kenward and Roger (1997) then developed an alternative estimator of $\mathbf{M}^{-1}$, denoted by $\hat{\boldsymbol{\Phi}}_A$.

Kenward and Roger (1997) also developed the test statistic

$$F^* \sim \lambda \frac{\bar{\mathbf{y}}' \mathbf{L}' (\mathbf{L} \hat{\Phi}_A \mathbf{L}')^{-1} \mathbf{L} \bar{\mathbf{y}}}{r} \quad (3)$$

where λ is a scaling factor and $F_{r,d}$ is the critical value where d is the approximate degrees of freedom. Both λ and d are estimated from the data. The Kenward-Roger procedure is implemented in SAS's PROC MIXED, but uses $\hat{\mathbf{m}}^@$ in place of $\hat{\Phi}_A$.

Keselman et al. (1993) and Algina and Keselman (1997) investigated the performance of the WJ test at controlling the Type I error rate in a split-plot design under several simulation conditions. In the former study the authors investigated (a) the number of levels of the within-subjects factor ($K = 4, 8$), (b) the ratio of total sample size N to $K - 1$ (i.e., $N/(K - 1)$), (c) the ratio of the smallest n_j to $K - 1$ (i.e., $n_{\min}/(K - 1)$), (d) sample size inequality, (e) pairing of n_j with covariance matrices, and (f) the shape of the distribution of the data. In all conditions the number of levels of the between-subjects factor was three ($J = 3$) and heterogeneity of covariance matrices was held constant at a ratio of 1:3:5.

The latter study added $J = 6$, degree of departure from sphericity measured by epsilon (ϵ), and heterogeneity of covariance matrices with a ratio of 1:5:9. The authors were interested in the sample sizes required to control the Type I error rate when testing the within-subjects main effect and the between- by within-subjects interaction. In the first study, the sample sizes ranged from 30 to 171 and in the second study they ranged from 20 to 714. From these two studies the authors provided sample size guidelines for the WJ test to control the Type I error under normal and non-normal data. The final sample size recommendations are summarized in Table 1.

Fai and Cornelius (1996) developed and compared four alternative test statistics (F_1 to F_4) that can be used to test linear hypotheses on means in multivariate studies. They showed how to use the data to estimate the

denominator degrees of freedom for the four statistics and the scaling factors λ_2 and λ_4 for the F_2 and F_4 statistics. The F_1 and F_2 statistics use $\hat{\mathbf{M}}^{-1}$ to estimate the covariance matrix of the mean vector whereas F_3 and F_4 use $\hat{\mathbf{m}}^@$. The F_4 statistic is similar to the statistic obtained by (3) using the KR option in PROC MIXED, but with a different formula for the scaling factor and the degrees of freedom. The F_1 test is available in SAS when the Satterthwaite option is used in PROC MIXED. For further details on F_1 through F_2 see Fai and Cornelius.

Fai and Cornelius (1996) applied their tests to split-plot designs with a three-level between-subjects factor (J) and a four-level within-subjects factor (K). The covariance structure was compound symmetric. The design was unbalanced in that the number of subjects varied across levels of the between-subjects factor and data were not generated for some combinations of subjects and the within-subjects factor. Because the missing data were never generated, the missing data mechanism was effectively MCAR. Estimated Type I error rates and power were reported for the main effect of the between-subjects factor. All four tests provided reasonable control of the Type I error rate. The performance of F_1 and F_3 , which do not include a scaling factor were very similar. Type I error rates and power for F_4 was always larger than for F_3 .

Schaalje, McBride, and Fellingham (2002), reporting on a study conducted by McBride (2002), reported Type I error rates for F_1 and the test obtained using the KR option in PROC MIXED. McBride investigated the performance of these tests in a split-plot design. The following provides a social science example of the design investigated by McBride. Suppose three methods for structuring interactions among students in a mathematics classroom are to be compared; n schools are randomly assigned to each method, where n was three in half of the conditions studied by McBride and five in the other half. The methods will be implemented for three, six, or nine weeks. Each school contributes K classes. Each class is assigned a single interaction quality score. In half of the conditions studied by McBride, $K = 3$ and the

Table 1. Final $n_{\min}/(K - 1)$ Recommendations for Distribution by Between-Subjects Factor (J) by Test by Within-Subjects Factor (K)

Distribution	J	Test	$n_{\min}/(K - 1)$	
			$K = 4$	$K = 8$
Normal	3	K	2.00	3.00
		$J \times K$	3.00	4.00
	6	K	1.33	1.43
		$J \times K$	4.75	5.00
Non-normal	3	K	3.00	4.00
		$J \times K$	8.00	6.00
	6	K	1.33	1.71
		$J \times K$	14.00	10.14

Note. Based on Keselman et al. (1993) and Algina and Keselman (1997)

design was balanced. In the other half, $K = 5$ so that within each school two classes would be assigned to two of the implementation periods and one class would be assigned to the remaining implementation period. In these conditions the design was unbalanced, but no data were missing.

McBride also investigated the effect of the covariance structure, which included the following five structures: compound symmetric (equal correlations and equal variance for the repeated measures), heterogeneous compound symmetric (equal correlations, but unequal variances for the repeated measures), Toeplitz, heterogeneous first-order autoregressive (correlations conform to a first-order autoregressive pattern, but the variances for the repeated measures are unequal), and first-order ante-dependence (see Wolfinger, 1996, for examples of these covariance structures). The results indicated that employing the KR option provided better control than did employing the

Satterthwaite option in PROC MIXED. Type I error rates were closer to the nominal level for balanced designs than for unbalanced designs. For unbalanced designs, Type I error rates improved as n increased.

Kenward and Roger (1997) investigated how well the original KR procedure controlled Type I error rates in four situations: (a) a four-treatment, two-period cross-over design, (b) a row-column- α design, (c) a random coefficients regression model for repeated measures data, and (d) a split-plot design. In (c) and (d) there were missing data. In (c) the missing data mechanism was MCAR. The missing data mechanism in (d) was not specified. In all situations, the KR test controlled the Type I error rate well.

Kowalchuk, Keselman, Algina, and Wolfinger (2004) compared the performance of the KR and the WJ procedures at controlling the Type I error rate under several simulation conditions for a $(J = 3) \times (K = 4)$ split-plot design. The simulation conditions they

investigated were (a) type of population covariance structure, (b) degree of group size inequality, (c) positive and negative pairings of covariance matrices and group sample sizes, (d) shape of the data, and (e) type of covariance structure fit to the data. All simulation conditions had heterogeneous covariance matrices across the levels of the between-subjects factor (J) with a ratio of 1:3:5. Data with missing values were not investigated. The KR test coupled with modeling the true covariance structure of the data performed better than did the WJ test under all conditions with small sample sizes. Also, the authors showed that always assuming an unstructured covariance structure performed comparably to modeling the true covariance structure when using the KR test.

Based on the previous results, the KR test and similar tests like the F_4 test (Fai & Cornelius, 1996) can control the Type I error rate for a variety of repeated measures designs when there are either missing data but no covariance heterogeneity or covariance heterogeneity but no missing data. The purpose of this study is to investigate control of the Type I error rate by the KR test as it is implemented in PROC MIXED when there are both missing data and covariance heterogeneity. Because of the similarities between the KR test and the WJ test and because Type I error rates for the WJ test have been extensively evaluated by Algina and Keselman and their colleagues, the KR test will be evaluated under conditions similar to those used by these authors to evaluate the WJ test, with the addition of missing value conditions.

Methodology

Study Variables

Eight variables were manipulated in this simulation. The variables of interest are (a) the number of levels of the between-subjects factor (A), (b) the number of levels of the within-subjects factor (B), (c) $n_{\min}/(K - 1)$ where K is the number of levels of the within-subjects factor, (d) sample size inequality across the between-subjects factor (SSI), (e) degree of sphericity as quantified with Box's (1954) epsilon (ϵ), (f) nature of pairing of group sizes with covariance matrices (NPSC), (g) type of

missing data mechanism (TMDM), and (h) percent of missing data (PM). For each combination of levels of the factors, five thousand replications were generated.

Both the number of levels of the between-subjects and within-subjects factors were investigated in the study. Each of these factors had two levels with $J = 3, 6$ and $K = 3, 6$. In the initial planning, the study was going to investigate $J = 3, 6$ and $K = 4, 8$, but preliminary simulations indicated that using PROC MIXED took an inordinate amount of time when $K = 8$.

The sample sizes investigated were $n_{\min}/(K - 1) = 4, 6$ for $J = 3$ and $n_{\min}/(K - 1) = 5, 7.7$ for $J = 6$. Within each pair of $n_{\min}/(K - 1)$ ratios, the smaller ratio corresponds to sample size recommendations in Table 1 for the between- by within-subjects interaction with normal data, $K = 8$, and $J = 3, 6$. The larger $n_{\min}/(K - 1)$ values were based on the recommendations from Table 1 and the higher demands missing values will place on the data analysis.

Keselman et al. (1998) found that unequal sample sizes in split-plot designs were common, occurring in a little over 50% of the split-plot designs. For this reason unequal sample sizes were investigated. In particular, moderate and severe group size inequalities were investigated as defined by Keselman et al. (1993) through the coefficient of variation:

$$C = (\bar{n}\sqrt{J})^{-1} \sqrt{\sum_{j=1}^J (n_j - \bar{n})^2}, \quad (4)$$

where $C \approx .16, .33$ describe moderate and severe group size inequality, respectively.

Departures from sphericity quantified by Box's (1954) epsilon (ϵ), were also investigated with $\epsilon = .60, .75, .90$, where $\epsilon = .60$ and $\epsilon = .75$ represent relatively severe and moderate violations of sphericity, respectively. In past studies $\epsilon = .40, .57, .75$ were investigated (Algina & Keselman, 1997; Keselman, Keselman, & Shaffer, 1991; Algina & Oshima, 1994). However, ϵ has a lower bound of $\epsilon = 1/(K - 1)$, so for $K = 3$ the lower bound is $\epsilon = .50$ and so $\epsilon = .40$ cannot be investigated. Also, according to Huynh and Feldt (1976) $\epsilon =$

.75 represents the lower limit of ε found in educational and psychological data. The epsilon values in this simulation study were chosen based on this contention. In particular, note that $\varepsilon = .75$ is the mid value and the other values are $\varepsilon \pm .15$. The actual covariance matrices are shown in Table 2.

ratio of sample size to heterogeneity of covariance matrices was set at 1:3:5 for $J = 3$ and 1:3:5:1:3:5 for $J = 6$ (Algina & Keselman, 1997; Keselman et al., 1993; Keselman, Algina, Kowalchuk, & Wolfinger, 1999). Furthermore,

Table 2. Pooled Covariance Matrices

	$K = 3$	$K = 6$
$\varepsilon = .90$	$\begin{bmatrix} 18.0 & 5.0 & 6.0 \\ & 8.0 & 5.0 \\ & & 7.0 \end{bmatrix}$	$\begin{bmatrix} 18.0 & 5.0 & 7.0 & 7.0 & 6.0 & 5.0 \\ & 12.0 & 8.0 & 7.0 & 6.0 & 5.0 \\ & & 10.0 & 6.0 & 6.0 & 5.0 \\ & & & 10.0 & 5.0 & 5.0 \\ & & & & 9.0 & 5.0 \\ & & & & & 8.0 \end{bmatrix}$
$\varepsilon = .75$	$\begin{bmatrix} 23.2 & 4.5 & 7.4 \\ & 10.3 & 5.3 \\ & & 4.3 \end{bmatrix}$	$\begin{bmatrix} 29.6 & 12.7 & 7.5 & 7.0 & 5.9 & 5.9 \\ & 15.1 & 7.9 & 6.0 & 6.4 & 4.9 \\ & & 13.2 & 6.9 & 6.0 & 5.4 \\ & & & 9.4 & 6.0 & 4.8 \\ & & & & 8.0 & 5.0 \\ & & & & & 5.9 \end{bmatrix}$
$\varepsilon = .60$	$\begin{bmatrix} 23.8 & 1.9 & 9.3 \\ & 9.5 & 5.7 \\ & & 3.9 \end{bmatrix}$	$\begin{bmatrix} 28.8 & 4.8 & 10.1 & 9.8 & 8.3 & 7.3 \\ & 17.4 & 8.1 & 7.4 & 6.9 & 4.1 \\ & & 9.9 & 7.7 & 6.5 & 5.7 \\ & & & 8.3 & 5.6 & 4.3 \\ & & & & 5.6 & 4.4 \\ & & & & & 4.3 \end{bmatrix}$

The pairing direction, positive or negative, between the unequal group sizes and the heterogeneous covariance matrices were also investigated. A pairing is positive when the largest n_j is paired with the covariance matrix with the largest elements and negative when the largest n_j is paired with the covariance matrix with the smallest elements. In order to have comparability with previous research results, the

previous studies have shown that this ratio and pairing can have a strong impact on the Type I error rate for approximate univariate *F*-tests, such as the Huynh-Feldt *F*-test (1976), and multivariate tests, particularly when the sample size is small (Keselman & Keselman, 1990). Specifically, positive pairings produce conservative Type I errors and negative pairing produce liberal Type I errors.

The MCAR and MAR missing data mechanisms were investigated in connection with 5%, and 15% probability of missing data at each level of the within-subjects factor except the first level; there were no missing data in the first level (see the Data Generation section for an explanation). Only the MCAR and MAR missing data mechanisms were investigated because Padilla and Algina (2004) demonstrated that the NMAR missing data mechanism negatively impacts the Type I error rate of the KR test statistic in a repeated measured design with no between-subjects factors.

Data Generation

The data were generated by using the model

$$y_{ijk} = \mu + e_{ijk} \quad (5)$$

The mean vector $\boldsymbol{\mu}_j = [\mu_1 \ \mu_2 \ \dots \ \mu_K]'$ was the same for all J groups and the elements μ_k were equal because the focus of the study was on control of the Type I error rate by the KR test. The common elements were arbitrarily set to zero. The $\mathbf{e}$ vector was a $K \times 1$ random vector such that $\mathbf{e} \sim NID(\mathbf{0}, \boldsymbol{\Sigma}_j)$.

All data simulations and analyses were conducted using SAS version 9.0. For each combination of levels of the simulation factors, the following steps were used to simulate the data in the j^{th} level of the between-subjects factor.

1. Simulate $\mathbf{Z}$, a $n_j \times K$ matrix of pseudorandom standard normal variables where n_j is the sample size for the j^{th} level of the between-subjects split-plot design.

2. Calculate $\mathbf{T}$ a $K \times K$ upper triangular Cholesky factor of the covariance matrix $\boldsymbol{\Sigma}$.

3. Calculate $\mathbf{y} = d_j \mathbf{Z} \mathbf{T}$, where d_j is a constant selected to create the required degree of covariance heterogeneity.

4. In all conditions there were no missing values on y_{il} :

- a. For MCAR, eliminate y_{ik} ($k = 2, \dots, K$) if $U_{ik} < \pi$ where π is the expected

proportion of the missing data on y_k and U_{ik} is a uniform random variable.

- b. For MAR, eliminate y_{ik} if $U_{ik} < \Phi(my_{i1} + c)$, where Φ is the cumulative standard normal distribution function and the parameters m and c will be described below.

In selecting data points for elimination, the parameter m controls how dependent the missing data are on y_1 in the MAR condition and was set to one. Let

$$r_{ik} = \begin{cases} 1 & \text{if } y_{ik} \text{ is missing} \\ 0 & \text{otherwise} \end{cases}.$$

With $m = 1$, the biserial correlation between r_{ik} and y_1 was .5 in the MAR condition. Hence, the missing data indicators depend fairly heavily on y_1 . With $m = 1$, the expected proportion of missing data on y_k is dependent on c . In the procedure described in the preceding paragraphs, the probability that $r_{ik} = 1$ is related to y_1 is modeled by a normal ogive (probit) model. Using well-known facts about the normal ogive model (see, for example, Lord & Novick, 1968, equations 16.9.3 and 16.94), it can be shown that

$$c = \{\Phi^{-1}(\pi)\} \sqrt{1+m^2}. \quad (6)$$

Thus, for $m = 1$, and for 5% and 15% missing data conditions, the expression becomes $c = -1.645\sqrt{2}$, and $c = -1.036\sqrt{2}$, respectively.

Data Analysis

The SAS PROC MIXED program used in this simulation is

```
proc mixed;
class Person A B;
model score = A B A*B/ ddfm=kenwardroger;
repeated B/ subject=Person group=A type=un;
run;
```

The following list describes various aspects of the code.

- **Person** is a variable that identifies simulated subjects.

- **Score** is the variable containing scores on the dependent variable.
- **A** is a variable that identifies the levels of the between-subjects factor.
- **B** is a variable that identifies the levels of the within-subjects factor.
- **ddfm = kenwardroger** instructs SAS to use the KR statistic to test the main effects and the interaction.
- **Repeated** is a key word that tells SAS that B is a repeated measures (within-subjects) factor and is necessary when there are missing data.
- **Group = A** tells SAS to model the covariance matrix for each level of A. That is, it specifies modeling heterogeneity of covariance matrices across the levels of A.
- **Subject = Person** tells SAS that the score values are correlated within each person.
- **Type = un** instructs SAS to estimate an unstructured covariance matrix with K estimated variances and $K(K - 1)/2$ estimated covariances.

Although there are several covariance structures that can be used to model the covariance matrix (Wolfinger, 1996), only the unstructured between-subjects heterogeneous structure (UN-H) covariance matrix was used in this simulation. Although using a UN-H covariance structure comes at the cost of estimating $K(K + 1)/2$ parameters, Kowalchuk et al. (2004) showed that under similar simulation conditions assuming an unstructured covariance structure performed comparably to modeling the true covariance structure when using the KR test.

The corresponding p -values of applying the KR test to 5,000 replications were available for each combination of the investigated conditions. The result of each test was summarized by a dichotomous variable, defined in the following manner:

$$Type\ I\ Error = \begin{cases} 0 & \text{if the } p - \text{value} < .05 \\ 1 & \text{otherwise} \end{cases}$$

For each of the between-subjects, within-subjects, and between- by within-subjects KR tests the Type I error variable was analyzed

by using logistic regression with the study variables as factors. A forward selection approach was used to select appropriate models. The models used were an intercept-only model, a model with main effects only, a model with main effects and two-way interactions, and so forth. A model was considered adequate for the data if the χ^2 goodness of fit test was non-significant or if Bentler's (1990) Comparative Fit Index (CFI) $\geq .95$. An index of fit was used because, due to the large number of replications, the χ^2 goodness of fit statistic for the logistic model could be very sensitive to small effects of the factors. The CFI in this context was calculated as follows:

$$CFI = 1 - (\lambda / \lambda_i) \quad (7)$$

where $\lambda = \max(\chi^2 - df, 0)$, χ^2 and df are the chi-squared goodness of fit statistic for the fitted model and the corresponding degrees of freedom, $\lambda_i = \max(\chi_i^2 - df_i, \chi^2 - df, 0)$, and χ_i^2 and df_i is the chi-squared goodness of fit statistic for the intercept-only model and its corresponding degrees of freedom.

Assessment of the Type I error rates were based on Bradley's (1978) liberal criterion for identifying conditions in which hypothesis testing procedures work adequately. His liberal criterion is $.5\alpha \leq \tau \leq 1.5\alpha$ where α is the nominal Type I error and τ is the actual Type I error. Using $\alpha = .05$, the liberal criterion is $.025 \leq \tau \leq .075$.

Results

Analysis of Type I Error Rates for the Between-Subjects Main Effect

The distribution of Type I error rates for the between-subjects main effect is shown in Figure 1 and has $M = .050$ and $SD = .003$. The range of the Type I error rate is $[.041, .057]$. The goodness of fit test for the intercept-only model was not significant, $\chi^2(383) = 398.64$, $p = .28$, suggesting that the effects of the factors were quite small. Because the Type I errors rates for the between-subjects main effect were predominately within Bradley's liberal criterion and because the intercept only model could not be rejected, it appears that the KR between-subjects omnibus test controls the Type

I error well at all levels of the investigated factors in this study.

The distribution of Type I error rates for the within-subjects main effect is shown in Figure 2 and has $M = .052$ and $SD = .005$. The range of the Type I error rate is $[.041, .070]$. Hence, in all conditions the Type I error rate was well within Bradley's (1978) liberal criterion interval. CFI for the model with main effects and two-way interactions was .98. In addition the goodness of fit test was non-significant, $\chi^2(339) = 354.24, p = .27$. Thus, the two-way interaction model was selected for further analysis. Wald tests indicated that all factors that had significant main effects also entered into significant two-way interactions. As might be expected from Figure 2, all effects were small. Mean Type I Error rates were between .048 and .061 in all two-way tables and no simple effect was as large as .01. Type I error rates tended to be larger when J , K , and percent missing data were larger. Type I error rates also tended to be larger for MAR data¹.

Analysis of Type I Error Rates for the Within-Subjects Main Effect

Because a major focus of this study is the effect of sample size on Type I error rates, two-way tables of means for the only interactions with sample size are presented in Table 3. These results indicate that control of the Type I error rate was good regardless of the sample size and that the effect of sample size on the Type I error rate was quite small.

Analysis of Type I Error Rates for the Between-Subjects Interaction

The distribution of Type I error rates for the interaction effect is presented in Figure 3 and has $M = .054$ and $SD = .007$. The range of the Type I error rate is $[.040, .075]$. Consequently, in all conditions the Type I error rate was once again within Bradley's liberal criterion interval. CFI for the model with main effects and two-way interactions was 1.00. In addition, the goodness of fit test was non-significant, $\chi^2(339) = 368.79, p = .23$. Wald tests indicated that all factors that had significant main effects also entered into significant two-way interactions. As might be expected from Figure 3, all effects of factor were small. Mean Type I Error rates were between .049 and .058 in all two-way tables and no simple effect was as large as .01. Type I error rates tended to be larger when K , sample size inequality, and percent missing were larger. Type I error rates also tended to be larger when the sample size-covariance pairing was negative. The effect of J was miniscule. The effect of type of missing data tended to be small and to vary in direction over levels of the factors with which it interacted.

Because a major focus of this study is the effect of sample size on Type I error rates, two-way tables of means for the interactions only with sample size are presented in Table 4. These results indicate that control of the Type I error rate was good regardless of the sample size and that the effect of sample size on the Type I error rate was quite small.

Figure 1. Distribution of Type I Error Rates: Between-Subjects KR F -Test Figure 2. Distribution of Type I Error Rates: Within-Subjects KR F -TestTable 3. Effect of $n_{\min}/(K - 1)$ on Type I Error Rates for the Within-Subjects Main Effect

Factor	Factor levels	$n_{\min}/(K - 1)$	
		Small	Large
K	3	.0503	.0514
	6	.0541	.0539
PM	5%	.0494	.0509
	15%	.0550	.0545

Note. Each proportion is out of 480,000 hypothesis tests.

Figure 3. Distribution of Type I Error Rates: Interaction KR F -TestTable 4. Effect of $n_{\min}/(K - 1)$ on Type I Error Rates for the Between- by Within-Subjects Interaction

Factor	Factor levels	$n_{\min}/(K - 1)$	
		Small	Large
K	3	.0509	.0507
	6	.0577	.0553
SSI	.16	.0527	.0524
	.33	.0559	.0537
NPSC	Positive	.0509	.0517
	Negative	.0577	.0543
TMDM	MCAR	.0552	.0519
	MAR	.0534	.0542
PM	5%	.0508	.0504
	15%	.0578	.0557

Note. Each proportion is out of 480,000 hypothesis tests.

Conclusion

The results of this study support the conclusion that sampling distribution based inferences on the means using ML estimates can control the Type I error rate under MCAR missing data mechanisms. Additionally, sampling distribution based inferences using ML estimates can control the Type I error rate when the missing data mechanism is MAR (Little & Rubin, 2002; Rubin, 1976). Most important this control can be obtained with relatively modest sample size requirements.

With respect to the between-subjects main effect, the KR test statistic controlled the Type I error rate well across all levels of the simulation factors. Most Type I error rates were within both Bradley's conservative criterion and all were well within the liberal criterion. None of the simulation factors affected the Type I error rate of the between-subjects main effect. In regard to the within-subjects main effect and the within- by between-subjects interaction, although a number of factors affected Type I error rates, all effects were very small and all Type I error rates were within Bradley's liberal criterion.

The effects of the factors on Type I error rates were generally quite small. Nevertheless it is clear that the effects of the factors on the Type I error rates must be due to their effects on the accuracy of the *F*-distribution as an approximation to the sampling distribution of the test statistic. The KR test statistic was selected because it uses a better estimator of the covariance matrix for small sample sizes and Satterthwaite (1946) type degrees of freedom based on the better estimate of the covariance matrix. However, when the data are incomplete in addition to being relatively small and paired with a MAR missing data mechanism, the accuracy of the approximation may be worse than when the data are complete.

Although the design investigated in this study was a popular split-plot design with one between- and one within-subjects factor, the positive findings open the door for further simulation work on using ML to directly estimate model parameters from split-plot designs with missing values. One condition that can be investigated is a non-normal distribution

of the dependent variable. In the present study, the data were generated under a multivariate normal distribution and since data from educational or psychological research cannot be presumed to be normal, investigation of a non-normal data condition can provide applied researchers with valuable information as to whether the KR test is robust to the normality assumption. In other words, can the KR test control the Type I error when the normality assumption is violated?

Even though all of the Type I error rates of the KR test were within Bradley's (1978) liberal criterion, it is not clear at what percent of missing data the KR test will begin to breakdown. Additionally, it is not clear how small the sample sizes can be and still have the KR test provide reasonable control of the Type I error. Consequently, future work could focus on what are the percent of missing data and sample size requirements needed for the KR test to provide reasonable control of the Type I error.

An alternative to the estimator of the sampling covariance matrix used in the KR test is the sandwich estimator (White, 1980, Liang & Zeger, 1986). The sandwich estimator provides a consistent estimator of the covariance matrix given that the model for the means is correct. That is the model for the covariance structure need not be correct. Hence, it may be fruitful to compare the performance of the *F*-test using the sandwich estimator to the KR test at controlling the Type I error in a simulation study with ignorable missing data.

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Reliability and Statistical Power: How Measurement Fallibility Affects Power and Required Sample Sizes for Several Parametric and Nonparametric Statistics

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The relationship between reliability and statistical power is considered, and tables that account for reduced reliability are presented. A series of Monte Carlo experiments were conducted to determine the effect of changes in reliability on parametric and nonparametric statistical methods, including the paired samples dependent t test, pooled-variance independent t test, one-way analysis of variance with three levels, Wilcoxon signed-rank test for paired samples, and Mann-Whitney-Wilcoxon test for independent groups. Power tables were created that illustrate the reduction in statistical power from decreased reliability for given sample sizes. Sample size tables were created to provide the approximate sample sizes required to achieve given levels of statistical power based for several levels of reliability.

Key words: Pseudorandom generation, effect size, Monte Carlo simulations.

Introduction

Students of statistics usually become familiar with the factors that affect statistical power. For example, most students learn that sample size, level of significance, and estimated effect size all determine the a priori power of a statistical analysis. Some know that how effectively a particular design reduces error variance affects power, as does the directionality of the alternative hypothesis. However, many students do not realize that the reliability of measurements may also affect the statistical power (Hopkins & Hopkins, 1979). Light, Singer, and Willett (1990) provided tables to illustrate the point. Unfortunately, their tables provide only a very few situations and are therefore limited in their usefulness. It is not

clear how the Light et al. tables were developed. The present study extends their tables and provides such information for additional statistical methods.

Using the information provided in these tables, researchers can account for different levels of reliability as they determine sample sizes for their studies. Perhaps the converse approach is even more useful; however, that is, researchers might be encouraged to improve the reliability of their instruments in order to need fewer participants in their studies. These tables can also be useful tools in teaching students the relationship between reliability of a survey instrument and statistical power.

Background

One of the chief concerns of research design is to ensure that a study has adequate statistical power to detect meaningful differences, if indeed they exist. There is a very good reason researchers should worry about power a priori: If researchers are going to invest a great amount of money and time in carrying out a study, then they would certainly want to have a reasonable chance, perhaps 70% or 80%, to find a difference between groups if it does exist. Thus, a priori power (the probability of rejecting a null hypothesis that is false) will inform researchers how many subjects per group

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will be needed for adequate power. Several factors affect statistical power. That is, once the statistical method and the alternative hypothesis have been set, the power of a statistical test is directly dependent on the sample size, level of significance, and effect size (Stevens, 2002). Often overlooked, however, is the relationship that variance has with power. Specifically, variance influences power through the effect size. For example, Cohen (1988) defined the effect for the t statistic as

$$\delta = (\mu_1 - \mu_0) / \sigma_X \quad (1)$$

If variance can be reduced, effect size increases. Variance reduction techniques include using a more homogeneous population and improving the reliability of measurements (Aron & Aron, 1997; Zimmerman, Williams, & Zumbo, 1993). Similarly, because variance is reduced, analysis of covariance is more powerful than analysis of variance when a useful covariate is incorporated into the design.

Reliability and Effect Size

Cleary and Linn (1969) reported that “in the derivation and interpretation of statistical tests, the observations are generally considered to be free of error of measurement” (p. 50). From a classical test theory perspective, an individual’s observed score (X) is the sum of true score (T) and error score (E); that is, $X = T + E$. Thus, if there is no error of measurement, then the observations are the true scores; implicitly, statistical hypotheses are proposed in terms of true scores. For a set of scores, however, measurements made without error occur only when the instruments provide perfectly reliable scores. Observed score variance, σ_X^2 , is defined as the sum of true score variance, σ_T^2 , and measurement error variance. Because reliability, $\rho_{XX'}$, is defined as the ratio of true score variance to observed score variance,

$$\rho_{XX'} = \sigma_T^2 / \sigma_X^2 = 1 - \sigma_E^2 / \sigma_X^2, \quad (2)$$

reliability can only be perfect (i.e., 1) when there is no measurement error (Lord & Novick, 1968). Because σ_X can be written as

$$\sigma_T / \sqrt{\sigma_{XX'}}, \quad (3)$$

the standardized effect size for the t test can be written as

$$\delta = (\mu_1 - \mu_0)(\sqrt{\sigma_{XX'}}) / \sigma_T \quad (4)$$

(Levin & Subkoviak, 1977; Williams & Zimmerman, 1989). Consequently, reliability affects statistical power indirectly through effect sizes. Cohen (1988) reported that reduced reliability results in reduced effect sizes in observed data (ES), which therefore reduces power. That is, observed effect sizes,

$$ES = ESP * \sqrt{r_{XX'}}, \quad (5)$$

where ESP is the population effect size. Therefore, when reliability is perfect, observed ES equals ESP; but when reliability is less than perfect, ES is a value smaller than the true ESP. Some introductory statistics textbooks discuss this problem in reference to attenuation in correlation due to unreliability of measures (e.g., Glass & Hopkins, 1996).

Reliability and Power

Controversy surrounds the relationship between power and reliability (Williams & Zimmerman, 1989). Good statistical power can exist with poor reliability and a change in variance unrelated to reliability can change power. However, there are persuasive reasons to consider reliability as an important factor in determining statistical power. For example, statistical power is a function of level of significance, sample size, and effect size only under the assumption of no measurement error, but measures in the social sciences are typically not measured perfectly (Cleary & Linn, 1969; Levin & Subkoviak, 1977). Indeed, the implicit assumption that our measures are perfectly reliable is not justified in practice and therefore measurement error should be considered a priori for sample size (Crocker & Algina, 1986; Subkoviak & Levin, 1977; Sutcliffe, 1958).

There is no controversy that statistical power depends on observed variance. Zimmerman and Williams (1986) noted that when speaking of statistical power it is irrelevant whether the observed variance is all true score

variance or contains some amount of measurement error; that is, “the greater the observed variability of a dependent variable, whatever its source, the less is the power of a statistical test” (p. 123). However, because reliability is defined by observed variance in conjunction with either true or error variance, one cannot be certain which source of variance is changed when reliability improves. That is, if observed variance increases, one cannot be certain whether the increase is due to an increase in true score variance or a increase in error variance, or both. Or as Zimmerman et al. (1993) reported, power changes as reliability changes only if observed score variance changes simultaneously.

Knowing that improved reliability results in less measurement error, if it is assumed that true variance is a fixed value for the given population, it follows that a change in reliability will result in a change in observed score variance. Indeed, statistical power is a mathematical function of reliability only if either true score variance or error variance is a constant; otherwise power and reliability are simply related (Cohen, 1988; Williams & Zimmerman, 1989). But, improvement in reliability is usually interpreted as a reduction in the measurement error variance that occurs from a more precise measurement (Zimmerman & Williams, 1986). Therefore, a reduction in reliability that is accompanied by an increase in observed score variance will indeed reduce statistical power (Zimmerman et al., 1993). That is, if true score variance remains constant but lower reliability leads to increased error variance, then statistical power will be reduced because of the increased observed score variance (Humphreys, 1993).

Based on such an assumption, Light et al. (1990) advised that when measurements are less than perfectly reliable, improving the power of statistical tests involves a decision either to increase sample size or to increase reliability—the researcher must compare the costs associated with instrument improvement to the costs of adding study participants (see also Cleary & Linn, 1969; Feldt & Brennan, 1993). Researchers may encounter such a situation if an instrument does not perform as reliably in a given study as it has elsewhere, leading to

increased variance in the current project. Assuming that the increased variance is not due to more heterogeneity in the population and that the true score variance of the population hasn't changed, the observed score variance will change as a consequence of the change in reliability.

Unfortunately, there are few easy ways to account for reliability when determining sample sizes. The tables found in Cohen (1988) do not provide the option to vary reliability. Computer programs such as Sample Power and PASS 2000 also assume perfect reliability. This article will report on the impact of reliability on power as well as provide tables to assist researchers in finding sample sizes necessary with fallible measures.

Methodology

Two Monte Carlo programs, MC2G (Brooks, 2002) and MC3G (Brooks, 2002) written in Borland Delphi Professional version 6.0, were used to create normally distributed but unreliable data and perform analyses for several statistical methods, namely: (a) paired samples dependent *t* test, (b) pooled-variance independent *t* test, (c) one-way analysis of variance with three levels, (d) Spearman rank correlation, (e) Wilcoxon signed-rank test for paired samples, and (f) Mann-Whitney-Wilcoxon test for independent groups. The program output was used to create power and sample size tables for these tests.

Reliability was varied from .70 to 1.0 in increments of 0.05. For power tables, power rates varied from .70 to .90 by .10. Population effect sizes were varied from small to large using Cohen's (1988) conventional standards. Specifically, for *t* tests and their nonparametric alternatives, a small standardized effect size was set at $d = .20$, medium was $d = .50$, and a large effect was set to be $d = .80$; for correlations, a small effect was set at $r = .10$, medium was $r = .30$, and a large effect was set to be $r = .50$; for ANOVA, a small standardized difference effect was set at $f = .10$, medium was $f = .25$, and a large effect was set to be $f = .40$. For the power tables, the sample sizes were obtained under the assumption of perfect reliability. That is, the sample sizes were fixed at the values needed to

achieve power levels of .70, .80 and .90, respectively, when reliability was 1.0. The remaining values in the power tables were determined by systematically varying the reliability with that given sample size. For the sample sizes tables, power was fixed, reliability was varied, and sample sizes were tried repeatedly until the desired power was achieved.

Data Generation

The two Monte Carlo programs generate uniformly distributed pseudorandom numbers that are used as input to the procedure that converts them into normally distributed data. All data were generated to follow the standard normal distribution. For each sample, the appropriate statistical analysis was performed. The number of correct rejections of the null hypothesis was stored and reported by the program. These procedures were repeated as necessary for each sample condition created. The programs use the L'Ecuyer (1988) uniform random number generator. Specifically, the Fortran code of Press, Teukolsky, Vetterling, and Flannery (1992), was translated into Delphi Pascal. The L'Ecuyer generator was chosen because of its large period and because combined generators are recommended for use with the Box-Muller method for generating random normal deviates (Park & Miller, 1988).

The computer algorithm for the Box-Muller method used by the MC2G and MC3G programs was adapted for Delphi Pascal from the standard Pascal code provided by Press, Flannery, Teukolsky, and Vetterling (1989). The programs generate normally distributed data of varying reliability based on classical test theory. That is, reliability is not defined using a particular measure of reliability (e.g., splithalf or internal consistency); rather it is defined as the proportion of raw score variance explained by true score variance (Equation 2). Each raw score generated is taken to be a standardized total score.

In order to generate data with less-than-perfect reliability, scores were generated using the true-score standard deviations provided by the researchers; then for each score, the programs added a random error component. Consequently, as reliability decreased, the variation of the random error component

increased, resulting in increased raw score variance. For correlation analyses, the same reliability was used for both measures; for independent sample analyses, the same reliability was used each for each group.

Monte Carlo

The number of iterations for the study is based on the procedures provided by Robey and Barcikowski (1992). Significance levels for both tests on which Robey and Barcikowski's method is based were set at .05 with a power level of .90; the magnitude of departure was chosen to be $\alpha \pm .2$, which falls between their intermediate and stringent criteria for accuracy. The magnitude of departure is justified by the fact that at $\pm .2 \alpha$, the accuracy range for $\alpha = .05$ is $.04 \leq \alpha \leq .06$.

Based on the calculations for these parameters (this set of values was not tabled), 5422 iterations would be required to "confidently detect departures from robustness in Monte Carlo results" (Robey & Barcikowski, 1992, p. 283), but applies to power studies also (Brooks, Barcikowski, & Robey, 1999). However, to assure even greater stability in the results, a larger number of simulations was chosen for each type of analysis. Specifically, 10,000 samples were used for the power tables. The sample size algorithm used by the programs runs repeated analyses beginning with 100 samples per analysis, gradually increasing to 10,000 samples per analysis. Sometimes, however, the algorithm aborts before the 10,000 sample level is reached when the desired power level is approximated closely enough earlier in the process (at least 1000 samples were run in every case).

Results

Tables 1 through 5 show the relationship between statistical power and reliability for the dependent t test, independent t test, one-way ANOVA with three groups, Wilcoxon signed ranks, and Mann-Whitney-Wilcoxon tests, respectively. The tables clearly show that, as reliability is reduced while true score variance remains constant, statistical power is reduced. There is a relatively linear relationship between statistical power and reliability when sample

size is fixed. For example, Table 1 shows that when statistical power is chosen to be .71 for the dependent t test, 12 cases are required when perfect reliability is assumed and a large effect size ($d = .8$) is expected. When reliability was changed to .90 with 12 cases, the actual

statistical power was observed to be .63. Reliability set at .80 resulted in observed statistical power of .54. Finally, actual power for 12 cases was .46 when reliability was set at .70. Such depreciation of power occurs for all other tests examined in the study.

Table 1. Actual statistical power for paired-samples dependent t tests resulting from different reliability values for given sample sizes at two-tailed $\alpha = .05$

Effect Size	N per group	Reliability						
		1.0	.95	.90	.85	.80	.75	.70
Large ($d = .8$)	12	.71	.67	.63	.59	.54	.50	.46
	15	.82	.78	.74	.70	.65	.61	.56
	19	.91	.88	.85	.81	.77	.73	.68
Medium ($d = .5$)	27	.71	.66	.62	.58	.53	.49	.45
	34	.81	.77	.73	.68	.64	.59	.55
	44	.90	.87	.83	.80	.75	.71	.66
Small ($d = .2$)	157	.70	.66	.62	.57	.53	.49	.45
	199	.80	.76	.72	.67	.63	.59	.54
	264	.90	.87	.83	.80	.75	.71	.66

Table 2. Actual statistical power for pooled-variance independent t tests resulting from different reliability values for given sample sizes at two-tailed $\alpha = .05$

Effect Size	N per group	Reliability						
		1.0	.95	.90	.85	.80	.75	.70
Large ($d = .8$)	21	.72	.70	.67	.65	.62	.59	.56
	26	.81	.79	.77	.74	.72	.69	.66
	34	.90	.89	.87	.85	.83	.81	.78
Medium ($d = .5$)	51	.70	.68	.66	.64	.61	.58	.55
	64	.80	.78	.76	.74	.71	.68	.65
	86	.90	.89	.87	.85	.83	.81	.78
Small ($d = .2$)	309	.70	.68	.65	.63	.60	.58	.54
	393	.80	.78	.76	.73	.71	.68	.65
	526	.90	.89	.87	.85	.83	.80	.77

Table 3. Actual statistical power for one-way analysis of variance with three groups resulting from different reliability values for given sample sizes at two-tailed $\alpha = .05$

Effect Size	N		Reliability					
	per group	1.0	.95	.90	.85	.80	.75	.70
Large ($f=.40$)	17	.70	.67	.65	.63	.60	.56	.53
	21	.80	.78	.75	.73	.71	.67	.64
	28	.91	.89	.87	.85	.83	.80	.77
Medium ($f=.25$)	41	.70	.67	.65	.62	.60	.57	.54
	51	.80	.78	.75	.73	.70	.67	.64
	66	.90	.88	.86	.84	.82	.79	.76
Small ($f=.10$)	269	.71	.68	.65	.62	.60	.57	.54
	333	.80	.78	.75	.73	.70	.67	.64
	441	.90	.89	.87	.85	.82	.80	.77

Table 4. Actual statistical power for Wilcoxon signed-rank tests resulting from different reliability values for given sample sizes at two-tailed $\alpha = .05$

Effect Size	N		Reliability					
	per group	1.0	.95	.90	.85	.80	.75	.70
Large ($d=.8$)	12	.70	.66	.62	.58	.54	.50	.45
	15	.80	.76	.71	.67	.63	.58	.54
	19	.90	.87	.83	.79	.75	.71	.66
Medium ($d=.5$)	28	.70	.65	.61	.57	.53	.48	.44
	35	.80	.76	.72	.68	.63	.58	.54
	46	.90	.87	.84	.80	.75	.71	.66
Small ($d=.2$)	164	.70	.66	.62	.57	.53	.49	.45
	208	.80	.76	.72	.68	.63	.59	.54
	276	.90	.87	.83	.80	.75	.71	.66

Table 5. Actual statistical power for Mann-Whitney-Wilcoxon tests resulting from different reliability values for given sample sizes at two-tailed $\alpha = .05$

Effect Size	N		Reliability					
	per group	1.0	.95	.90	.85	.80	.75	.70
Large ($d=.8$)	21	.69	.67	.64	.62	.59	.57	.53
	27	.80	.78	.76	.74	.71	.68	.65
	35	.90	.88	.86	.84	.82	.80	.77
Medium ($d=.5$)	53	.70	.68	.66	.63	.61	.60	.55
	67	.80	.78	.76	.73	.71	.68	.65
	90	.90	.89	.87	.85	.83	.81	.78
Small ($d=.2$)	323	.70	.67	.65	.62	.59	.57	.54
	411	.80	.78	.76	.73	.71	.68	.65
	550	.89	.88	.87	.85	.82	.80	.77

Tables 6 through 10 show the sample sizes required to maintain a given power level when reliability is less than perfect. Again, there are relatively linear relationships for all tests at all power levels. For example, Table 6 shows that when the desired statistical power level is set at .80 and a large effect size ($d = .8$) is expected,

the use of 15 cases results in power of .80 when reliability is 1.0; but when reliability is reduced to .90, 17 cases are required. If reliability is .80, then the study needs 21 participants. Finally, 25 cases must be used to achieve power of .80 when reliability is .70.

Table 6. Sample sizes required for paired-samples dependent t tests in order to achieve the given statistical power values under different reliability conditions at two-tailed $\alpha = .05$

Effect Size	Power	Reliability						
		1.0	.95	.90	.85	.80	.75	.70
Large ($d=.8$)	.70	12	13	14	15	17	18	20
	.80	15	16	17	19	21	23	25
	.90	19	20	22	24	27	29	33
Medium ($d=.5$)	.70	27	29	32	35	39	43	48
	.80	34	37	40	44	49	54	60
	.90	44	49	53	59	65	72	80
Small ($d=.2$)	.70	157	172	192	214	234	258	287
	.80	199	220	243	266	289	329	369
	.90	264	286	328	364	400	440	492

Table 7. Sample sizes required for pooled-variance independent t tests in order to achieve the given statistical power values under different reliability conditions at two-tailed $\alpha = .05$

Effect Size	Power	Reliability						
		1.0	.95	.90	.85	.80	.75	.70
Large ($d=.8$)	.70	21	22	23	24	25	27	29
	.80	26	27	28	30	32	34	37
	.90	34	36	38	40	42	45	48
Medium ($d=.5$)	.70	51	53	56	59	63	67	72
	.80	64	67	71	75	79	85	91
	.90	86	89	95	102	107	114	121
Small ($d=.2$)	.70	309	327	345	365	387	415	443
	.80	393	415	438	466	492	527	566
	.90	526	557	583	618	658	702	755

Table 8. Sample sizes required for one-way analysis of variance with three groups in order to achieve the given statistical power values under different reliability conditions at two-tailed $\alpha = .05$

Effect Size	Reliability							
	Power	1.0	.95	.90	.85	.80	.75	.70
Large ($f=.40$)	.70	17	18	19	20	21	22	24
	.80	21	22	23	25	26	28	30
	.90	28	29	30	32	34	36	39
Medium ($f=.25$)	.70	41	44	45	48	50	54	58
	.80	51	54	56	61	65	68	73
	.90	66	70	75	78	83	88	95
Small ($f=.10$)	.70	269	288	300	314	332	356	382
	.80	333	353	374	395	419	451	482
	.90	441	464	488	516	551	583	619

Table 9. Sample sizes required for Wilcoxon signed-ranks tests in order to achieve the given statistical power values under different reliability conditions at two-tailed $\alpha = .05$

Effect Size	Reliability							
	Power	1.0	.95	.90	.85	.80	.75	.70
Large ($d=.8$)	.70	12	13	14	16	17	19	20
	.80	15	17	18	20	21	24	26
	.90	19	21	23	25	28	31	34
Medium ($d=.5$)	.70	28	31	34	37	40	45	50
	.80	35	39	42	46	51	57	63
	.90	46	51	56	62	68	75	85
Small ($d=.2$)	.70	164	181	201	222	246	273	304
	.80	208	225	253	282	314	346	387
	.90	276	307	338	376	417	462	511

Table 10. Sample sizes required for Mann-Whitney-Wilcoxon tests in order to achieve the given statistical power values under different reliability conditions at two-tailed $\alpha = .05$

Effect Size	Reliability							
	Power	1.0	.95	.90	.85	.80	.75	.70
Large ($f=.40$)	.70	21	22	23	25	27	28	30
	.80	27	28	30	32	34	36	39
	.90	35	37	40	42	44	47	51
Medium ($f=.25$)	.70	53	56	58	62	67	69	75
	.80	67	70	74	79	84	89	96
	.90	90	93	97	105	113	117	127
Small ($f=.10$)	.70	323	339	358	386	405	437	463
	.80	411	430	458	484	517	551	593
	.90	550	575	611	653	692	733	796

Conclusion

In social sciences, few things are measured perfectly (Subkoviak & Levin, 1977). Researchers should therefore make an effort to minimize the effects of measurement error. Although some authors suggest that lower reliability is acceptable for group studies of attitudes or personality variables (e.g., Fink & Kosecoff, 1998; McMillan & Schumacher, 2001), it becomes obvious based on the tables provided here that improving reliability will increase power and therefore fewer members of these groups will be needed to participate in the study.

For example, in a two group study using a dependent measure that produces scores with a reliability of .70, 91 participants are required for a medium effect size at a power of .80; if reliability is improved to .85, the number of participants can be reduced to 75 (see Table 7). Perhaps for some studies, the additional effort required to improve the instrument is not justifiable; but for research with high per-subject costs, investment to improve the instrument may be very worthwhile. As well, the effect of measurement fallibility is even more dramatic for small effect sizes. In the same example as above, but for a small effect size, an improvement from reliability of .70 to .85 will result in a sample size reduction of around 100 (see Table 7).

Perhaps the most advantageous way for researchers to use the sample size information provided here is to make informed decisions about the trade-off between sample size and reliability. That is, researchers can make informed decisions about the costs and benefits of spending time and effort to improve an instrument. The issue really isn't how many more people do we need because our instrument is not perfectly reliable? Researchers would already have an estimate of variance based on that level of unreliability from pilot studies or previous research—after all, the effect size would be based on that observed variance—not true score variance. Rather, the implication intended from this work is more emphasis on the development of reliable and valid instruments. As instruments and reliability improve, because the true score variance of participants would

(presumably) remain the same, observed score variance will decrease and would provide additional power. There are several strategies that have been developed for minimizing the effects of measurement error and increasing reliability. These include revising items, increasing the number of items, lengthening item scales, administering the instrument systematically, timing of data collection and use of multiple raters or scores (Light et al., 1990).

Before choosing a final sample size, the possibility of measurement error should be considered. To determine sample sizes “without simultaneously considering errors of measurement is to live in a ‘fool’s paradise’” (Levin & Subkoviak, 1977, p. 337). If one suspects that measurement error exists and there is no viable means to reduce it, sample size should be increased accordingly. Researchers can identify potential problems with measurement error through pilot studies or previous research. Where reliability information is lacking, the researcher should use cautious estimates, with a preference toward more conservative values, when deciding sample sizes (Levin & Subkoviak, 1977).

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Comparison of the t vs. Wilcoxon Signed-Rank Test for Likert Scale Data and Small Samples

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The one sample t-test is compared with the Wilcoxon Signed-Rank test for identical data sets representing various Likert scales. An empirical approach is used with simulated data. Comparisons are based on observed error rates for 27,850 data sets. Recommendations are provided.

Key words: Nonparametric, Wilcoxon's signed-rank test, one sample t-test, Likert scales, Type I and Type II error rates.

Introduction

There has been disagreement since the 1940s concerning the use of the t-test versus its nonparametric equivalents when the assumptions of the t-test may not be valid, particularly those of normality. Similarly, controversies have raged at various times over the past 60 years about the use of classical or parametric procedures versus distribution-free or nonparametric procedures when the level of measurement is less than interval. The discussions in the literature began with Stevens (1946) and Siegel (1956) who stated that the level of measurement attained in the data should be a major factor in test selection. Siegel (1956) took a definite stance that nonparametric procedures should be utilized whenever the level is no more informative than ordinal.

In the behavioral sciences, particularly in psychology, Baggaley (1960) and Binder (1984) fueled the fire started by Stevens (1946). The extensive use of Likert scales in the behavioral sciences continues to make test selection a debatable issue. The debate is not restricted to the social sciences, because Likert scales also are widely used in opinion-based research in marketing, human resource management and other areas of business as well as in education and nursing. The liveliness of the discussions surrounding this issue in presentations at various conferences provided the motivation for this investigation.

Comparisons of distribution-free and parametric procedures initially were based upon theoretical considerations involving asymptotic relative efficiency (ARE), which is a large sample property. It pertains to the limit of the ratio of the sample sizes required to attain a specified power as the alternative, or true value, approaches the value under the null hypothesis and the sample size goes to infinity. Although the ARE is theoretically appealing, infinite sample sizes are difficult to obtain in practice.

According to Conover (1999) and Siegel (1956), the ARE of the one sample Wilcoxon signed-rank (WSR) test for location as compared with the one sample t-test for a normal population is 0.955. Conover (1999) stated that if the underlying population is uniformly distributed the ARE is 1.0 and for most non-normal populations exceeds 1.0, but is never less than 0.864.

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The ARE is an important theoretical consideration for comparing the theoretical power of two different statistical procedures. However, it is considered to be of limited value when working with small samples. Sawilowsky (1990) stated that at best, Monte Carlo studies have shown that ARE may be indicative of the promise of relative power of non-parametric procedures versus their parametric counterparts for small samples.

Conover (1999) pointed out that the t-test is more powerful than its rank-sum alternatives when populations are normally distributed. However, as most statisticians would agree, normality is a very difficult property to obtain. Sawilowsky and Blair (1992) demonstrated that when populations are not normally distributed, the Wilcoxon rank-sum procedure is more powerful than the t-test.

For the correlated layout, Siegel (1956, p. 83) stated that, for small sample sizes, the efficiency of the Wilcoxon signed-rank test to the t-test is near 95 percent. Most textbooks that include the Wilcoxon signed-rank procedure and discuss its assumptions versus the t-test recommend using the Wilcoxon signed-rank test in small sample situations whenever there is any question about normality or an interval level of measurement, but symmetry is reasonable and the differences are ordinal. Therefore, the purpose of this article is to compare the performance of these two procedures with Likert scale data in small sample situations where the assumptions of normality and interval measurement, are not satisfied.

Some Literature Review for Independent and Dependent Tests with Ordinal Scaled Data

There is limited evidence of practical comparisons of parametric versus nonparametric procedures based on the actual scale of measurement available in the data. The term practical is used because discussion in the literature, Stevens (1946), Siegel (1956), Baggaley (1960), Binder (1984) and Conover (1999), has historically been predicated on philosophical issues or asymptotic properties. Sawilowsky (1991) presented an excellent summary of the level of measurement issue and the weak measurement versus strong statistics controversy.

Some studies that have considered scale of measurement in comparing parametric vs. nonparametric tests are Blair and Higgins (1985), Nanna and Sawilowsky (1998), Nanna (2002), and two preliminary studies done by Meek, et al., (2000) and (2001).

Blair and Higgins (1985) used Monte Carlo methods with ten theoretical distributions to compare power of the paired samples t-test and the Wilcoxon signed ranks test for paired data, utilizing samples of 10, 25 and 50. They found the paired t-test to have a slight power advantage over the Wilcoxon procedure under normal and uniform distributions but little or no advantage under the other distributions for $n = 10$ and none at the larger sample sizes.

The first study by Meek, et al., (2000) used an identical approach to that utilized in this paper but compared the two independent samples t-test to the Mann-Whitney procedure under various combinations of Likert scales and sample sizes. Their findings indicated that, for small samples, there appeared to be little difference in precision between the t-test and the Mann-Whitney for data collected on a Likert scale. More germane to this article, the second article by Meek, et al., (2001) used a similar approach to compare the performances of the Wilcoxon signed-rank test and the t-test with Likert scales but was limited by having only slightly more than 2400 cases, and therefore, the results are not discussed further here.

Nanna and Sawilowsky (1998) compared the power of the independent samples t-test to that of the Wilcoxon rank-sum procedure with actual data sets measured on an ordinal scale. Their data were based on Functional Independence Measure (FIM) scores in medical rehabilitation. FIM scores used a 7-point Likert scale and often are highly skewed. Nanna and Sawilowsky (1998) found that the Wilcoxon rank-sum procedure had higher power than the t-test test for almost all combinations of sample size and alpha level examined. Nanna (2002) found that the rank transformation procedure provided an increase in power over Hotelling's T^2 when testing for equality of centroids using Likert scale data. Nanna (2002) used essentially the same FIM data sets as Nanna and Sawilowsky (1998).

Many of the current textbooks that include coverage of the Wilcoxon signed-rank procedure are quite limited in their discussions of its assumptions and make no specific recommendations for its use compared to the t-test other than to indicate it should be used if the assumptions of normality and interval measurement are questionable, particularly in small sample situations. Although robustness of the t-test is often cited as a reason for choosing t over the Wilcoxon signed rank and other nonparametric procedures, Bradley (1980) found that both the Z test and t-test were very non-robust for L-shaped distributions when comparing average p-values to nominal alphas.

Sawilowsky (1990) stated that the concept of robustness relates to both Type I and Type II errors and that choosing a test procedure requires one to consider other issues and properties too. Sawilowsky (1991) pointed out that there are no hard and fast rules for choosing between parametric and nonparametric procedures and Sawilowsky (2005) presented a summary of misconceptions regarding such choices. Heeren and D'Agostino (1987) found the independent samples t-test to be robust with ordinal data while Sawilowsky and Blair (1992) found that the t-test was reasonably robust when sample sizes were equal and at least of size $n = 30$ per group.

Several current statistics texts in the business field were reviewed to determine how they presented nonparametric versus parametric procedures. Anderson, et al., (2005), Moore, et al., (2003) and Newbold (1995) did not mention the assumptions underlying the Wilcoxon signed-rank test and made no recommendations regarding its use. Bowerman, et al., (2007) stated that when n is small, the distribution is non-normal and the measurement is ordinal the t-test is not valid and the Wilcoxon signed-rank test should be used. Keller (2005), Berenson, et al., (2004) and Chou (1989) made statements similar to those of Bowerman, et al., (2007). Keller (2005, p.738) further stated that the t-test cannot be used if the data are ordinal, thus eliminating its use with Likert scales. Doane and Seward (2007) recommended the use of the Wilcoxon signed-rank test in small sample situations because it is free of the normality assumption, uses ordinal data, is robust to

outliers and has fairly good power over a range of non-normal population shapes. Conover (1999) differed, and stated that, as does the t-test, the Wilcoxon signed-rank test requires an interval scale of measurement that also should eliminate its use with a Likert scale. Siegel (1956) specified that the Wilcoxon signed-rank test requires a level of measurement that is between ordinal and interval, called an ordered metric scale.

All of the textbooks cited above stress that the basis for their recommendations is to be able to calculate an exact probability of making a Type I error. If the assumptions underlying any procedure are questionable then it is not possible to do so. However, it is seldom possible to completely verify that all assumptions of any procedure are totally satisfied and, sometimes, it is of more interest to protect against a Type II error than against a Type I error.

Simulation of the Data

In order to generate data that would be typical of Likert scale responses from distributions with specified means, the simulations were obtained using the method detailed in the study by Meek, et al., (2000). That is, binomial distributions were used to generate integer results from a population whose range was 0 to $k-1$ and had a mean of $\mu-1$. These distributions, and the resulting data, were then shifted one unit to the right to obtain a range of observed values from 1 to k with a population mean of μ . Data were generated to represent five-point and seven-point Likert scales. A total of 27,850 simulations were conducted with 8,750 (31.4%) of them representing symmetric distributions. Because the one sample Wilcoxon signed-rank procedure is a test of the population median the symmetric cases are the only ones where it is truly appropriate, assuming that a Likert scale truly generates ordinal data. Based on Doane and Seward's (2007) statement that the Wilcoxon signed-rank procedure is fairly robust to non-normal or asymmetric shapes it should be reasonable for use on the majority of the remaining cases, too.

In addition to the level of measurement's being ordinal, at best, the underlying distributions used to generate observations were discrete, though infinite, and

the actual distributions were skewed in slightly more than two-thirds of the cases rather than symmetric. Thus, in all cases, the basic assumptions of the t -test were violated while in approximately 69% of the cases at least one assumption for the Wilcoxon signed-rank test was violated. Of the 27,850 data sets on which comparisons were made 11,350 represent a five-point Likert scale and 16,500 a seven-point Likert scale with varying sample sizes of 5, 10 and 15 for both scales.

Experimental Design

Comparisons of the one sample t -test and the Wilcoxon signed-rank test for location were based on corresponding p -values and the number of incorrect decisions that resulted from each. The p -values were calculated for each test procedure's results using Minitab® and the numbers of rejections and non-rejections at various nominal significance levels were tabulated for combinations of scale size, sample size, hypothesized mean and actual mean. The numbers of rejections for each test procedure were determined by comparing the p -values to nominal significance levels of 0.01, 0.05 and 0.10. The absolute differences between the hypothesized and actual means that were evaluated were 0.0, 0.5 and 1.0. Differences greater than 1.0 were not considered because both tests were rejecting H_0 with sample sizes of 10 and 15 approximately 90% of the time at that difference at the 0.10 level using a 5-point scale. A similar percentage of rejections occurred for the 7-point scale when the sample size was 15.

Two-way contingency tables were constructed for each combination by numbers of rejections and non-rejections versus the test procedure used. The Chi-square test of association was used to test for a relationship between the statistical decision and the procedure used. It is recognized that the use of the Chi-square test is questionable since both the t -test and the Wilcoxon signed-rank test were run on the same samples. The Chi-square test results do help to highlight disparities in the numbers of rejections between the two procedures. Tables were constructed identifying for which combinations significant differences occurred and at what level. It should be noted that Chi-square tests could not be run for

combinations having alphas of 0.01 and 0.05 when n is five because the theoretical (expected) number of rejections by the Wilcoxon signed-rank test is zero in those cases.

Another, and possibly more informative, way of comparing the two procedures is to look at their corresponding error rates. Thus, tables were constructed to compare the error rates of the two test procedures for all of the various combinations indicated above. Because the majority of samples simulated were from asymmetric distributions a separate table was constructed showing error rates for the procedures when the actual distributions were symmetric. In a very limited number of cases (eighteen) the Wilcoxon signed-rank procedure had more rejections than the t -test. These are tabulated.

Results

One of the assumptions underlying the Wilcoxon signed-rank procedure is that the distribution is symmetric. Several comparisons were made for which this assumption is violated; for example, data on the 7-point scale when the actual mean is 2.0 or when it is 6.0. These simulations and corresponding tests were conducted to see what happens in that situation. It is recognized that any results under those conditions are questionable but, in terms of actual errors, are useful because Doane and Seward (2007) indicated that the Wilcoxon signed-rank test is robust to non-normal, and somewhat asymmetrical, population shapes. In fact, the assumptions underlying the t -test are violated in every situation because there is neither an underlying normal distribution nor an interval level of measurement. Even so, the results indicate that, in almost every case when the null hypothesis was false, the t -test performed as well or better than the Wilcoxon signed-rank test. There were a total of 13 cases in which the Wilcoxon signed-rank test rejected more times than the t -test when H_0 was false and in only one of those was the difference significant, and that was at the 0.10 level.

The results of comparing the numbers of rejections for the two procedures using contingency tables are presented in Tables 1 through 6. In each of those tables, the first two

columns represent the values for the hypothesized mean and the actual mean, respectively. Columns 3 and 4 identify the sample size and the number of samples generated for that combination of hypothesized and actual means. The alpha values listed at the tops of columns 5, 6 and 7 represent the nominal significance levels at which the t and Wilcoxon signed-rank tests were run. Except for Tables 1 and 4, the last three columns in each table give the levels at which the Chi-square tests comparing corresponding results of the t and Wilcoxon signed-rank procedures were significant. In Tables 1 and 4, columns 5 and 6 have asterisks entered because the Wilcoxon signed-rank test cannot reject at alphas of 0.05 and 0.01 when $n = 5$.

A brief explanation of the entries in columns 5, 6 and 7 follows. For example, an entry of NS in the column headed by $\alpha = 0.10$ indicates that the numbers of rejections by t and the Wilcoxon signed-rank test were not significantly different at a nominal alpha of 0.10 for the combination of hypothesized and actual means listed for that row. Similarly, an entry of 0.05 under the column headed by $\alpha = 0.01$ indicates that the numbers of rejections by the two tests were significantly different at the 0.05 level of significance for the set of means in that row.

As an example, in the second row of Table 3, below, where the hypothesized mean is 1.5 and the actual mean is 2.0 the t-test rejected 139 times (not presented) out of 200 runs at 0.10 while the Wilcoxon signed-rank test rejected 125 times (not presented) at 0.10. Thus, t and Wilcoxon signed-rank test each failed to reject at that level 61 and 75 times, respectively. Casting those values into a contingency table using tests as columns and decisions as rows results in a calculated Chi-square value of 2.18 which is not significant at $\alpha = 0.10$. This is the significance level, NS, entered in row 2 and column 7 of Table 3. Other than the asterisks in Tables 1 and 4, already explained above, all other entries in columns 5, 6 and 7 of Tables 1 through 6 were obtained similarly. It should be noted that corrections for 1 degree of freedom for the Chi-square test are not incorporated in Minitab®.

Tables 1, 2 and 3 correspond to data generated for a 5-point Likert scale while Tables 4, 5 and 6, given below, are for data generated on a 7-point Likert scale. All of the significant differences between the numbers of rejections for the two procedures for the 5-point scale correspond to more rejections by the t-test than by the Wilcoxon signed-rank test. From Table 1, it is seen that the t-test rejected the null hypothesis significantly more times than the Wilcoxon signed-rank test in 18 of the 25 comparisons, or 16 of 23 if we ignore the cases where H_0 corresponds to a boundary value.

As the sample size increases, the cases where the numbers of rejections for the two procedures differ significantly drops correspondingly for significance levels of 0.10 and 0.05, to 8 and 12, respectively, out of 23 for $n = 10$ and 3 and 5, respectively, out of 23 for $n = 15$. However, they stay about the same for 0.01, 18 and 17 for $n = 10$ and $n = 15$, respectively. These numbers ignore boundary value cases.

As with the 5-point scale, ignoring boundary values, in the 7-point scale we see that at $\alpha = 0.10$ the significant differences decrease from 25 to 4 as the sample size increases from 5 to 15. Correspondingly, at 0.05 and 0.01, the significant differences decrease from 13 to 3 and 27 to 21, respectively, as n increases from 10 to 15.

A better way to compare the two test procedures, rather than looking at significant differences between the numbers of rejections, is to look at their estimated Type I and Type II error rates. These are presented below for all distributions in Table 7.

In Table 7, it is obvious that the Wilcoxon signed-rank procedure protects better against a Type I error because its average Type I error rate was always less than that of the t-test, whose Type I error rate exceeded the nominal significance level five times with the 7-point scale. It should be noted though that, except for $n = 15$ with the 7-point scale, the actual Type I error rate for the t-test was closer to the nominal level in all other comparisons. The average Type

Table 1: Five-point scale comparison of t test and Wilcoxon signed-rank test for a sample size of 5

Hypothesized Mean	Actual Mean	N	# of runs	$\alpha = .01$	$\alpha = .05$	$\alpha = .1$
1.0 ⁽¹⁾	2.0	5	100	*	*	.01
1.5	2.0	5	100	*	*	NS
2.0	2.0	5	100	*	*	.01
2.5	2.0	5	100	*	*	NS
3.0	2.0	5	100	*	*	.01
1.5	2.5	5	100	*	*	NS
2.0	2.5	5	100	*	*	.01
2.5	2.5	5	100	*	*	NS
3.0	2.5	5	100	*	*	.01
3.5	2.5	5	100	*	*	.10
2.0	3.0	5	300	*	*	.01
2.5	3.0	5	300	*	*	.10
3.0	3.0	5	300	*	*	.01
3.5	3.0	5	300	*	*	.05
4.0	3.0	5	300	*	*	.01
2.5	3.5	5	100	*	*	.05
3.0	3.5	5	100	*	*	.01
3.5	3.5	5	100	*	*	NS
4.0	3.5	5	100	*	*	.01
4.5	3.5	5	100	*	*	NS
3.0	4.0	5	100	*	*	.01
3.5	4.0	5	100	*	*	.10
4.0	4.0	5	100	*	*	.01
4.5	4.0	5	100	*	*	NS
5.0 ⁽¹⁾	4.0	5	100	*	*	.01

(1) When the hypothesized value equals a boundary value a better test would be to reject H_0 if any other value occurs in the sample.

* H_0 cannot be rejected at a significance level of 0.05 or 0.01 for samples of size 5 using Wilcoxon signed-rank test.

Table 2: Five-point scale comparison of t test and Wilcoxon signed-rank test for a sample size of 10

Hypothesized Mean	Actual Mean	n	# of runs	$\alpha = .01$	$\alpha = .05$	$\alpha = .1$
1.0 ⁽¹⁾	2.0	10	100	.01	.01	.01
1.5	2.0	10	100	.05	.05	NS
2.0	2.0	10	100	NS	.10	NS
2.5	2.0	10	100	.01	NS	NS
3.0	2.0	10	100	.01	.10	NS
1.5	2.5	10	100	.01	NS	NS
2.0	2.5	10	100	.05	NS	.10
2.5	2.5	10	100	NS	NS	NS
3.0	2.5	10	100	.01	.10	.10
3.5	2.5	10	100	.01	NS	NS
2.0	3.0	10	300	.01	.01	NS
2.5	3.0	10	300	.01	NS	NS
3.0	3.0	10	450	.05	.05	.05
3.5	3.0	10	300	.01	.10	.10
4.0	3.0	10	300	.01	.01	.05
2.5	3.5	10	100	NS	NS	NS
3.0	3.5	10	100	.01	.05	NS
3.5	3.5	10	100	NS	NS	NS
4.0	3.5	10	100	.10	.05	.10
4.5	3.5	10	100	.01	NS	NS
3.0	4.0	10	100	.01	.01	.05
3.5	4.0	10	100	.05	NS	NS
4.0	4.0	10	100	NS	.10	.10
4.5	4.0	10	100	.05	NS	NS
5.0 ⁽¹⁾	4.0	10	100	.01	.05	.05

(1) When the hypothesized value equals a boundary value a better test would be to reject H_0 if any other value occurs in the sample.

Table 3: Five-point scale comparison of t test and Wilcoxon signed-rank test
for a sample size of 15

Hypothesized Mean	Actual Mean	n	# of runs	$\alpha = .01$	$\alpha = .05$	$\alpha = .1$
1.0 ⁽¹⁾	2.0	15	200	.01	NS	NS
1.5	2.0	15	200	.10	.10	NS
2.0	2.0	15	200	NS	NS	NS
2.5	2.0	15	200	.10	NS	NS
3.0	2.0	15	300	.01	NS	NS
1.5	2.5	15	100	.05	NS	NS
2.0	2.5	15	100	.01	NS	NS
2.5	2.5	15	100	NS	NS	NS
3.0	2.5	15	100	.01	NS	NS
3.5	2.5	15	100	.05	NS	NS
2.0	3.0	15	300	.01	NS	NS
2.5	3.0	15	300	.01	NS	NS
3.0	3.0	15	400	NS	.05	NS
3.5	3.0	15	300	.01	.05	.05
4.0	3.0	15	300	.01	NS	NS
2.5	3.5	15	100	.01	NS	NS
3.0	3.5	15	100	.01	NS	NS
3.5	3.5	15	100	NS	NS	NS
4.0	3.5	15	100	.01	.10	NS
4.5	3.5	15	100	.05	NS	NS
3.0	4.0	15	100	.01	.10	NS
3.5	4.0	15	100	.05	NS	NS
4.0	4.0	15	100	NS	NS	.05
4.5	4.0	15	100	NS	NS	.10
5.0 ⁽¹⁾	4.0	15	100	.01	NS	NS

⁽¹⁾ When the hypothesized value equals a boundary value a better test would be to reject H_0 if any other value occurs in the sample.

Table 4: Seven-point scale comparison of t test and Wilcoxon signed-rank test for a sample size of 5

Hypothesized Mean	Actual Mean	N	# of runs	$\alpha = .01$	$\alpha = .05$	$\alpha = .1$
1.0 ⁽¹⁾	2.0	5	100	*	*	.01
1.5	2.0	5	100	*	*	NS
2.0	2.0	5	100	*	*	.01
2.5	2.0	5	100	*	*	NS
3.0	2.0	5	100	*	*	.01
1.5	2.5	5	100	*	*	NS
2.0	2.5	5	100	*	*	.01
2.5	2.5	5	100	*	*	NS
3.0	2.5	5	100	*	*	.01
3.5	2.5	5	100	*	*	NS
2.0	3.0	5	100	*	*	.01
2.5	3.0	5	100	*	*	NS
3.0	3.0	5	100	*	*	.01
3.5	3.0	5	100	*	*	NS
4.0	3.0	5	100	*	*	.01
2.5	3.5	5	100	*	*	.10
3.0	3.5	5	100	*	*	.01
3.5	3.5	5	100	*	*	NS
4.0	3.5	5	100	*	*	.01
4.5	3.5	5	100	*	*	.05
3.0	4.0	5	300	*	*	.01
3.5	4.0	5	300	*	*	.05
4.0	4.0	5	300	*	*	.01
4.5	4.0	5	300	*	*	.05
5.0	4.0	5	300	*	*	.01
3.5	4.5	5	100	*	*	NS
4.0	4.5	5	100	*	*	.01
4.5	4.5	5	100	*	*	NS
5.0	4.5	5	100	*	*	.01
5.5	4.5	5	100	*	*	NS
4.0	5.0	5	100	*	*	.01
4.5	5.0	5	100	*	*	NS
5.0	5.0	5	100	*	*	NS
5.5	5.0	5	100	*	*	NS
6.0	5.0	5	100	*	*	.01
4.5	5.5	5	100	*	*	.05
5.0	5.5	5	100	*	*	.01
5.5	5.5	5	100	*	*	NS
6.0	5.5	5	100	*	*	.01
6.5	5.5	5	100	*	*	NS
5.0	6.0	5	100	*	*	.01
5.5	6.0	5	100	*	*	NS
6.0	6.0	5	100	*	*	.01
6.5	6.0	5	100	*	*	NS
7.0 ⁽¹⁾	6.0	5	100	*	*	.01

⁽¹⁾ When the hypothesized value equals a boundary value a better test would be to reject H_0 if any other value occurs in the sample.

* H_0 cannot be rejected at a significance level of 0.05 or 0.01 for samples of size 5 using Wilcoxon signed-rank test.

Table 5: Seven-point scale comparison of t test and Wilcoxon signed-rank test
for a sample size of 10

Hypothesized Mean	Actual Mean	N	# of runs	$\alpha = .01$	$\alpha = .05$	$\alpha = .1$
1.0 ⁽¹⁾	2.0	10	100	.01	.01	NS
1.5	2.0	10	100	NS	NS	NS
2.0	2.0	10	100	NS	.05	NS
2.5	2.0	10	100	.01	NS	NS
3.0	2.0	10	100	.01	.05	NS
1.5	2.5	10	100	.01	NS	NS
2.0	2.5	10	100	NS	.05	NS
2.5	2.5	10	100	NS	NS	NS
3.0	2.5	10	100	.01	.05	NS
3.5	2.5	10	100	.01	NS	NS
2.0	3.0	10	100	.01	.05	NS
2.5	3.0	10	100	NS	NS	NS
3.0	3.0	10	100	NS	NS	NS
3.5	3.0	10	100	NS	NS	NS
4.0	3.0	10	100	.01	.05	NS
2.5	3.5	10	100	.01	.01	NS
3.0	3.5	10	100	NS	.10	NS
3.5	3.5	10	100	NS	NS	NS
4.0	3.5	10	100	.01	.05	NS
4.5	3.5	10	100	.01	NS	NS
3.0	4.0	10	200	.01	.01	.10
3.5	4.0	10	200	.01	NS	NS
4.0	4.0	10	200	NS	NS	NS
4.5	4.0	10	200	.05	NS	NS
5.0	4.0	10	200	.01	NS	NS
3.5	4.5	10	100	.01	NS	NS
4.0	4.5	10	100	.05	NS	NS
4.5	4.5	10	100	NS	NS	NS
5.0	4.5	10	100	.05	NS	NS
5.5	4.5	10	100	.01	NS	NS
4.0	5.0	10	200	.01	.01	NS
4.5	5.0	10	200	.01	NS	NS
5.0	5.0	10	200	NS	NS	.10
5.5	5.0	10	200	NS	NS	NS
6.0	5.0	10	200	.01	.05	.05
4.5	5.5	10	100	.01	NS	NS
5.0	5.5	10	100	.01	NS	NS
5.5	5.5	10	100	NS	NS	NS
6.0	5.5	10	100	.10	.10	NS
6.5	5.5	10	100	.01	NS	NS
5.0	6.0	10	100	.01	NS	NS
5.5	6.0	10	100	.01	NS	NS
6.0	6.0	10	100	NS	NS	.10
6.5	6.0	10	100	NS	NS	NS
7.0 ⁽¹⁾	6.0	10	100	.01	.05	.05

⁽¹⁾ When the hypothesized value equals a boundary value a better test would be to reject H_0 if any other value occurs in the sample.

Table 6: Seven-point scale comparison of t test and Wilcoxon signed-rank test
for a sample size of 15

Hypothesized Mean	Actual Mean	N	# of runs	$\alpha = .01$	$\alpha = .05$	$\alpha = .1$
1.0 ⁽¹⁾	2.0	15	100	.01	NS	NS
1.5	2.0	15	100	NS	NS	NS
2.0	2.0	15	100	NS	NS	NS
2.5	2.0	15	100	NS	NS	.10
3.0	2.0	15	100	.10	NS	NS
1.5	2.5	15	100	NS	NS	.10
2.0	2.5	15	100	.05	NS	NS
2.5	2.5	15	100	NS	NS	NS
3.0	2.5	15	100	NS	NS	NS
3.5	2.5	15	100	.10	NS	NS
2.0	3.0	15	100	.01	NS	.10
2.5	3.0	15	100	NS	NS	NS
3.0	3.0	15	100	NS	NS	NS
3.5	3.0	15	100	NS	NS	NS
4.0	3.0	15	100	.01	NS	NS
2.5	3.5	15	100	.05	NS	NS
3.0	3.5	15	100	.05	NS	NS
3.5	3.5	15	100	NS	NS	NS
4.0	3.5	15	100	NS	NS	NS
4.5	3.5	15	100	.05	NS	NS
3.0	4.0	15	300	.01	NS	NS
3.5	4.0	15	300	.05	NS	NS
4.0	4.0	15	300	NS	.10	NS
4.5	4.0	15	300	.05	NS	.10
5.0	4.0	15	300	.01	.05	NS
3.5	4.5	15	100	NS	NS	NS
4.0	4.5	15	100	.10	NS	NS
4.5	4.5	15	100	NS	NS	NS
5.0	4.5	15	100	.05	NS	NS
5.5	4.5	15	100	.10	.01	NS
4.0	5.0	15	100	.05	NS	NS
4.5	5.0	15	100	NS	NS	NS
5.0	5.0	15	100	NS	NS	NS
5.5	5.0	15	100	NS	NS	NS
6.0	5.0	15	100	.01	NS	NS
4.5	5.5	15	100	.10	NS	NS
5.0	5.5	15	100	NS	NS	NS
5.5	5.5	15	100	NS	NS	NS
6.0	5.5	15	100	NS	NS	NS
6.5	5.5	15	100	NS	NS	NS
5.0	6.0	15	100	.05	NS	NS
5.5	6.0	15	100	.10	NS	NS
6.0	6.0	15	100	.05	NS	NS
6.5	6.0	15	100	NS	NS	NS
7.0 ⁽¹⁾	6.0	15	100	NS	NS	NS

⁽¹⁾ When the hypothesized value equals a boundary value a better test would be to reject H_0 if any other value occurs in the sample.

Table 7: Average error rates (%)

$\Delta = \mu_o - \mu_a$	n	Error Type	Runs	WSR test average @ α of			t-test average @ α of		
				0.01	0.05	0.10	0.01	0.05	0.10
Five	Point	Scale							
-1.0 ⁽¹⁾	5	II	600	*	*	74.2	89.0	59.0	38.2
-0.5	5	II	700	*	*	88.4	98.4	88.1	76.4
0.0	5	I	700	*	*	1.9	0.1	3.7	9.0
+0.5	5	II	700	*	*	87.6	98.4	87.0	76.4
+1.0 ⁽¹⁾	5	II	600	*	*	73.2	87.3	59.0	36.5
-1.0 ⁽¹⁾	10	II	600	84.7	32.2	14.7	47.5	17.5	9.0
-0.5	10	II	700	99.1	83.6	68.4	92.3	75.4	63.7
0.0	10	I	850	0.0	1.9	5.1	1.2	4.1	9.5
+0.5	10	II	700	96.9	78.4	65.0	88.0	70.1	57.6
+1.0 ⁽¹⁾	10	II	600	82.5	30.5	11.8	48.0	19.2	7.3
-1.0 ⁽¹⁾	15	II	600	39.3	7.0	2.2	20.0	4.2	1.0
-0.5	15	II	800	89.8	62.0	46.6	79.9	54.8	41.9
0.0	15	I	900	0.3	2.1	6.0	0.9	4.6	8.9
+0.5	15	II	800	87.6	60.5	44.8	76.4	53.4	40.0
+1.0 ⁽¹⁾	15	II	700	38.1	7.3	3.3	16.9	4.6	1.7
Seven	Point	Scale							
-1.0 ⁽¹⁾	5	II	1000	*	*	76.0	89.1	70.3	51.5
-0.5	5	II	1100	*	*	88.7	97.7	87.9	78.6
0.0	5	I	1100	*	*	3.5	0.6	5.4	11.5
+0.5	5	II	1100	*	*	89.5	97.8	88.9	79.8
+1.0 ⁽¹⁾	5	II	1000	*	*	77.2	90.3	70.4	53.8
-1.0 ₍₁₎	10	II	1000	88.2	44.2	28.1	61.7	35.4	23.1
-0.5	10	II	1100	98.8	83.2	69.6	91.6	76.8	63.7
0.0	10	I	1100	0.0	3.0	6.5	0.9	4.7	10.2
+0.5	10	II	1100	98.4	84.9	72.9	92.6	79.2	68.6
+1.0 ⁽¹⁾	10	II	1000	89.7	47.1	29.4	66.9	39.0	23.9
-1.0 ⁽¹⁾	15	II	1000	58.0	21.9	12.3	42.8	17.3	10.4
-0.5	15	II	1100	93.1	72.5	58.5	86.5	67.1	53.0
0.0	15	I	1100	0.5	4.8	9.3	1.8	6.4	11.4
+0.5	15	II	1100	91.8	73.3	58.7	87.5	69.4	54.8
+1.0 ⁽¹⁾	15	II	1000	60.1	22.3	11.4	43.7	17.3	9.6

⁽¹⁾ If the hypothesized value equals a boundary value the result was deleted since a better test is to reject H_0 if any value other than μ_0 occurs in the sample.

* H_0 cannot be rejected at a nominal α value of either 0.01 or 0.05 for a sample of size 5.

Bold-faced entries indicate cases where the nominal α was exceeded.

If error rates using the t -test were lower than those using the Wilcoxon signed-rank test for every set of mean differences. Of the total of 630 combinations of mean comparisons and significance levels, the Wilcoxon signed-rank test rejected more times than the t -test when H_0 was false in only 13 combinations and the difference was significant, at 0.10, in only one of those. Because many of these cases involve distributions that are not symmetric and means are compared rather than medians it may not be fair to compare the Wilcoxon signed-rank test's Type II error rates to those of the t -test, even though at least two of the t -test's assumptions are violated in every case. Therefore, error rates for cases involving only symmetric distributions, where means and medians are the same, are presented in Table 8 below.

As can be seen in Table 8 the pattern of error rates is very similar to that shown in Table 7 for all distributions. That is, even though the Wilcoxon signed-rank test's assumptions are satisfied in all cases, assuming data generated on a Likert scale can be considered ordinal, and the t -test's assumptions are not satisfied in any cases the average Type II error for the t -test is smaller than that of the Wilcoxon signed-rank test. As before, the Wilcoxon signed-rank test protects

better against a Type I error with smaller average error rates. Surprisingly, and contrary to popular belief, the t -test, even though its assumption are violated, appears to protect substantially better against Type II errors for sample sizes of 5 and for larger mean differences at a significance level of 0.01. This phenomenon occurred for both symmetric and non-symmetric distributions. For the cases involving distributions that were not symmetric there did not seem to be any substantial differences between distributions that were skewed to the left from those that were skewed to the right.

In all, 630 combinations of means, sample sizes, Likert scales and nominal α -levels were run. The Wilcoxon signed-rank test rejected more times than the t -test in only eighteen of those combinations and only once did it do so significantly. The combination for which the Wilcoxon signed-rank test rejected significantly more times than the t -test at a level of 0.10 was: $n = 15$, 7-point scale, hypothesized mean of 2.5 vs. actual mean of 2.0 and a nominal α of 0.10. Cases for which Wilcoxon signed-rank test rejections exceeded t rejections are given in Table 9. Of the 18 cases in Table 9, five correspond to cases where H_0 was true and 13 to cases where H_0 was false.

Table 8: Average error rates (in %) for symmetric distributions

Scale	N	Runs	$\Delta=\mu_o-\mu_a$	Type Error	WSR test error @ $\alpha =$			t-test error @ $\alpha =$		
					0.01	0.05	0.10	0.01	0.05	0.10
5	5	300	-1.0	II	*	*	87	92	62	41
5	5	300	-0.5	II	*	*	87	99	92	82
5	5	300	0.0	I	*	*	0	0	4	10
5	5	300	0.5	II	*	*	84	98	87	78
5	5	300	1.0	II	*	*	84	87	59	35
5	10	300	-1.0	II	89	35	16	49	20	12
5	10	300	-0.5	II	99	81	67	92	76	70
5	10	450	0.0	I	0	2	5	1	4	9
5	10	300	0.5	II	97	78	67	90	72	61
5	10	300	1.0	II	88	33	12	53	19	7
5	15	300	-1.0	II	45	7	2	23	4	1
5	15	300	-0.5	II	92	67	52	84	61	48
5	15	400	0.0	I	0	2	6	1	5	8
5	15	300	0.5	II	90	64	49	78	56	42
5	15	300	1.0	II	42	7	3	18	5	2
7	5	300	-1.0	II	*	*	86	91	71	51
7	5	300	-0.5	II	*	*	85	98	89	77
7	5	300	0.0	I	*	*	1	1	5	11 ¹
7	5	300	0.5	II	*	*	90	98	94	84
7	5	300	1.0	II	*	*	91	95	75	62
7	10	200	-1.0	II	92	49	28	64	36	20
7	10	200	-0.5	II	99	85	72	91	79	66
7	10	200	0.0	I	0	4	7	1	6 ¹	10
7	10	200	0.5	II	98	85	75	94	82	69
7	10	200	1.0	II	93	38	27	66	35	21
7	15	300	-1.0	II	65	23	15	44	18	12
7	15	300	-0.5	II	94	75	62	89	71	56
7	15	300	0.0	I	0	3	9	1	5	11 ¹
7	15	300	0.5	II	93	73	61	88	69	54
7	15	300	1.0	II	65	23	11	45	16	8

¹ Identifies cases where the nominal α was exceeded.

* Indicates cases where n is too small for Wilcoxon signed-rank test to reject at the nominal significance level.

the study. Contrary to what was expected, based on the literature, the t-test was much better at

Table 9: Cases where Wilcoxon signed-rank rejections exceed t rejections

Scale	N	Runs	Actual μ	Hypoth. μ	Nom. α	WSR rej.	t-test rej.	Sig.
5	5	100	2.5	2.5	0.10	6	2	NS
5	10	300	3.0	2.5	0.10	99	91	NS
5	15	200	2.0	2.5	0.10	115	114	NS
5	15	100	2.5	2.5	0.10	6	4	NS
5	15	100	4.0	3.5	0.10	66	65	NS
7	5	100	2.5	2.5	0.10	9	8	NS
7	5	100	5.5	5.5	0.10	9	8	NS
7	5	100	6.0	6.5	0.10	14	11	NS
7	10	100	2.0	2.5	0.10	55	50	NS
7	10	100	5.5	4.5	0.10	64	63	NS
7	10	100	6.0	5.5	0.10	49	48	NS
7	15	100	2.0	2.5	0.10	67	55	0.10
7	15	100	2.0	2.5	0.05	51	47	NS
7	15	100	2.0	3.0	0.05	84	81	NS
7	15	100	2.5	2.5	0.10	17	13	NS
7	15	100	5.5	4.5	0.10	88	87	NS
7	15	100	5.5	4.5	0.05	81	79	NS
7	15	100	6.0	5.5	0.05	42	39	NS

Conclusion

Based on the 27,850 simulations conducted in this study, of which 8,750 involved symmetric distributions, it appears that the t-test may be preferred over the signed-rank procedure, even for very small sample sizes, unless it is imperative that one be able to calculate the exact probability of committing a Type I error. As in the Meek, et al., (2000) and (2001) studies, the Blair and Higgins (1985) study, and the Nanna (2002) study the level of measurement does not appear to be an important factor in test selection, at least in the case of a Likert scale. A more important consideration, at least with respect to the one sample test of location, is which error is more critical to guard against. The limitations of this study are that all data were generated from binomial distributions, the assumptions for the t-test are violated in all cases and the symmetry assumption of the signed-rank test is violated in 69% of the cases. Even with these limitations the t-test showed a lower average Type II error rate across all of the sample sizes that were used in

protecting against a Type II error for the sample size of five than was the signed-rank test, even when the Wilcoxon signed-rank test's assumptions were all satisfied. As the sample size increased the number of significant differences between the two procedures decreased dramatically for the 0.10 and 0.05 significance levels, to the point that the tests had similar error rates for those significance levels when $n = 15$. Although the results of this study seem to be in conflict with those of Blair and Higgins (1985), Nanna and Sawilowsky (1998), and Nanna (2002) their studies involved testing either two populations or the multivariate case and used different underlying distributions.

In summary, the results of these simulations indicated:

1. Except for a sample size of 5, the numbers of significant differences were fewest at a nominal α of 0.10 while significant differences decreased for both 0.10 and 0.05 as the sample size increased, but not for 0.01;

2. The t-test tended to have a higher Type I error rate, but closer to the nominal value, on average, while the Wilcoxon signed-rank test had a higher Type II error rate;

3. There did not appear to be any dramatic differences between error rates when the distributions were symmetric as opposed to being asymmetric;

4. The t-test actually appears to reject false hypotheses better; i.e., to have higher power, than the Wilcoxon signed-rank test when the sample sizes are small, even though its assumptions are violated in every case; and,

5. This study appears to contradict statements and recommendations about the use of the t-test vs. the Wilcoxon signed-rank test in small sample applications involving these particular non-normal distributions and ordinal data.

Further study needs to be done using different types of underlying distributions to generate the data to determine if these results might be attributed to having used a binomial generator. Additional points that might be considered in the future are other Likert scales, such as a 9-point, and ordinal measurements that do not correspond to Likert scale data. Regardless of this study's limitations it is quite surprising to find that all of the recommendations in the literature for using Wilcoxon's signed-rank procedure over the t-test, particularly with small sample sizes and Likert scale data, appear to be groundless, even when the t-test's assumptions are violated. Under conditions similar to the ones in this study it seems the only justification for using the Wilcoxon signed-rank procedure over the t-test is that it be imperative that an exact Type I error be able to be calculated.

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Another Look at Confidence Intervals for the Noncentral T Distribution

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An alternative approach to the computation of confidence intervals for the noncentrality parameter of the Noncentral t distribution is proposed. It involves the percent points of a statistical distribution. This conceptual improvement renders the technical process for deriving the limits more comprehensible. Accurate approximations can be derived and easily used.

Key words: Confidence intervals, noncentral t distribution, lambda-prime distribution, Bayesian inference.

Introduction

In spite of several recent presentations (see especially, Fidler & Thompson, 2001; Bird, 2002), many potential users, as well as statistical instructors, consider computing or teaching confidence intervals for the noncentrality parameter of the Noncentral t distribution to be very complex tasks. One of the conceptual difficulties is the lack of explicit formula. Although the considerable advances in computing techniques are supposed to render the task easy, they do not solve the conceptual difficulties.

The latter state is all the more deceptive in that when the number of degrees of freedom is large enough so that the Normal approximation holds the solution is very simple: the confidence limits are given by the percent points of a Normal distribution, as for the familiar case of an unstandardized difference between means. Thus, it can be expected that in the general case the limits would also be

computed as the percent points of a statistical distribution. Unfortunately, this is not the case with the usual presentations.

Moreover, warnings about the accuracy of some computer programs of the Noncentral t distribution (typically, the Noncentral t algorithm fails for large sample size or effect size) cast doubt on some numerical results. Consequently, there remains the need for accurate approximations that are not currently easily available. Even when an exact computation is wanted, it needs an iterative algorithm, for which an accurate approximation constitutes a good starting point.

An alternative approach is proposed in this article that results in computing the confidence limits as the percent points of a statistical distribution as in the most familiar situations. An interesting consequence of this conceptual improvement is that standard techniques to approximate statistical distributions can be used in order to find easy to use very accurate approximations. In conclusion, the question of the justification and interpretation of confidence intervals will be briefly examined.

Considerations and discussions regarding how and when to use confidence intervals for the Noncentral t distribution, may be found elsewhere. Therefore, this article is not methodological. In this perspective, it will be sufficient, with no loss of generality, to consider the elementary case of the inference about a standardized difference between two means.

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Computing confidence intervals from the Noncentral t distribution

When comparing two means, the t test statistic is the ratio $(\bar{Y}_1 - \bar{Y}_2)/E$ of the two statistics, $\bar{Y}_1 - \bar{Y}_2$ that is an estimate of the population difference $\mu_1 - \mu_2$ and the standard error E of that estimate (see e.g., Fidler & Thomson, 2001, p. 587). In other words, E is an estimate of the standard deviation ε of the sampling distribution for $\bar{Y}_1 - \bar{Y}_2$. For instance, in the particular case of two independent groups, assuming a common variance σ^2 , one has $\varepsilon = \sigma\sqrt{1/n_1 + 1/n_2}$.

The sampling distribution of the ratio $(\bar{Y}_1 - \bar{Y}_2)/E$ is a Noncentral t distribution with df degrees of freedom and a noncentrality parameter λ , equal to $(\mu_1 - \mu_2)/\varepsilon$. This distribution is usually written $t'_{df}(\lambda)$. The noncentrality parameter is termed λ , as in Algina and Keselman (2003), in order to avoid confusion with the population effect size. Formally, the Noncentral t distribution is the noncentrality parameter λ plus the standard Normal z distribution, all divided by the square root of the usual Chi-square distribution divided by the degrees of freedom (see e.g., Fidler & Thomson, 2001, p. 589):

$$t'_{df}(\lambda) = (\lambda + z) / \sqrt{\chi^2_{df} / df}.$$

The traditional approach for finding the lower (for instance) limit λ_L of the noncentrality parameter λ uses the probability p_λ that $t'_{df}(\lambda)$ exceeds the value t_{CALC} observed in the data in hand:

$$p_\lambda = \Pr(t'_{df}(\lambda) > t_{CALC}).$$

Then, one must vary the λ value in order to find, by successive approximations, the particular value λ_L such that $p_{\lambda_L} = \alpha/2$:

$$p_\lambda = \Pr(t'_{df}(\lambda) > t_{CALC}) = \alpha/2. \quad (1)$$

The conceptual difficulties come from the fact that finding the limit λ_L involves as many different distributions as considered λ values. A practical consequence is that it is a highly difficult task to derive accurate approximations.

An alternative approach: computing confidence intervals as percent points of the Lambda-prime distribution

An alternative solution consists in computing the confidence limits for the noncentrality parameter as percent points of a statistical distribution. When df is large enough so that the normal approximation holds, λ_L is simply the $100\alpha/2$ percent point of the standardized Normal distribution with mean t_{CALC} . This can be generalized by introducing an appropriate statistical distribution. Even if it has not been made explicit in the usual presentations, this distribution is in fact not unfamiliar (without mentioning the fiducial and Bayesian presentations discussed in the conclusion).

Indeed, it is usual to plot p_λ (or its complement $1-p_\lambda$) as a function of λ . An illustration is given in Figure 1 for $t_{CALC} = +1.0076$ with $df = 22$ (hence a p -value $p = 0.3246$, two-sided), which corresponds to the two-group A way data example given by Fidler & Thomson (2001, p. 586). The p_λ value increasingly varies from zero (when λ tends to $-\infty$) to one (when λ tends to $+\infty$), so that the corresponding curve is nothing else than the cumulative distribution function of a probability distribution. Such a graphical representation is commonly proposed to get a graphical solution for the confidence limits (see, for instance, Steiger & Fouladi, 1997, pp. 240), but the proponents fail to recognize that, in doing this, they implicitly define the confidence limits as the percent points of this probability distribution.

Figure 1 - Plot of p_λ as a function of λ for $t_{\text{CALC}} = +1.0076$ and $df = 22$ and graphical solution for the 95% confidence interval for λ . The curve is the cumulative distribution function of the $\Lambda'_{22}(+1.0076)$ distribution.

As for the Noncentral t , this distribution can be easily defined from the Normal and Chi-square distributions, but the result has not been so popularized. $(\bar{Y}_1 - \bar{Y}_2)/E > t_{\text{CALC}}$ can be equivalently written as $\bar{Y}_1 - \bar{Y}_2 - t_{\text{CALC}} E > 0$. Consequently, p_λ is the probability that $\bar{Y}_1 - \bar{Y}_2 - t_{\text{CALC}} E$ exceeds zero.

The sampling distribution of $\bar{Y}_1 - \bar{Y}_2 - t_{\text{CALC}} E$ can be formally defined from independent standard Normal and Chi-square distributions as:

$$\varepsilon(\lambda + z - t_{\text{CALC}} \sqrt{\chi_{df}^2 / df}).$$

so that

$$\begin{aligned} p_\lambda &= \Pr(\bar{Y}_1 - \bar{Y}_2 - t_{\text{CALC}} E > 0) \\ &= \Pr(-z + t_{\text{CALC}} \sqrt{\chi_{df}^2 / df} < \lambda) \\ &= \Pr(z + t_{\text{CALC}} \sqrt{\chi_{df}^2 / df} < \lambda), \end{aligned}$$

because the Normal distribution is symmetric around zero.

Thus, p_λ can be computed from the distribution characterized by $z + t_{\text{CALC}} \sqrt{\chi_{df}^2 / df}$. This distribution, which was considered (with no name) by Fisher (1990/1973, pp. 126-127) in the fiducial framework, was called Lambda-prime in Lecoutre (1999). It is also a noncentral distribution, again with df degrees of freedom, but with noncentrality t_{CALC} . Formally:

$$\Lambda'_{df}(t_{\text{CALC}}) = z + t_{\text{CALC}} \sqrt{\chi_{df}^2 / df}.$$

Consequently, it is possible to inverse in some sense the problem in (1) and compute p_λ as the probability that the *Lambda-prime* distribution with noncentrality t_{CALC} is smaller than λ :

$$p_\lambda = \Pr(\Lambda'_{df}(t_{\text{CALC}}) < \lambda).$$

Thus, the curve in Figure 1 is the cumulative distribution function of the *Lambda-prime* distribution with 22 degrees of freedom and noncentrality +1.0076.

In order to find the limit, solve

$$p_\lambda = \Pr(\Lambda'_{df}(t_{\text{CALC}}) < \lambda_L) = \alpha/2. \quad (2)$$

(2) is technically equivalent to (1) and requires a similar iterative process, but it has a conceptual advantage. Indeed, it involves a unique distribution, so that λ_L is the $100\alpha/2$ percent point of the $A'_{df}(t_{CALC})$ distribution. In the same way, the upper limit λ_U is its $100(1-\alpha/2)$ percent point. For instance, in Figure 1, the limits $\lambda_L = -0.986$ and $\lambda_U = +2.979$ of the 95% confidence interval are respectively the 2.5 and 97.5 percent points of the $A'_{22}(+1.0076)$ distribution.

Note again that the statistic $\bar{Y}_1 - \bar{Y}_2 - t_{CALC}E$ should not be regarded as less natural than the t test statistic. Indeed, it is similar to the familiar limits $\bar{Y}_1 - \bar{Y}_2 \pm t_{1-\alpha/2}E$ of the $100(1-\alpha)\%$ confidence interval for a raw difference. This analogy will be discussed in the conclusion.

Approximations of the 100π percent point of the $A'_{df}(t)$ distribution

Beyond its conceptual simplification, the alternative approach allows to derive accurate approximations. In this Section, in order to simplify the notations, t_{CALC} will be written t .

Numerical example

Consider Bird's first example (Bird, 2002, p. 206), which is also considered in

Algina and Keselman (2003). There were three independent groups of size 30 each, with means $\bar{Y}_1 = 22.467$, $\bar{Y}_2 = 24.933$, and $\bar{Y}_3 = 32.000$ and within group standard deviation 7.435. Bird reported the 97.5% confidence intervals of two standardized contrasts $(\bar{Y}_1 + \bar{Y}_2)/2 - \bar{Y}_3$ and $\bar{Y}_1 - \bar{Y}_2$. The computations for the first contrast will be detailed to illustrate the approximation methods. For this contrast, the t test statistic is $t = -4.9924$ ($df = 87$). The exact confidence interval of λ is: $[-7.3766, -2.5844]$.

It can be computed by the usual method based on the Noncentral t distribution using the available programs (for instance the Noncentral Distribution Calculator of Steiger, 2004), or alternatively as the 1.25 and 98.75 percent points of the Lambda-prime distribution with 87 degrees of freedom and eccentricity -4.9924.

Three approximation methods will be considered. The results for the two contrasts of interest are presented in Table 1. The limits for the standardized contrast $(\bar{Y}_1 + \bar{Y}_2)/2 - \bar{Y}_3$ in Table 1 are obtained by multiplying the limits for λ by the appropriate constant (0.223607) referred as SE in Bird's table, page 208. Note that this constant can be simply computed as the ratio of the observed standardized contrast to the t test value: $-1.1163/-4.9924 = 0.2236$.

Table 1. Bird's example: comparison of the three approximation methods

Contrast	Value	T	97.5%CI	Exact	Approximation		
					Bird	Normal	Chi-square
$(\bar{Y}_1 + \bar{Y}_2)/2 - \bar{Y}_3$	-1.1163	-4.9924	LowerLimit	-1.6495	-1.6264	-1.6489	-1.6495
			UpperLimit	-0.5779	-0.6063	-0.5773	-0.5779
$\bar{Y}_1 - \bar{Y}_2$	-0.3318	-1.2849	LowerLimit	-0.9123	-0.9207	-0.9123	-0.9123*
			UpperLimit	+0.2506	+0.2572	+0.2506	+0.2506*

Note. * Normal approximation

Three Approximation Methods - Bird's Approximation

Reconsidered in the new approach, the Bird (2002, p. 203) approximation of the 100π percent point of the Lambda-prime consists in adding t and the 100π percent point of the standard (central) t distribution with the same degrees of freedom:

$$\Lambda'_{df,\pi}(t) \approx t + t_{df,\pi}.$$

The approximate $100(1-\alpha)\%$ confidence interval for λ is obtained:

$$t \pm t_{df,1-\alpha/2},$$

hence here for $t_{87,0.9875} = +2.2809$ the approximate confidence interval: $-4.9924 \pm 2.2809 \rightarrow [-7.2733, -2.7116]$.

Algina and Keseleman (2003) found that the accuracy of this approximation does vary with the magnitude of the parameter, which can be verified in Table 1.

A simple normal approximation

The Lambda-prime distribution is generally asymmetric. However, when $t = 0$ it reduces to the standard Normal distribution, and when df is large it tends to the $N(t,1)$ distribution. So we can expect that a Normal approximation with the same mean and variance is appropriate, at least for small t and for large df .

The $\Lambda'_{df}(t)$ distribution has mean $M = kt$ where

$$k = \sqrt{\frac{2}{df}} \frac{\Gamma(\frac{df+1}{2})}{\Gamma(\frac{df}{2})},$$

and variance

$$V = 1 + t^2(1 - k^2) = 1 + t^2 - M^2,$$

so, that it can be approximated by the $N(M, V)$ distribution:

$$\Lambda'_{df,\pi}(t) \approx kt + z_{\pi} \sqrt{1 + t^2(1 - k^2)}.$$

The approximate $100(1-\alpha)\%$ confidence interval for λ is obtained:

$$kt \pm z_{1-\alpha/2} \sqrt{1 + t^2(1 - k^2)}.$$

In order to find k , one can compute its logarithm:

$$\begin{aligned} \log(k) &= (\log(2) - \log(df))/2 + \log\Gamma((df+1)/2) \\ &\quad - \log\Gamma(df/2), \end{aligned}$$

and then take the exponential of $\log(k)$. $\log\Gamma(x)$ is the logarithm of the Gamma function $\Gamma(x)$, that generalizes factorials to numbers beyond the integers. It is standard and for instance available in Excel. k can also be computed using the series expansion (Johnson & Welch, 1939):

$$\begin{aligned} k = & 1 - \frac{1}{4df} + \frac{1}{32df^2} + \frac{5}{128df^3} \\ & - \frac{21}{2048df^4} - \frac{399}{8192df^5} + \frac{869}{65536df^6} + \dots \end{aligned}$$

Alternatively, Table 2 can be used for finding the wanted value.

Table 2 - k values for df ranking from 1 to 100. For $k > 100$ the approximation $k \approx 1-1/(4df)$ gives an error less than 10^{-5} .

df	k	df	k	df	k	df	k	df	k
1	0.797885	2	0.886227	3	0.921318	4	0.939986	5	0.951533
6	0.959369	7	0.965030	8	0.969311	9	0.972659	10	0.975350
11	0.977559	12	0.979406	13	0.980971	14	0.982316	15	0.983484
16	0.984506	17	0.985410	18	0.986214	19	0.986934	20	0.987583
21	0.988170	22	0.988705	23	0.989193	24	0.989640	25	0.990052
26	0.990433	27	0.990786	28	0.991113	29	0.991418	30	0.991703
31	0.991969	32	0.992219	33	0.992454	34	0.992675	35	0.992884
36	0.993080	37	0.993267	38	0.993443	39	0.993611	40	0.993770
41	0.993922	42	0.994066	43	0.994203	44	0.994335	45	0.994460
46	0.994580	47	0.994695	48	0.994806	49	0.994911	50	0.995013
51	0.995110	52	0.995204	53	0.995294	54	0.995381	55	0.995465
56	0.995546	57	0.995624	58	0.995699	59	0.995772	60	0.995842
61	0.995910	62	0.995976	63	0.996040	64	0.996102	65	0.996161
66	0.996219	67	0.996276	68	0.996330	69	0.996383	70	0.996435
71	0.996485	72	0.996534	73	0.996581	74	0.996627	75	0.996672
76	0.996716	77	0.996759	78	0.996800	79	0.996841	80	0.996880
81	0.996918	82	0.996956	83	0.996993	84	0.997028	85	0.997063
86	0.997097	87	0.997131	88	0.997163	89	0.997195	90	0.997226
91	0.997257	92	0.997286	93	0.997315	94	0.997344	95	0.997372
96	0.997399	97	0.997426	98	0.997452	99	0.997478	100	0.997503

In Bird's example, it is found that $k = 0.997131$, $M = -4.9781$, and $V = 1.1428$, hence for $z_{0.9875} = +2.2414$ the approximate confidence interval for λ : $-4.9781 \pm 2.2414\sqrt{1.1428} \rightarrow [-7.3742, -2.5820]$ that is close to the exact interval.

A Chi-square approximation

For large t values, a better approximation can be found that takes into account the asymmetry of the distribution. This needs to consider the third central moment that can be deduced from the mean:

$$W = 2k^2 - \frac{2df-1}{df}kt^3 = 2M^3 - \frac{2df-1}{df}t^2M.$$

Next, compute the skewness of the distribution as the ratio of W to the third power of the square root of the variance V (i.e. $W/V^{3/2}$). The

skewness is a measure of the degree of asymmetry of the distribution. When it is small, one can use the Normal approximation $N(M, V)$ above. For practical applications, it was empirically found that a more sophisticated approximation is not necessary when the skewness is smaller than 0.001. Otherwise, the following Chi-square approximation that fits the skewness can be used. It involves again reasonably simple computations. Let

$$c = \frac{W}{4V}, q = \frac{V}{2c^2} \text{ and } a = M - qc.$$

Then the approximation is given by percent points of the Chi-square distribution with q degrees of freedom:

$$\Lambda'_{df,\pi}(t) \approx a + c\chi_{q,\pi}^2 \text{ if } c > 0,$$

$$\Lambda'_{df,\pi}(t) \approx a + c\chi_{q,1-\pi}^2 \text{ if } c < 0.$$

If $t > 0$ (which is equivalent to $c > 0$), we get the approximate $100(1-\alpha)\%$ confidence interval for λ : $[a + c\chi^2_{q,\alpha/2}, a + c\chi^2_{q,1-\alpha/2}]$. If $t < 0$, the limits are exchanged.

In practice q is generally very large and the Wilson and Hilferty (1931) approximation can be used (this is needed if your computer program does not work for high degrees of freedom values):

$$\chi^2_{q,\pi} \approx q \left(\sqrt{\frac{2}{9q}} z_\pi + 1 - \frac{2}{9q} \right)^3$$

Some programs for the Chi-square distribution accepts only integer degrees of freedom. In this case, the 100π percent point of the Gamma distribution with parameter $q/2$ can be used alternatively:

$$\chi^2_{q,\pi} = 2\text{Gamma}_\pi(q/2).$$

In Bird's example, it is found that $W = -0.0041$, $c = -0.0009016$, $q = 702948.01$ and $a = 628.7998$, hence the approximate confidence interval (computations have been performed with the maximum number of decimals for intermediate values): $[628.7998 - 0.0009016 \times$

$705608.34, 628.7998 - 0.0009016 \times 700293.06] \rightarrow [-7.3766, -2.5844]$, where $\chi^2_{702948.01, 0.0125} = 700293.06$ and $\chi^2_{702948.01, 0.09875} = 705608.34$ are computed using the Wilson-Hilferty approximation. This interval coincides with the exact interval with four decimal place accuracy.

A Comparison of the Three Methods

Table 3 gives a more systematic comparison of the three approximation methods. The exact probability levels associated with the different approximations of the 100π percent point of the $\Lambda'_{df}(t)$ distribution are reported for $100\pi = 2.5$ and $100\pi = 97.5$ (which gives the limits of the 95% confidence interval), and for $100\pi = 0.5$ and $100\pi = 99.5$ (which gives the limits of the 99% confidence interval). In the two cases, results are given for 10 and 50 degrees of freedom. They are reported only for positive values of t ; the results for negative values can be deduced by symmetry.

Bird's approximation is very inaccurate for small df or large t and can hardly be recommended. By contrast, the simple Normal approximation works very well. The Chi-square approximation is quasi exact for most practical applications.

Table 3. Exact probability levels associated with the three approximations of the 100π percent point of the $\mathcal{A}'_{df}(t)$ distribution

2.50% and 97.50% percent points

t	Bird's approximation				Normal approximation				Chi square approximation			
	$df=10$		$df=50$		$df=10$		$df=50$		$df=10$		$df=50$	
	2.50	97.50	2.50	97.50	2.50	97.50	2.50	97.50	2.50	97.50	2.50	97.50
0	1.29	98.71	2.23	97.77	2.50	97.50	2.50	97.50	2.50*	97.50*	2.50*	97.50*
0.25	1.33	98.72	2.24	97.77	2.50	97.50	2.50	97.50	2.50*	97.50*	2.50*	97.50*
0.50	1.38	98.70	2.26	97.77	2.50	97.50	2.50	97.50	2.50*	97.50*	2.50*	97.50*
0.75	1.46	98.66	2.28	97.76	2.50	97.50	2.50	97.50	2.50	97.50	2.50*	97.50*
1.00	1.57	98.60	2.31	97.74	2.49	97.49	2.50	97.50	2.50	97.50	2.50*	97.50*
1.50	1.86	98.41	2.39	97.69	2.48	97.48	2.50	97.50	2.50	97.50	2.50*	97.50*
2.00	2.27	98.10	2.50	97.61	2.46	97.46	2.50	97.50	2.50	97.50	2.50*	97.50*
2.50	2.81	97.68	2.63	97.50	2.42	97.43	2.50	97.50	2.50	97.50	2.50	97.50
3.00	3.50	97.14	2.80	97.37	2.39	97.39	2.49	97.49	2.50	97.50	2.50	97.50
4.00	5.31	95.75	3.22	97.01	2.30	97.31	2.49	97.49	2.50	97.50	2.50	97.50
5.00	7.63	94.01	3.77	96.53	2.22	97.24	2.47	97.48	2.49	97.50	2.50	97.50
10.00	21.04	84.57	8.19	92.66	1.95	97.04	2.40	97.40	2.47	97.51	2.50	97.50
15.00	30.54	77.72	14.10	87.58	1.84	96.97	2.33	97.34	2.46	97.52	2.50	97.50
20.00	36.36	73.27	19.72	82.78	1.80	96.94	2.29	97.31	2.45	97.52	2.50	97.50
25.00	40.12	70.25	24.39	78.77	1.78	96.93	2.27	97.28	2.45	97.52	2.50	97.50

Note. *Normal approximation (exact for $t = 0$)

0.50% and 99.50% percent points

t	Bird's approximation				Normal approximation				Chi square approximation			
	$df=10$		$df=50$		$df=10$		$df=50$		$df=10$		$df=50$	
	0.50	99.50	0.50	99.50	0.50	99.50	0.50	99.50	0.50	99.50	0.50	99.50
0	0.08	99.92	0.37	99.63	0.50	99.50	0.50	99.50	0.50*	99.50*	0.50*	99.50*
0.25	0.08	99.92	0.37	99.63	0.50	99.50	0.50	99.50	0.50*	99.50*	0.50*	99.50*
0.50	0.08	99.92	0.38	99.63	0.50	99.50	0.50	99.50	0.50*	99.50*	0.50*	99.50*
0.75	0.09	99.92	0.38	99.63	0.50	99.50	0.50	99.50	0.50	99.50	0.50*	99.50*
1.00	0.11	99.91	0.39	99.62	0.50	99.50	0.50	99.50	0.50	99.50	0.50*	99.50*
1.50	0.14	99.88	0.41	99.60	0.49	99.49	0.50	99.50	0.50	99.50	0.50*	99.50*
2.00	0.20	99.83	0.44	99.58	0.48	99.48	0.50	99.50	0.50	99.50	0.50*	99.50*
2.50	0.30	99.74	0.48	99.55	0.46	99.46	0.50	99.50	0.50	99.50	0.50	99.50
3.00	0.44	99.61	0.53	99.50	0.45	99.45	0.50	99.50	0.50	99.50	0.50	99.50
4.00	0.92	99.17	0.67	99.38	0.41	99.41	0.49	99.49	0.50	99.50	0.50	99.50
5.00	1.77	98.44	0.86	99.21	0.37	99.37	0.49	99.49	0.49	99.51	0.50	99.50
10.00	11.13	91.64	3.03	97.23	0.25	99.27	0.45	99.45	0.47	99.52	0.50	99.50
15.00	21.38	84.59	7.25	93.53	0.21	99.23	0.42	99.42	0.45	99.53	0.50	99.50
20.00	28.67	79.33	12.32	89.21	0.19	99.22	0.40	99.40	0.44	99.53	0.49	99.50
25.00	33.67	75.54	17.15	85.12	0.18	99.21	0.39	99.39	0.44	99.53	0.49	99.51

Note. *Normal approximation (exact for $t = 0$)

Conclusion

Returning to the analogy between the statistic $\bar{Y}_1 - \bar{Y}_2 - t_{\text{CALC}} E$ and the familiar limits $\bar{Y}_1 - \bar{Y}_2 \pm t_{1-\alpha/2} E$ of the $100(1-\alpha)\%$ confidence interval for a raw difference, it can be tempting to consider the interval $\bar{Y}_1 - \bar{Y}_2 \pm t_{\text{CALC}} E$. Assume for instance that t_{CALC} is positive, then one can remark that t_{CALC} is the $100(1-p)/2$ percent point $t_{1-p/2}$ of the t distribution, where p is the two-sided p -value of the usual t test. Thus, the analogy seems again more compelling.

By the definition of t_{CALC} , for the data in hand the bounds of this interval are zero, the traditional null hypothesis value, and two times the observed difference, what Rosnow and Rosenthal (1996) called the counter-null value. In their methodological article, Rosnow and Rosenthal (page 336) considered such an interval. Taking the example of an observed difference between two means $+0.266$ and a p -value $p = 0.23$, they interpreted the specific null counter-null interval $[0, +0.532]$ as a 77% confidence interval, that is as a $100(1-p)\%$ confidence interval. This interpretation reveals a typical confusion between Frequentist and Bayesian probabilities.

In the Frequentist conception of confidence intervals, the confidence level is the proportion of repeated intervals that contain the (fixed) parameter; it is usually termed the coverage probability. The procedure, and in particular the confidence level, must be determined before knowing the data. In the case of the Rosnow and Rosenthal interval $[0, +0.532]$, two possibilities can be envisaged to define the procedure and thus to compute the coverage probability.

Nevertheless, the procedure can proceed by computing the interval $\bar{Y}_1 - \bar{Y}_2 \pm t_{\text{CALC}} E$, with the data dependent value t_{CALC} . For each repeated sample the bounds of this interval are zero and the particular counter-null value for this sample. Of course, the coverage probability of this interval varies with the parameters and it is not equal to 0.77 (except for two particular values of the ratio $(\mu_1 - \mu_2)/\varepsilon$ symmetrical around zero).

The procedure can also proceed by computing the interval $\bar{Y}_1 - \bar{Y}_2 \pm t_{1-p/2} E$, with the fixed value $p = 0.23$ for each repeated sample. The coverage probability of this interval is 0.77. However, this is not a Frequentist approach, because 0.77 has been determined by the data in hand. Clearly, 0.77 is a data dependent probability, which needs a Bayesian approach to be correctly interpreted. The Bayesian inference associates to the interval $[0, +0.532]$ the posterior probability that this interval contains the parameter, given the data.

Although confidence intervals refer to a Frequentist justification, they are often (mis)interpreted in Bayesian terms. The distinction between the Frequentist coverage probability and the Bayesian posterior probability is all the more subtle in the present situation that it turns out that it is correct from a Bayesian viewpoint to say that there is a 77% chance that the interval $[0, +0.532]$ contains $(\mu_1 - \mu_2)/\varepsilon$, or again in the example in Figure 1 to say that there is a 95% chance that the interval $[-0.986, +2.979]$ contains the noncentrality parameter λ . This simply assumes a prior distribution that does not favor any particular value of the parameters, what Bayesian called a non-informative prior.

This distribution is revised by the data and the corresponding posterior distribution for the noncentrality parameter λ is just the $\Lambda'_{\text{df}(t_{\text{CALC}})}$ distribution. Consequently, the Lambda-prime distribution, in addition to its status of sampling distribution gains the status of a probability distribution that expresses the uncertainty about the unknown parameter λ . One can use the confidence interval for λ with the benefits of both the Frequentist and Bayesian interpretations and without worrying about the correct justification (not to speak of Fisher's fiducial argument).

The fact that even experts in statistics are not immune to conceptual confusions and interpret Frequentist intervals in Bayesian terms should not be regarded as an error. Rather this means that, as most statistical inference users, they are also, perhaps without knowing it, interested in the Bayesian probability. This should invite us not to radicalize the opposition between the Bayesian and Frequentist inferences

but rather to consider their interplay. This is a difficult challenge, but it is already well advanced in the statistical literature (see Bayarri & Berger, 2004).

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Tests for Treatment Group Equality When Data are Nonnormal and Heteroscedastic

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Several tests for group mean equality have been suggested for analyzing nonnormal and heteroscedastic data. A Monte Carlo study compared the Welch tests on ranked data and heterogeneous, nonparametric statistics with previously recommended procedures. Type I error rates for the Welch tests on ranks and the heterogeneous, nonparametric statistics were well controlled with a slight power advantage for the Welch tests on ranks.

Key words: Welch test on ranks, nonparametric statistics, nonnormality, heteroscedasticity, mean equality

Introduction

Researchers in the behavioral sciences are often interested in comparing the typical performance of subjects across independent groups, and they often select traditional test statistics (e.g., two-sample *t*, ANOVA *F*) without regard for their underlying assumptions, even though it has been pointed out that these assumptions may frequently be violated (e.g., Micceri, 1989; Keselman et al., 1998; Wilcox, 1988). Many authors have highlighted available procedures for analyzing data that violate either the assumption of normality or the assumption of variance homogeneity. Brown and Forsythe (1974), Kohr and Games (1974), and many

others demonstrated the general effectiveness (i.e., Type I error control) of Welch's (1938, 1951) two-sample and omnibus test statistics with heterogeneous variances. In addition, Keselman, Cribbie and Zumbo (1997), Wilcox (1995; 1997), Yuen and Dixon (1973), and Zimmerman and Zumbo (1993a), among many others, have demonstrated the effectiveness of several alternatives to traditional parametric tests that can be used with nonnormal data, including nonparametric test statistics and tests with robust estimators (e.g., trimmed means).

However, there has been little success in discovering a test that is robust (with respect to Type I and Type II errors) to the simultaneous violations of both assumptions. That is, although procedures have been proposed for analyzing data that violate both the normality and variance heterogeneity assumptions concurrently (described below), there has not been a thorough investigation and comparison of the Type I error and power properties of these procedures. Therefore, the current article compares potential strategies for analyzing nonnormal and heteroscedastic data, with the goal of being able to recommend a procedure that provides a good balance between Type I error control and power.

One possibility for analyzing nonnormal and heteroscedastic data is to utilize the Welch two-sample and omnibus tests, which have been found to provide excellent Type I error control

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and power for some patterns of nonnormality (with unequal variances); however, for other patterns the Type I error rates can deviate considerably from the nominal rate (e.g., Cressie & Whitford, 1986; Keselman, Lix & Kowalchuk, 1998). Another potential solution when variances are heterogeneous and distribution shapes are nonnormal is to use a heteroscedastic statistic, such as Welch's (1938, 1951) tests, with sample estimators that are intended to be robust to the biasing effects of nonnormality, e.g., trimmed means and Winsorized variances (see Yuen & Dixon, 1973; Wilcox, 1995, 1997). By minimizing the effects of extreme observations the trimmed mean can provide a more accurate representation of the central tendency of the majority of the distribution. An increase in power may also be experienced if eliminating the extreme observations reduces the standard error of the mean. However, Keselman, Lix, et al. (1998) reported that under some patterns of nonnormality power could be depressed relative to utilizing the usual means and variances.

Nonparametric test statistics (e.g., Wilcoxon, Mann-Whitney, Kruskal-Wallis) have been studied for unequal variances and nonnormal data. Zimmerman (1987; 1996) and Zimmerman and Zumbo (1993a), among others, showed that nonparametric test statistics are not robust to unequal variances, regardless of whether the data are normal or nonnormal.

Zimmerman and Zumbo (1993a) explained that, "an attractive hypothesis is that both problems [nonnormality and variance heterogeneity] can be solved at once by the Welch *t* test performed on the ranks of measures instead of the measures themselves" (p. 507). Thus, with this approach, researchers would convert nonnormal, heteroscedastic data to ranks, and analyze the data with the Welch two-sample or omnibus tests. Zimmerman and Zumbo (1993a; 1993b) conducted simulation studies with several patterns of nonnormality and variance heterogeneity and report that the Welch test on ranks "counteracts effects of nonnormality and unequal variances at the same time" (p. 535). More specifically, for many patterns of nonnormality and variance homogeneity, the Welch test on ranks provided better overall Type I and Type II error control

relative to the two-sample *t* and Welch *t* on unranked data or the two-sample *t* on ranks. However, it should be noted that for some patterns of nonnormality (e.g., lognormal) Type I error rates were not controlled within Bradley's (1978) liberal criterion ($\pm .5 \alpha$).

Another potential solution is the heteroscedastic rank-based test statistics proposed by Brunner and Munzel (2000) and Brunner, Dette and Munk (1997). Specifically these authors presented two-sample and omnibus, respectively, heteroscedastic rank-based test statistics that, unlike the traditional Kruskal-Wallis nonparametric statistic, consider the variance heterogeneity of the group distributions in the computational procedure. Munzel and Hothorn (2001) presented findings on the Type I error and power properties of the Brunner and Munzel two-sample procedure for nonnormal distributions with unequal variances, indicating that Type I error and power rates were considerably better than those of the parametric and nonparametric competitors. However, results were only reported for a many-to-one multiple comparisons setting for the discretized normal distribution.

The purpose of this article is to compare the Type I error control and power of the above strategies under several conditions of nonnormality and/or heteroscedasticity. It extends the conditions investigated by Zimmerman and Zumbo (1993a; 1993b) and Munzel and Hothorn (2001) to independent groups designs with more than two levels of the independent variable and, with respect to nonnormality, investigates skewed distributions not previously investigated and that have been reported to be representative of many behavioral science variables (Micceri, 1989; Wilcox, 1995). The Type I error control and power of the procedures in a multiple comparisons setting is also examined.

Test Statistics

Five omnibus test statistic and data configuration combinations were evaluated and compared in this study. These included: a) Welch's (1951) test statistic on unranked data (Welch); b) Welch's test statistic on trimmed means and Winsorized variances (20% symmetric trimming) (Welch-t); c) Welch's test

statistic on ranked data (Welch-r); d) the Kruskal-Wallis (Kruskal & Wallis, 1952) omnibus nonparametric test statistic (which utilizes ranked data) (KW); and e) the Brunner, Dette and Munk (1997) heterogeneous nonparametric test statistic (BDM).

Welch

Welch's (1938) two-sample test statistic can be expressed as:

$$t_w = \frac{\overline{X}_j - \overline{X}_{j'}}{\sqrt{\frac{s_j^2}{n_j} + \frac{s_{j'}^2}{n_{j'}}}}$$

which is distributed as a t variable with degrees of freedom due to Satterthwaite (1946),

$$v_w = \frac{\left(\frac{s_j^2}{n_j} + \frac{s_{j'}^2}{n_{j'}} \right)^2}{\left[\frac{s_j^4}{n_j^2(n_j-1)} + \frac{s_{j'}^4}{n_{j'}^2(n_{j'}-1)} \right]},$$

where $\overline{X}_j$, s_j^2 and n_j represent the sample means, variances, and sample sizes, respectively, for the jth group ($j \neq j'$, $j = 1, \dots, J$).

Welch's (1951) omnibus test can be expressed as:

$$F_w = \frac{\frac{\sum_j w_j (\overline{X}_j - \overline{X}_j^*)^2}{J-1}}{1 + \left(\frac{2(J-2)}{J^2-1} \right) \left(\frac{\sum_j \left(1 - w_j / \sum_j w_j^2 \right)^2}{n_j - 1} \right)},$$

which is distributed as an F variable with J-1 and v_w degrees of freedom, where

$$w_j = \frac{n_j}{s_j^2},$$

$$\overline{X}_j^* = \frac{\sum_j w_j \overline{X}_j}{\sum_j w_j},$$

and

$$v_w = \frac{J^2 - 1}{3 \sum_j \frac{\left(1 - w_j / \sum_j w_j \right)^2}{n_j - 1}}.$$

Kruskal-Wallis

The Kruskal-Wallis nonparametric procedure begins by ranking the observations in the combined sample. Let the rank of the i th observation in the j th group be represented by r_{ij} and the sum of the ranks for the j th group be represented by $a_j = \sum_i r_{ij}$. The statistic tests the null hypothesis $H_0: \lambda_1 = \dots = \lambda_J$ (where λ represents the population mean only under the assumption that the population shapes are identical) and rejects H_0 if $KW \geq \chi^2_{(J-1)}$ where:

$$KW = 12 \left(\frac{\sum_j a_j^2 / n_j}{N(N+1)} \right) - 3(N+3),$$

and $N = \sum_j n_j$. Multiple comparisons are performed with a modified two-sample version of the omnibus Kruskal-Wallis test (see Sprent & Smeeton, 1993). The null hypothesis $H_0: \lambda_j = \lambda_{j'}$ is rejected if $|t_{KW}| \geq t_{\alpha, N-J}$, where:

$$t_{KW} = \frac{\bar{X}_1 - \bar{X}_2}{\sqrt{\frac{(S_r - C)(N-1-KW)(n_j + n_{j'})}{n_j n_{j'}(N-J)(N-1)}}},$$

$$S_r = \sum_i \sum_j r_{ij}^2$$

and

$$C = \frac{N(N+1)^2}{4}.$$

Welch-t

Trimmed means are computed by removing a percentage of observations from each of the tails of a distribution. Let $g_j = [\gamma n_j]$, where γ represents the proportion of observations to be trimmed from each tail of the distribution and $[x]$ is the largest integer less than or equal to x . Further, let h_j represent the remaining (effective) sample size following removal of the trimmed observations. Recommendations have been made in the literature for 15% symmetric trimming (Mudholkar, Mudholkar & Srivastava, 1991) and 20% symmetric trimming (Wilcox, 1995). The j th sample trimmed mean can be represented as:

$$\bar{X}_{tj} = \frac{1}{h_j} \sum_{i=g_j+1}^{n_j-g_j} X_{ij}$$

and the j th sample Winsorized mean as

$$\bar{X}_{wj} = \frac{1}{n_j} \sum_{i=1}^{n_j} Y_{ij}$$

where:

$$\begin{aligned} Y_{ij} &= X_{(g_j+1)j} \text{ if } X_{ij} \leq X_{(g_j+1)j}, \\ &= X_{ij} \text{ if } X_{(g_j+1)j} < X_{ij} < X_{(n_j-g_j)j}, \\ &= X_{(n_j-g_j)j} \text{ if } X_{ij} \geq X_{(n_j-g_j)j}. \end{aligned}$$

An associated Winsorized variance is computed by replacing the censored observations from the lower tail with the lowest uncensored observation and the censored observations from the upper tail with the highest uncensored observation. The Winsorized variance is:

$$s_{wj}^2 = \frac{1}{h_j - 1} \sum_{i=1}^{n_j} (Y_{ij} - \bar{X}_{wj})^2.$$

The sample trimmed means and Winsorized variances can then be substituted into Welch's (1938; 1951) two-sample and omnibus test statistics. For example, substituting the trimmed means and Winsorized variances into the Welch (1938) two-sample test yields the statistic:

$$t_w = \frac{\bar{X}_{tj} - \bar{X}_{tj'}}{\sqrt{\frac{s_{wj}^2}{h_j} + \frac{s_{wj'}^2}{h_{j'}}}}.$$

with error degrees of freedom,

$$v_w = \frac{\left(\frac{s_{wj}^2}{h_j} + \frac{s_{wj'}^2}{h_{j'}} \right)^2}{\left[\frac{s_{wj}^4}{h_j^2(h_j-1)} + \frac{s_{wj'}^4}{h_{j'}^2(h_{j'}-1)} \right]}.$$

Welch-r.

The Welch test can be performed on the ranked data, where ranks are established regardless of group membership. The null hypothesis, $H_0: \lambda_1 = \dots = \lambda_J$, is rejected if $F_w \geq F_{\alpha, J-1, v_w}$.

Brunner, Dette, and Munk

Brunner, Dette and Munk (1997) proposed the following heterogeneous, rank-based F statistic:

$$F_B = \frac{N}{tr(M_{11}V)} QMQ',$$

where

$$M = \underline{I} - \frac{1}{J} \underline{J}, \quad \underline{I} = \text{identity matrix of rank } J,$$

$$\underline{J} = J \text{ by } J \text{ matrix of } 1s,$$

$$V = N * \text{diag} \left(\frac{s_1^2}{n_1}, \dots, \frac{s_J^2}{n_J} \right),$$

$$s_j^2 = \frac{1}{N^2(n_j - 1)} \sum_j (R_{ij} - \bar{R}_j)^2,$$

$$Q = \frac{1}{N} \left(\bar{R}_1 - \frac{1}{2}, \dots, \bar{R}_J - \frac{1}{2} \right),$$

$$\bar{R}_j = \frac{1}{n_j} \sum_{i=1}^{n_j} R_{ij},$$

and R_{ij} is the rank of X_{ij} after the data are pooled. The null hypothesis, $H_0: \lambda_1 = \dots = \lambda_J$ is rejected if $F_B \geq F_{\alpha, v_1, v_2}$ where:

$$v_1 = \frac{M_{11}[tr(V)]^2}{tr(MVMV)}$$

$$v_2 = \frac{[tr(V)]^2}{tr(V^2\Lambda)}$$

and $\Lambda = \text{diag} \{ (n_1 - 1)^{-1}, \dots, (n_J - 1)^{-1} \}$. Multiple comparisons are performed with the two-sample version of the Brunner, Dette and Munk (1997) procedure (see Brunner & Munzel, 2000).

It is important to note that the null hypotheses associated with the above tests differ based on the characteristic(s) of the data that each test is sensitive to. The Welch test evaluates the null hypothesis that all population means are equal (i.e., $H_0: \mu_1 = \dots = \mu_J$). The Welch-t evaluates the null hypothesis that all population trimmed means are equal (i.e., $H_0: \mu_{t1} = \dots = \mu_{tJ}$). The K-W, Welch-r and BDM procedures evaluate the null hypothesis that all distribution functions are equal (i.e., $H_0: \lambda_1 = \dots = \lambda_J$). It is important to note that with the K-W, Welch-r and BDM procedures that the null hypotheses only relate to a test of location when population distribution shapes and variances are equal, where the procedures are sensitive to differences in the mean ranks (see Brunner, Dette & Munk, 1997, p. 1498; Kruskal & Wallis, 1952; Sprent & Smeeton, 2001). Hence, an important component of this article is to evaluate the rates of rejection for these procedures when variances are unequal.

Pairwise Multiple Comparison Procedures (MCPs)

Tukey

The Tukey (1953) procedure rejects $H_0: \mu_j = \mu_{j'}$ ($j \neq j'$) if $|t| \geq q(\alpha, J, v) / (2)^{1/2}$, where q is a value from the Studentized range distribution with J groups and v degrees of

freedom, and t and v represents the appropriate two-sample t -distributed test statistic and associated degrees of freedom, respectively.

REGWQ

Ryan (1960) proposed a modification to the Newman-Keuls (Newman, 1939; Keuls, 1952) procedure that ensures that the familywise (overall) Type I error rate is maintained at α , even in the presence of partial null hypotheses. Ryan's original procedure became known as the REGWQ after modifications to the procedure proposed by Einot and Gabriel (1975) and Welsch (1977). The REGWQ MCP sequentially tests all ordered mean differences for stretch sizes (inclusive ranges between rank-ordered means) $p = J, J - 1, \dots, 2$, and rejects $H_0: \mu_j = \mu_{j'}$ ($j \neq j'$) if an associated omnibus test has been rejected and:

$$|t| \geq q(\alpha_p, p, v) / (2)^{1/2},$$

where $\alpha_p = \alpha$ for $p = J, J - 1$, and $\alpha_p = 1 - (1 - \alpha)^{p/J}$, for $p = J - 2, \dots, 2$. If any H_0 s are retained for $p = p'$ then all H_0 s contained in that stretch are retained and not tested at later stages (i.e., $p < p'$). If all H_0 s are retained for $p = p'$ then all H_0 s with $p \leq p'$ are retained.

Methodology

A Monte Carlo study was used to compare the Type I error and power rates of the Welch test on ranks and the Brunner heteroscedastic rank-based statistics with that of the Welch test on unranked data, the Welch test with trimmed means and Winsorized variances and the Kruskal-Wallis (Kruskal & Wallis, 1952) nonparametric test in a one-way independent groups design. In addition, the procedures were compared in a pairwise multiple comparison framework, with the Tukey (1953) and REGWQ (Ryan, 1960; Einot & Gabriel, 1975; Welsch, 1977) procedures.

Seven variables were manipulated in this study: a) number of levels of the independent variable; b) total sample size; c) degree of sample size imbalance; d) degree of variance inequality; e) pairings of group sizes and variances; f) configuration of population means; and g) population distribution shape.

The number of levels of the independent variable was set at $J = 4$ and $J = 7$, resulting in 6 and 21 pairwise comparisons, respectively. This permits evaluation of the effect of the number of pairwise comparisons computed on Type I error control and power.

In order to investigate the effects of sample size, the total sample size (N) was manipulated by setting the average $n_j = 10, 15$, and 20 resulting in $N = 40, 60$ and 80 for $J = 4$, and $N = 70, 105$ and 140 for $J = 7$. The sample sizes were selected to be similar to those used by Zimmerman and Zumbo (1993a, b) in their investigations of the two-sample Welch (1938) test on ranked data. For the nonnull mean configurations used in this study, the group sizes 10, 15 and 20 result in *a priori* omnibus (ANOVA F statistic) power estimates of approximately .80, .95, and .98, respectively (assuming equal group sizes and variances).

Sample size balance or imbalance was also manipulated. Keselman et al. (1998) reported that unbalanced designs were more common than balanced designs in a review of studies published in educational and psychological journals. In addition, the effects of variance heterogeneity can be exacerbated when paired with unequal sample sizes. Therefore, three sample size conditions were examined (equal, moderately unequal and extremely unequal). The sample sizes used are enumerated in Table 1.

Degree of variance heterogeneity was also manipulated. According to Keselman et al. (1998), ratios of largest to smallest variances of 8:1 are not uncommon in educational and psychological studies and can have deleterious effects on the performance of many test statistics, especially when paired with unequal sample sizes. Therefore, three levels of variance equality/inequality were examined in this study: a) equal variances; b) largest to smallest variance ratio of 4:1; and c) largest to smallest variance ratio of 8:1. See Table 1 for group variances.

Pairings of variances and sample sizes can have differing effects on the Type I error and power rates of many test statistics. Specifically, when variances and sample sizes are directly (positively) paired Type I error estimates for the usual t/F tests can be

Table 1. Sample Sizes and Population Variances Used in the Simulation Study.

J	Sample Sizes	Population Variances
4	10, 10, 10, 10	1, 1, 1, 1
	9, 10, 10, 11	1, 2, 4, 4
	5, 8, 12, 15	1, 3, 5, 8
	15, 15, 15, 15	
	13, 15, 15, 17	
	7, 12, 18, 23	
	20, 20, 20, 20	
	17, 20, 20, 23	
	9, 16, 24, 31	
7	10, 10, 10, 10, 10, 10, 10	1, 1, 1, 1, 1, 1, 1
	9, 9, 10, 10, 10, 11, 11	1, 1, 2, 2, 3, 3, 4
	5, 6, 8, 10, 12, 14, 15	1, 2, 2, 4, 7, 7, 8
	15, 15, 15, 15, 15, 15, 15	
	13, 14, 15, 15, 15, 16, 17	
	7, 9, 12, 15, 18, 21, 23	
	20, 20, 20, 20, 20, 20, 20	
	17, 18, 20, 20, 20, 22, 24	
	9, 12, 16, 20, 24, 28, 31	

conservative (with correspondingly deflated power). On the other hand, when variances and sample sizes are inversely (negatively) paired Type I error estimates for the usual t/F tests can be liberal (with correspondingly inflated power). Therefore, both positive and negative pairings were examined.

Several configurations of nonnull population means were investigated, in addition to the complete null case. Following Toothaker's (1991) definitions of mean configuration, equally spaced, minimum variability and maximum variability configurations were utilized. See Table 2 for a listing of the mean configurations.

Another factor examined in this study was population distribution shape. The three distribution shapes investigated were: 1) normally distributed data; 2) moderately skewed

data from the g- and h- distribution (Hoaglin, 1985), where $g = .5$ and $h = 0$ (Skewness = 1.75, Kurtosis = 8.90); and 3) substantially skewed data from the g- and h- distribution, where $g = 1$ and $h = 0$ (Skewness = 6.20, Kurtosis = 114).

Empirical Type I error rates were recorded for all procedures, with familywise error rates reported for the MCPs. In this paper, the robustness of a procedure, with respect to Type I error control, will be determined using Bradley's (1978) liberal criterion. That is, a procedure is deemed robust with respect to Type I errors if the empirical rate of Type I error falls within the range $\pm .5 \alpha$. Power rates were also recorded for all the procedures, with power rates for the MCPs quantified with respect to average per-pair power (where per-pair power is the probability of rejecting a false pairwise null

Table 2. Population Mean Configurations Used in the Simulation Study.

Population Means						
μ_1	μ_2	μ_3	μ_4	μ_5	μ_6	μ_7
J = 4						
0.00	0.00	0.00	0.00			
0.00	0.00	0.00	1.28			
0.00	0.00	0.66	1.32			
0.00	0.00	1.09	1.09			
0.00	0.50	1.00	1.50			
J = 7						
0.00	0.00	0.00	0.00	0.00	0.00	0.00
0.00	0.00	0.00	0.00	0.00	0.00	1.30
0.00	0.00	0.00	0.00	0.00	1.04	1.04
0.00	0.00	0.00	0.51	1.02	1.02	1.02
0.00	0.00	0.62	0.62	0.62	1.24	1.24
0.00	0.23	0.46	0.69	0.92	1.15	1.38

hypothesis) and all-pairs power (the probability of rejecting all false pairwise null hypothesis).

The simulation program was written in SAS/IML (SAS Institute, Inc., 1999). Pseudorandom normal variates were generated with the SAS generator RANNOR. If Z_{ij} is a standard normal deviate, then $X_{ij} = \mu_j + (\sigma_j Z_{ij})$ is a normal variate with mean μ_j and variance σ_j^2 . To generate data from the g- and h-distributions, standard unit normal variables were converted to the random variable:

$$X_{ij} = \left[\frac{\exp(gZ_{ij})}{g} \right] \left[\exp\left(\frac{hZ_{ij}^2}{2}\right) \right].$$

To obtain a distribution with standard deviation σ_j , each X_{ij} was multiplied by a value of σ_j . When $g > 0$ the g- and h- distribution population

mean is not 0 and therefore the population mean was subtracted from X_{ij} before being multiplied by σ_j . When working with trimmed means, the population trimmed mean for the jth group was also subtracted from the variate before multiplying by σ_j . In order to ensure that the null hypothesis associated with the rank-based procedures was true when distribution shapes were nonnormal and variances were unequal, the Nelder and Mead (1965) minimization function was implemented through an S-Plus version of the FORTRAN code in Olsson (1974. See also Olsson & Nelson, 1975).

Distributions were shifted accordingly. Specifically, the S-Plus function 'nelder' was used, which is available in the library of R and S-Plus functions described in Wilcox (2005). Five thousand replications were performed for each condition, using a nominal significance level of .05.

Results

The pattern of Type I error and power results were consistent across sample size inequality, variance inequality, and nonnull mean configurations, and were therefore averaged over these conditions. Further, the pattern of results was similar across sample size conditions and therefore only the results for the largest sample size condition are presented and discussed (except when noted otherwise). For the pairwise MCPs, partial null familywise error rates were controlled within Bradley's limits in all cases where complete null Type I error rates were controlled, and therefore are not reported.

Omnibus Tests

Type I error Control

Type I error rates (%) for $J = 4$ and $J = 7$ are presented in Table 3. When the distribution shapes were normal, Type I error rates were maintained within Bradley's liberal bounds (2.5%-7.5%) by all, but one, procedure for $J = 4$ and $J = 7$; the Kruskal-Wallis procedure was liberal (7.8%) for $J = 4$ when sample sizes and variances were negatively paired. When the distribution shapes were skewed, the Welch and Kruskal-Wallis tests did not always maintain Type I error rates within Bradley's bounds when $J = 4$ and sample sizes and variances were negatively paired. The Welch test in particular became very liberal (e.g., 16.9%), whereas the Kruskal-Wallis test exhibited some inflation (e.g., 7.9%). The remaining procedures were able to maintain Type I error rates within Bradley's bounds under all conditions.

Power

Power rates (%) for $J = 4$ and $J = 7$ are presented in Table 4. When the variances were equal there was very little difference between the procedures, with the exception that the Welch test had reduced power for the $g=1, h=0$ distribution. In general, the power for the Welch test on ranks, the Brunner heteroscedastic nonparametric procedure and the Kruskal-Wallis procedure was slightly larger than that for either of the other Welch statistics. With unequal variances, the usual Welch test and the Welch test with trimmed means had deflated power relative to the remaining procedures for both

nonnormal distributions, although the Brunner heteroscedastic nonparametric procedure had especially low power with negatively paired sample sizes and variances, particularly for $J = 7$. There was very little difference between the power rates of the Kruskal-Wallis and the Welch test on ranks. Caution, however, should be taken in interpreting the power rates of the Welch and Kruskal-Wallis procedures with negatively paired sample sizes and variances given that the Type I error rates were not adequately controlled in some of these conditions.

Pairwise MCPs

The pattern of familywise error and average per-pair power results for the MCPs were consistent across $J = 4$ and $J = 7$ and therefore only results for $J = 7$ are displayed and discussed. The all-pairs power rates for $J = 4$ are displayed and discussed. (The $J = 7$ rates were too low for meaningful comparisons.)

Type I error Control

Complete null familywise error rates (%) for the REGWQ and Tukey pairwise MCPs are presented in Table 5. The REGWQ procedure maintained rates within Bradley's bounds under all conditions, with the exception that the procedure became conservative (i.e., empirical familywise error rates less than 2.5%) when it was used with either the Welch test or the Welch test on trimmed means and the data were $g=1, h=0$ distributed. The Tukey procedure maintained rates within Bradley's limits when applied with Welch's statistic on trimmed means, the Welch on ranks, or the Brunner-Munzel heteroscedastic statistic, although the Type I error rates became liberal when the Tukey procedure was applied with the usual Welch test or the Kruskal-Wallis test when sample sizes and variances were negatively paired.

Power

Average per-pair and all-pairs power rates for the REGWQ and Tukey pairwise MCPs are presented in Tables 6 and 7, respectively. Power rates overall were very low given the strict familywise error control and the inflated variances in the heteroscedastic conditions. There was very little difference in the overall

pattern of results for the Tukey and REGWQ procedures so given that the power was generally slightly larger for the REGWQ procedure (especially all-pairs power) only its' results will be discussed. When the variances were equal, there was very little difference between the procedures in terms of per-pair or all-pairs power across all distributions, although the REGWQ procedure when applied with the

Kruskal-Wallis statistic was generally the most powerful. When variances were unequal, the Welch test with trimmed means had less power than the Welch test on ranks or the Brunner-Munzel procedure across all distributions, with a slight advantage going to the Welch test on ranks (the usual Welch and Kruskal-Wallis procedures are not discussed because, when the variances were not equal, the Type I error rates were not controlled).

Table 3. Type I Error Percentages for $n = 20$ for the Welch test (Welch), the Welch test with trimmed means and Winsorized variances (Welch-t), the Welch test with ranked data (Welch-r), the Kruskal-Wallis nonparametric test (K-W) and the Brunner, Dette and Munk (1997) heteroscedastic nonparametric test (BDM).

	Normal Distribution			g=.5, h=0 Distribution			g=1, h=0 Distribution		
	$= \sigma^2_j$	PP	NP	$= \sigma^2_j$	PP	NP	$= \sigma^2_j$	PP	NP
J = 4									
Welch	5.3	5.1	5.3	5.9	5.7	7.2	6.5	7.4	13.5
Welch-t	5.7	5.5	5.8	5.6	5.3	6.2	4.9	4.9	6.7
Welch-r	5.7	6.4	6.6	5.7	5.9	6.4	5.7	6.0	6.4
K-W	4.8	4.0	7.8	4.8	3.9	7.9	4.8	4.1	7.9
BDM	6.8	7.0	7.0	6.8	7.2	7.1	6.8	7.3	7.2
J = 7									
Welch	5.0	4.9	5.0	6.7	6.5	8.4	9.6	10.0	16.9
Welch-t	6.2	5.7	6.4	6.0	5.8	6.7	6.0	6.1	7.5
Welch-r	5.6	5.7	6.2	5.6	5.8	6.4	5.7	5.8	6.6
K-W	4.3	3.6	7.0	4.3	3.7	7.2	4.3	3.8	7.4
BDM	5.7	5.6	6.5	5.7	5.6	6.5	5.7	6.0	6.6

Note: $= \sigma^2_j$ = equal population variances; PP and NP = positive and negative pairings of sample sizes and variances, respectively. Values exceeding Bradley's liberal limits (2.5% - 7.5%) are presented in bold.

Table 4. Power percentages for $n = 20$ for the Welch test (Welch), the Welch test with trimmed means and Winsorized variances (Welch-t), the Welch test with ranked data (Welch-r), the Kruskal-Wallis nonparametric test (K-W) and the Brunner, Dette and Munk (1997) heteroscedastic nonparametric test (BDM).

	Normal Distribution			g=.5, h=0 Distribution			g=1, h=0 Distribution		
	$= \sigma_j^2$	PP	NP	$= \sigma_j^2$	PP	NP	$= \sigma_j^2$	PP	NP
J = 4									
Welch	98.3	57.8	66.8	93.5	45.4	62.8	69.8	22.0	52.4
Welch-t	95.8	54.2	60.0	94.2	47.8	60.0	88.7	40.3	56.4
Welch-r	98.0	57.5	66.5	97.7	63.0	65.3	96.9	73.4	65.0
K-W	98.2	49.5	65.8	98.2	57.4	64.1	97.4	71.3	63.5
BDM	97.8	60.7	51.3	95.8	63.8	47.1	93.1	70.8	45.3
J = 7									
Welch	98.6	54.4	69.5	95.3	43.3	68.4	75.1	24.9	59.7
Welch-t	96.3	47.7	63.4	95.5	44.9	65.1	91.7	38.9	63.2
Welch-r	98.5	54.5	70.0	98.7	59.6	71.8	98.7	69.5	74.4
K-W	98.6	46.7	66.8	98.9	53.1	68.5	98.9	65.1	70.5
BDM	98.1	54.8	49.4	97.1	56.9	48.0	95.6	63.3	48.1

Note: $= \sigma_j^2$ = equal population variances; PP and NP = positive and negative pairings of sample sizes and variances, respectively. Conditions for which values exceeding Bradley's liberal limits (2.5% - 7.5%) are presented in bold.

Table 5. Type I Error Percentages for $J = 7$ and $n = 20$ for the for the Tukey and REGW MCPs with the Welch test (W), the Welch test with trimmed means and Winsorized variances (WT), the Welch test with ranked data (WR), the Kruskal-Wallis nonparametric test (KW) and the Brunner and Munzel (2000) heteroscedastic nonparametric test (BM).

	Normal Distribution			g=.5, h=0 Distribution			g=1, h=0 Distribution		
	= σ_j^2	PP	NP	= σ_j^2	PP	NP	= σ_j^2	PP	NP
Tukey-W	5.3	5.0	5.0	4.2	4.5	7.2	2.5	4.8	13.4
REGW-W	3.6	3.2	2.6	3.2	2.9	3.3	1.3	1.4	3.6
Tukey-WT	6.2	6.0	6.3	5.1	5.1	6.4	3.0	3.5	6.5
REGW-WT	4.3	3.5	3.3	3.4	3.0	2.9	1.9	1.8	2.1
Tukey-WR	5.9	6.0	6.6	6.0	6.1	6.5	6.0	6.3	6.6
REGW-WR	4.5	4.5	4.2	4.5	4.5	4.3	4.5	4.6	4.5
Tukey-KW	4.5	4.2	8.1	4.5	4.2	8.0	4.5	4.3	8.4
REGW-KW	3.3	3.0	5.6	3.3	3.0	5.7	3.3	3.1	6.0
Tukey-BM	5.7	5.2	5.9	5.7	5.2	6.1	5.7	5.5	6.2
REGW-BM	3.6	3.3	3.2	3.6	3.4	3.2	3.6	3.6	3.4

Note: = σ_j^2 = equal population variances; PP and NP = positive and negative pairings of sample sizes and variances, respectively. Values exceeding Bradley's liberal limits (2.5% - 7.5%) are presented in bold.

Table 6. Per-Pair Power Percentages for $J = 7$ and $n = 20$ for the Tukey and REGW MCPs with the Welch test (W), the Welch test with trimmed means and Winsorized variances (WT), the Welch test with ranked data (WR), the Kruskal-Wallis nonparametric test (KW), and the Brunner and Munzel (2000) heteroscedastic nonparametric test (BM).

	Normal Distribution			g=.5, h=0 Distribution			g=1, h=0 Distribution		
	= σ_j^2	PP	NP	= σ_j^2	PP	NP	= σ_j^2	PP	NP
Tukey-W	44.3	10.4	14.3	34.5	6.2	14.7	17.0	1.6	11.6
REGW-W	45.8	10.4	9.7	34.7	5.8	10.1	13.2	1.1	5.7
Tukey-WT	37.1	8.5	12.1	35.1	7.1	13.5	29.7	4.9	13.4
REGW-WT	36.4	7.8	7.4	34.5	6.4	8.8	31.9	4.0	7.9
Tukey-WR	44.1	10.0	16.8	44.8	11.5	16.3	43.8	14.8	16.2
REGW-WR	46.5	10.5	14.8	46.8	12.0	14.2	45.6	15.5	14.0
Tukey-KW	46.6	8.5	17.0	47.7	10.0	16.7	46.8	13.9	16.7
REGW-KW	50.9	9.1	18.3	52.4	10.7	18.0	51.7	15.1	18.0
Tukey-BM	43.7	9.1	13.9	40.2	10.4	12.2	35.4	12.9	11.3
REGW-BM	44.8	9.1	8.8	39.5	9.8	7.4	33.5	11.9	6.7

Note: = σ_j^2 = equal population variances; PP and NP = positive and negative pairings of sample sizes and variances, respectively. Conditions for which values exceeding Bradley's liberal limits (2.5% - 7.5%) are presented in bold .

Table 7. All-Pairs Power Percentages for $J = 4$ and $n = 20$ for the Tukey and REGW MCPs with the Welch test (W), the Welch test with trimmed means and Winsorized variances (WT), the Welch test with ranked data (WR), the Kruskal-Wallis nonparametric test (KW), and the Brunner and Munzel (2000) heteroscedastic nonparametric test (BM).

	Normal Distribution			g=.5, h=0 Distribution			g=1, h=0 Distribution		
	= σ_j^2	PP	NP	= σ_j^2	PP	NP	= σ_j^2	PP	NP
Tukey-W	28.8	4.2	2.3	17.2	1.6	2.1	4.3	0.2	1.2
REGW-W	36.0	7.4	4.6	23.8	3.2	3.7	7.1	0.4	2.1
Tukey-WT	22.4	3.1	1.5	18.4	2.0	1.7	12.6	1.0	1.5
REGW-WT	29.9	5.5	3.1	25.3	3.9	3.2	18.0	2.2	2.7
Tukey-WR	27.9	3.3	3.8	26.7	3.7	3.1	23.8	5.5	2.7
REGW-WR	35.1	6.1	6.5	33.7	6.8	5.6	30.9	9.5	5.1
Tukey-KW	31.4	3.1	6.0	31.2	3.8	5.1	28.3	6.1	4.6
REGW-KW	38.4	5.7	9.7	38.2	6.8	8.5	35.7	10.4	7.9
Tukey-BM	26.8	3.2	1.8	21.6	3.0	1.1	15.8	3.7	0.8
REGW-BM	33.5	5.6	3.4	28.5	5.5	2.3	22.7	6.7	1.8

Note: = σ_j^2 = equal population variances; PP and NP = positive and negative pairings of sample sizes and variances, respectively. Conditions for which values exceeding Bradley's liberal limits (2.5% - 7.5%) are presented in bold.

Conclusion

This article addressed the problem of testing for differences in the central tendency of independent groups with nonnormal (skewed) data and heterogeneous variances. This is an especially important issue for researchers in the behavioral sciences because these assumptions are rarely satisfied (e.g., Micceri, 1989; Keselman et al., 1998; Wilcox, 1988).

Of the omnibus tests evaluated in this paper, the Welch (1951) test with trimmed means and Winsorized variances, the Welch (1951) test on ranked data (Zimmerman & Zumbo, 1993a), and the Brunner heteroscedastic rank-based procedures (Brunner, Dette & Munk, 1997; Brunner & Munzel, 2000) provided superior Type I error control relative to the remaining procedures. The Type I error rates of the omnibus Welch test became liberal when distributions were skewed, and the Kruskal-Wallis test had liberal Type I error rates when variances were unequal (specifically when sample sizes and variances were negatively paired). These results concerning the liberal Type I error control of the Welch test with skewed and heteroscedastic data, and the Kruskal-Wallis procedure with unequal variances are consistent with previous reports (e.g., Algina, Oshima & Lin, 1994; Zimmerman & Zumbo, 1993a, 199b). With respect to power, there was very little difference between the procedures when the distributions were normal, although the power rates of the Welch test on ranks, the Brunner heteroscedastic nonparametric procedure, and the Kruskal-Wallis procedure were generally the largest.

These tests were also contrasted when they were applied to the set of all possible pairwise comparisons. In this case, the REGWQ MCP was able to maintain Type I error rates below Bradley's upper liberal bound (7.5%) with all of the tests investigated. The test statistics with a Tukey critical value also maintained their empirical Type I error rates below Bradley's upper liberal bound under most conditions; however, the Kruskal-Wallis statistic became slightly liberal when sample sizes and variances were negatively paired. These results are not unexpected given that the omnibus Kruskal-Wallis procedure also became liberal

under these conditions. Adopting an REGWQ critical value generally resulted in more powerful tests than adopting a Tukey critical value, especially with respect to all-pairs power. Further, when the distributions were nonnormal, adopting an REGWQ critical value resulted in the largest power when used with one of the ranked data procedures (Welch on ranks, Kruskal-Wallis, or the Brunner & Munzel heteroscedastic nonparametric procedure).

In summary, when treatment distributions were skewed and variances heterogeneous, both the Welch (1938; 1951) tests with ranked data and the heteroscedastic, nonparametric procedures proposed by Brunner and colleagues (Brunner, Dette & Munk, 1997; Brunner & Munzel, 2000) provided good Type I error control (in both omnibus and pairwise multiple comparison settings). However, the Welch tests on ranked data are recommended as they were generally more powerful than the Brunner procedures. Further, the Welch tests on ranked data can easily be implemented in any software program that allows the user to rank the observations and run the Welch heteroscedastic procedures (e.g., SAS, SPSS, R).

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The Effects of Heteroscedasticity on Tests of Equivalence

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Tests of equivalence, which are designed to assess the similarity of group means, are becoming more popular, yet very little is known about the statistical properties of these tests. Monte Carlo methods are used to compare the test of equivalence proposed by Schuirmann with modified tests of equivalence that incorporate a heteroscedastic error term. It was found that the latter were more accurate than the Schuirmann test in detecting equivalence when sample sizes and variances were unequal.

Key words: Null hypothesis testing, heteroscedasticity, tests of equivalence.

Introduction

Over a half century ago, Hotelling, Bartky, Deming, Friedman & Hoel (1948) wrote that “Unfortunately, too many people like to do their statistical work as they say their prayers – merely substitute in a formula found in a highly respected book written a long time ago” (p. 103). This quote, which can be found cited in *The Task Force on Statistical Inference in Psychology*’s report outlining recommendations for the effective use of statistics (Wilkinson, 1999), underscores the fact that many researchers apply statistical methods thoughtlessly, without considering the methods’ appropriateness to the research questions under consideration.

Many empirical questions in behavioral research involve testing the null hypothesis of no difference between groups on a specific dependent variable. In fact, formulating research

questions involving two groups as tests of this null hypothesis is almost a conditioned reflex among scholars, even though such an hypothesis is frequently irrelevant to the research question (Westlake, 1976). Testing the null hypothesis of no difference is inappropriate for studies in which the primary objective is to demonstrate that two groups are equivalent, rather than different, on a particular measure. More specifically, when the research question deals with the equivalence of groups on a dependent measure, an equivalence test is the appropriate (and necessary) statistical method to be used. The present article will highlight the importance of equivalence tests in behavioral research and use a Monte Carlo study to compare tests of equivalence when the variances of the groups are not equal.

Researchers frequently conduct studies in which assessing the equivalence of two groups is the main purpose. For example, consider an investigation of two therapies for dealing with perfectionism. One therapy is lengthy and expensive; the other short and inexpensive. The pertinent research question may be to determine whether the therapies are equivalent in terms of their effectiveness. If they are equivalent, then the shorter, less expensive method can be implemented with considerable cost and time savings. Traditional statistical procedures such as t-tests and ANOVAs are ill-suited to answering these questions because they focus, conceptually and statistically, on assessing group differences. For research

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questions pertaining to the equivalence of conditions, researchers require a statistical technique designed specifically to test the degree to which different conditions produce similar results. Tests of equivalence serve this purpose.

When employing tests of equivalence the goal is not to show that treatment conditions are perfectly identical, but only that the differences between the treatments are too small to be considered meaningful. Consider, for example, an investigation in which an attempt is made to demonstrate that scores on a computer-based test are equivalent to those from a paper and pencil based test (e.g., Epstein, Klinkenberg, Wiley & McKinley, 2001). In this example, the researchers may not need to show that the test scores are exactly equivalent (as with the traditional null hypothesis $H_0: \mu_1 = \mu_2$, but only that differences in test scores are inconsequential (i.e., $|\mu_1 - \mu_2| < D$, where D represents an a priori critical difference for determining equivalence).

A specific example may elucidate this issue more clearly. Alkhader, Clarke & Anderson (1998) conducted an investigation designed to assess the equivalence of the paper-and-pencil version and a computer adaptive version of three subtests from the Differential Aptitude Tests (DAT), namely numerical ability (NA), abstract reasoning (AR) and mechanical reasoning (MR). It is noteworthy that the title of their article specifically underscores the equivalence of these subtests and that in their introduction they highlight that "their equivalence must be established empirically" (p.206). However, as a means of demonstrating the equivalence of the measures, Alkhader et al. proceeded to conduct ANOVAs, which are expressly designed to detect statistically significant group differences. Based on their analyses they claimed to have demonstrated the equivalence of two of the three subtests (AR and MR). However, what Alkhader et al. in fact demonstrated was merely that scores on the NA subtest on the computer adapted version of the DAT were statistically significantly different from the paper and pencil method as traditionally defined.

The question of the equivalence of the different administration methods on subtest scores remains a mystery. As Cribbie, Gruman & Arpin-Cribbie (2004) and Rogers, Howard &

Vessey (1993) note, the rejection or nonrejection of the null hypothesis of traditional tests tells us very little about the potential equivalence of the groups in question. Effectively establishing whether the computer adapted version of the DAT produced subtest scores that were equivalent to the paper and pencil version would have required the use of a statistical technique that could assess the degree to which these measures produced similar results. This can be accomplished through the use of equivalence testing, the purpose of which is to demonstrate that two (or more) conditions are functionally the same (Stegner, Bostrom & Greenfield, 1996).

This approach to statistical analysis has been popular for many years in biology, where researchers interested in the interchangeability of genetically equivalent drugs have used the technique to determine drugs' comparative bioavailability, or bioequivalence (Westlake, 1976). However, researchers outside of biology have been slow to recognize the utility of this procedure and continue to use inappropriate statistics when conducting studies that consider the similarity of alternative conditions, tests, treatments, or procedures.

One of the more commonly discussed tests of equivalence was developed by Schuirmann (1987). Schuirmann's test of equivalence has been introduced to the behavioral sciences through influential articles by Rogers et al. (1993), Seaman & Serlin (1998) and others. The first step in applying Schuirmann's test of equivalence is to establish a critical mean difference for declaring two population means equivalent (D). Any mean difference smaller than D would be considered meaningless within the framework of the experiment. The selection of an equivalency interval (D) is an important aspect of equivalence testing that is primarily dependent on a subjective level of confidence with which to declare two (or more) populations equivalent. This level of confidence can take on many different forms including a raw value (e.g., mean test scores different by 10 points), a percentage difference (e.g., $\pm 10\%$), a percentage of the pooled standard deviation difference, etc.

Researchers debating an appropriate value of D should consider the nature of the

research. For example, if the paper-and-pencil test discussed above was ten times more expensive to administer than the computer-based test, even a very significant difference in outcomes (e.g., +20%) might be acceptable for concluding that the tests are equivalent; Whereas if the paper-and-pencil test was only twice as expensive to administer as the computer based test a difference in outcomes of no more than 5% might be required for concluding that the tests are equivalent. For a further discussion on establishing D readers are referred to Greene, Concato & Feinstein (2000).

When using this procedure it is assumed that the two samples are randomly and independently selected from normally distributed populations with equal variances. Two one-sided hypothesis tests can be used to establish equivalence, where the null hypothesis relates to the nonequivalence of the population means and can be expressed as two separate composite hypotheses:

$$H_{01} : \mu_1 - \mu_2 \geq D; H_{02} : \mu_1 - \mu_2 \leq -D.$$

Rejection of H_{01} implies that $\mu_1 - \mu_2 < D$, and rejection of H_{02} implies that $\mu_1 - \mu_2 > -D$. Further, rejection of both hypotheses implies that $\mu_1 - \mu_2$ falls within the bounds of $(-D, D)$ and the means are deemed equivalent.

H_{01} is rejected if $t_1 \leq -t_{\alpha}^{\alpha}$ where:

$$t_1 = \frac{(\bar{X}_1 - \bar{X}_2) - D}{\sqrt{\frac{(n_1 + n_2)[(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2]}{n_1 n_2 (n_1 + n_2 - 2)}}}$$

and H_{02} is rejected if $t_2 \geq t_{\alpha, df}$ where:

$$t_2 = \frac{(\bar{X}_1 - \bar{X}_2) - (-D)}{\sqrt{\frac{(n_1 + n_2)[(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2]}{n_1 n_2 (n_1 + n_2 - 2)}}}.$$

$\bar{x}_1$ and $\bar{x}_2$ are the group means, n_1 and n_2 are the group sample sizes, s_1 and s_2 are the group standard deviations and $t_{\alpha, df}$ is the upper-tailed α -level t critical value with $df = n_1 + n_2 - 2$ degrees of freedom.

One concern with the adoption of Schuirmann's test of equivalence is the potential effects of variance heterogeneity on the standard error of the statistic. This is an important consideration given that unequal variances (heteroscedasticity) appear to be the norm, rather than the exception in behavioral research (Keselman et al., 1998; Grissom, 2000). Keselman et al. have noted that researchers often report largest to smallest variance ratios as large as four to one, and largest to smallest variance ratios as large as eight to one are not uncommon. The standard error used with the Schuirmann test is identical to that used in the two independent samples t-test, and problems with this error term have a long history, termed the Behrens-Fisher problem (see, e.g., Scheffe, 1970).

One potential option is to use the heteroscedastic solution developed by Welch (1938) and Satterthwaite (1946). This idea was originally presented by Dannenberg, Dette & Munk (1994), although the procedure has received little attention given that in biopharmaceutical equivalence trials independent groups designs (where these methods would be appropriate) are rare relative to crossover designs (see Hauschke, Steinijans & Hothorn, 1996). However, independent groups designs are extremely common in behavioural research areas such as education, psychology, and management. Combining the numerator of Schuirmann's test with the error term of Welch's (1938) heteroscedastic test may provide an equivalence test that is robust to sample size and variance heterogeneity. For the Schuirmann-Welch test of equivalence H_{01} is rejected if $t_{w1} \leq -t_{\alpha, dfw}$ and H_{02} is rejected if $t_{w2} \geq t_{\alpha, dfw}$ where :

$$t_{w1} = \frac{(\bar{X}_1 - \bar{X}_2) - D}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}},$$

$$t_{w2} = \frac{(\bar{X}_1 - \bar{X}_2) - (-D)}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}},$$

and

$$df_w = \frac{\left(\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2} \right)^2}{\frac{s_1^4}{n_1^2(n_1-1)} + \frac{s_2^4}{n_2^2(n_2-1)}}.$$

Recently, Tryon (2001) proposed a novel approach to equivalence testing that uses inferential confidence intervals to make decisions regarding the equivalence of two groups. Specifically, with Tryon's equivalence test two groups are declared equivalent if $Rg \leq D$, where:

$$Rg = \frac{\left| \left[\bar{X}_1 - (t_{1-\alpha})(E)(s_{x_1}^-) \right] \right|}{\left| \left[\bar{X}_2 + (t_{1-\alpha})(E)(s_{x_2}^-) \right] \right|}$$

and

$$E = \frac{\sqrt{s_{x_1}^2 + s_{x_2}^2}}{s_{x_1}^- + s_{x_2}^-}.$$

$s_{\bar{x}}$ represents the usual standard error of the mean (i.e., $s_x / \sqrt{n}$) and $t_{1-\alpha}$ represents the (positive) two-tailed critical t value with $df = n-1$. A heteroscedastic version of the Tryon test is available by substituting the original degrees of freedom ($df = n-1$) by the Welch-Satterthwaite df divided by two (i.e., $df_w / 2$).

Methodology

Monte Carlo Study

A simulation study was used to compare the probability of detecting equivalence by: 1) Student t; 2) Welch t; 3) Schuirmann's equivalence test; 4) Schuirmann-Welch equivalence test; 5) Tryon equivalence test; and 6) Tryon-Welch equivalence test. Several variables were manipulated in this study including: a) sample size; b) population variances; and c) population mean configuration. Total sample sizes were set at $N = 20$ and $N = 60$. Sample sizes for $N = 20$ were: 1) $n_1=10$, $n_2=10$; 2) $n_1=8$, $n_2=12$; and 3) $n_1=5$, $n_2=15$. Sample sizes for $N = 60$ were: 1) $n_1=30$, $n_2=30$; 2) $n_1=25$, $n_2=35$; and 3) $n_1=20$, $n_2=40$.

Population variances were set at: 1) 1, 1; 2) .5, 1.5; 3) 1.5, .5; 4) .2, 1.8; and 5) 1.8, .2. These conditions were crossed resulting in: 1) equal n or σ^2 ; 2) positively paired n and σ^2 (largest n with largest σ^2 , smallest n with smallest σ^2); and 3) negatively paired n and σ^2 (largest n with smallest σ^2 , smallest n with largest σ^2).

Six mean configurations were evaluated in this study, including equivalent population means ($\mu_1 = \mu_2$) and five nonequivalent population means ($\mu_2 = \mu_1 + .4$, $\mu_2 = \mu_1 + .8$, $\mu_2 = \mu_1 + 1$, $\mu_2 = \mu_1 + 1.2$ and $\mu_2 = \mu_1 + 1.6$). The critical mean difference for establishing population equivalence (D) was maintained at 1 throughout all conditions. Given that D is set at 1, the equivalent mean configuration and nonequivalent configurations with $\mu_2 - \mu_1 < 1$ fall under the alternate hypothesis of the Schuirmann and Tryon tests of equivalence (i.e., the population mean difference does not exceed the critical mean difference and thus the means are expected to be declared equivalent), and nonnull configurations with $\mu_2 - \mu_1 > 1$ fall under the null hypothesis of the Schuirmann and Tryon tests of equivalence (i.e., the population mean difference exceeds the critical mean difference and thus the means are expected to be declared nonequivalent). For the case where $\mu_2 - \mu_1 = 1 = D$, the expected probability of declaring the two populations equivalent is α .

Five thousand simulations were conducted for each condition using a nominal significance level of $\alpha = 0.05$.

Results

The probability of declaring the two independent populations equivalent for $N = 20$ and $N = 60$ are presented in Tables 1 and 2, respectively.

$$\mu_2 - \mu_1 = 1 = D$$

The Schuirmann-Welch maintained rejection (i.e., rejecting H_{01} and H_{02}) rates at approximately α (.039-.048) for $N = 20$ and exactly at α for $N = 60$ when $\mu_2 - \mu_1 = 1$ [recall that $D=1$ so $E(t_{w1}) = 0$], regardless of the pattern of sample sizes and variances. However, the Schuirmann test had rejection rates ranging from .019 to .092 under positively and negatively

Table 1. Probability of declaring the two populations equivalent for $N = 20$ under each of the testing conditions.

Pairing	$\mu_2 - \mu_1$	t	t-w	sch	sch-w	try	try-w
Equal n or σ	0	.948	.949	.352	.340	.289	.261
	.4	.867	.873	.251	.243	.217	.195
	.8	.621	.641	.094	.091	.091	.081
	1	.462	.487	.045	.044	.048	.043
	1.2	.309	.338	.018	.018	.022	.020
	1.6	.099	.123	.002	.002	.003	.003
Positive	0	.980	.951	.212	.454	.318	.299
	.4	.932	.858	.145	.318	.228	.213
	.8	.749	.582	.047	.107	.085	.079
	1	.600	.406	.019	.048	.040	.037
	1.2	.437	.252	.007	.018	.016	.015
	1.6	.166	.065	.001	.001	.002	.001
Negative	0	.865	.947	.403	.189	.218	.161
	.4	.773	.894	.317	.146	.175	.130
	.8	.536	.738	.156	.067	.092	.067
	1	.399	.632	.092	.039	.057	.041
	1.2	.273	.516	.051	.019	.033	.023
	1.6	.096	.300	.011	.004	.008	.006

Note. t = independent samples t; t-w = Welch t; sch = Schuirmann test of equivalence; sch-w = Schuirmann-Welch test of equivalence; try = Tyron test of equivalence; try-w = Tyron-Welch test of equivalence.

paired sample sizes and variances respectively, for $N = 20$, and rates ranging from .028 to .084 under positively and negatively paired sample sizes and variances respectively, for $N = 60$. Both the Tryon and Tryon-Welch equivalence tests had reasonably accurate rejection rates for

$\mu_2 - \mu_1 = 1$ when $N = 20$, although rates were consistently mildly deflated under the unequal sample size and variance conditions when $N = 60$ (.032 - .036).

Rejection rates for the two independent samples t and Welch t for $\mu_2 - \mu_1 = 1$ reflect the power of these tests for detecting a true difference in means (see Table 1).

Table 2. Probability of declaring the two populations equivalent for $N = 60$ under each of the testing conditions.

Pairing	$\mu_2 - \mu_1$	t	t-w	sch	sch-w	try	try-w
Equal n or σ	0	.949	.950	.965	.964	.924	.918
	.4	.676	.680	.732	.729	.657	.650
	.8	.149	.153	.186	.185	.161	.157
	1	.037	.038	.050	.050	.044	.043
	1.2	.006	.006	.009	.009	.008	.008
	1.6	.000	.000	.000	.000	.000	.000
Positive 0		.975	.949	.961	.983	.944	.943
	.4	.757	.639	.682	.781	.671	.668
	.8	.189	.107	.131	.200	.144	.143
	1	.048	.021	.028	.050	.035	.035
	1.2	.007	.002	.003	.007	.005	.005
	1.6	.000	.000	.000	.000	.000	.000
Negative	0	.900	.950	.958	.913	.758	.725
	.4	.612	.732	.747	.647	.495	.466
	.8	.141	.239	.241	.165	.116	.106
	1	.041	.087	.084	.050	.036	.032
	1.2	.008	.023	.020	.010	.007	.007
	1.6	.000	.001	.000	.000	.000	.000

Note. t = independent samples t; wel-t = Welch t; sch = Schuirmann test of equivalence; sch-w = Schuirmann-Welch test of equivalence; try = Tyron test of equivalence; try-w = Tyron-Welch test of equivalence.

A Priori Equivalence ($\mu_2 - \mu_1 < D$)

When a priori population mean differences were less than the critical mean difference ($D = 1$), and either the sample sizes or variances were equal, the probability of declaring the two populations equivalent was almost identical for the Schuirmann, Schuirmann-Welch, Tyron and Tyron-Welch test statistics. The rates for the equivalence tests were significantly less than the rates for the Student t and Welch t when the total sample size was small ($N = 20$), although the rates were larger than those for the Student t and Welch t when the total sample size was large ($N = 60$).

The probability of declaring the two populations equivalent was greater for the Schuirmann-Welch test than the Schuirmann test when the sample sizes and variances were positively paired, whereas the probability of declaring the two populations equivalent was greater for the Schuirmann test than the Schuirmann-Welch test when the sample sizes and variances were negatively paired. This is due to the known bias in the non-heteroscedastic standard error, which becomes inflated when sample sizes and variances are positively paired and deflated when sample sizes and variances are negatively paired.

This bias can also be seen in the results for the traditional tests as the probability of declaring the two populations equivalent (i.e., a statistically non significant effect) was greater for the Student *t* than the Welch when the sample sizes and variances were positively paired, and the probability of declaring the two populations equivalent was greater for the Welch than the Student *t* when sample sizes and variances were negatively paired. The rates for the Tryon and Tryon-Welch tests were very similar across all conditions (primarily because the original Tryon test does not use the pooled standard error like the Schuirmann test) but consistently less than those of the Schuirmann-Welch test.

A Priori Nonequivalence ($\mu_2 - \mu_1 > D$)

When a priori population mean differences were greater than the critical difference ($D = 1$), and either the sample sizes or variances were equal, the probability of declaring the two populations equivalent was identical (and very low) for the Schuirmann and Schuirmann-Welch test statistics under all conditions and demonstrates an excellent ability to detect differences greater than D . This is due to the fact that the numerators of t_1 and t_{w1} have an expected positive value, whereas a rejection would only occur if t_1 and t_{w1} are LESS THAN $-t_{\alpha, df}$.

One way to think of this effect would be to relate it to traditional null hypothesis testing when testing a one-tailed alternative hypothesis (i.e., $H_1: \mu_1 - \mu_2 > 0$). We expect the Type I error rates to be approximately α when $\mu_1 - \mu_2 = 0$, but when $\mu_1 - \mu_2 < 0$ (i.e., an effect in the wrong direction) the Type I error rates will approach zero. The rates for the Schuirmann and Schuirmann-Welch tests were significantly less than the rates for the Student *t* and Welch *t* when the total sample size was small ($N = 20$), reflecting the fact that the Student *t* and Welch *t* have less power when $N = 20$, although the rates were very similar for all tests when the total sample size was large ($N = 60$). Similar to the results for a priori equivalence, the probability of declaring the two populations equivalent was greater for the Schuirmann-Welch test than the Schuirmann test when the sample sizes and variances were positively paired, whereas the

probability of declaring the two populations equivalent was greater for the Schuirmann test than the Schuirmann-Welch test when the sample sizes and variances were negatively paired. The rates for the Tryon and Tryon-Welch tests were very similar across all conditions, and were also very similar to rates for the Schuirmann-Welch procedure.

Conclusion

Behavioral researchers reliably use traditional statistical procedures such as Student's *t*-test when comparing groups even when the primary objective is to demonstrate that groups are equivalent, rather than different, on a particular measure. The present article highlights the need for tests of equivalence and compared alternatives to the original Schuirmann (1987) and Tryon (2001) tests of equivalence for situations in which treatment group variances are unequal. The Schuirmann-Welch test incorporated a heteroscedastic error term and error degrees of freedom, while the Tryon-Welch test incorporated heteroscedastic degrees of freedom. It was expected that these modifications would improve the performance of the test statistics when sample sizes and variances were unequal. The results of this study support the hypothesis that equivalence rates for the Schuirmann-Welch were more accurate than for the Schuirmann test, correcting for a bias in the standard error of the Schuirmann test that dates back to Fisher and Behrens in the 1930s. Equivalence rates were also more accurate (and more powerful) for the Schuirmann test than for either of the Tryon or Tryon-Welch statistics.

The results also highlight the fact that traditional test statistics such as the Student *t* and Welch *t* are not appropriate for testing research hypotheses that relate to the equivalence of two populations. The traditional null hypothesis testing procedures have an extreme bias towards declaring equivalence when sample sizes are small (i.e., a lack of power for detecting small treatment group differences), and are less likely to be able to detect equivalence relative to the Schuirmann or Schuirmann-Welch tests when sample sizes become large.

Tests of equivalence are popular in biopharmaceutical studies for demonstrating that

the effects of two drugs are practically equivalent. It is expected that as the number of studies outlining the methodologies of equivalence tests grow, the popularity of tests of equivalence will increase in behavioral fields such as education, psychology, and management. Thus, methodologists should provide recommendations for applying these tests. The findings of this study emphasize the need for robust tests of equivalence (such as the Schuirmann-Welch test investigated in this paper) for situations in which data conditions are not optimal. Empirical data rarely meet all of the underlying assumptions of test statistics (Keselman et al., 1998; Micceri, 1989; Welch, 1988), and instead one should be cognizant of assumption violations and apply appropriate test statistics that minimize the likelihood that incorrect inferences are drawn regarding the results.

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Approximate Bayesian Confidence Intervals for the Mean of an Exponential Distribution Versus Fisher Matrix Bounds Models

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The aim of this article is to obtain and compare confidence intervals for the mean of an exponential distribution. Considering respectively the square error and the Higgins-Tsokos loss functions, approximate Bayesian confidence intervals for parameters of exponential population are derived. Using exponential data, the obtained approximate Bayesian confidence intervals will then be compared to the ones obtained with Fisher Matrix bounds method. It is shown that the proposed approximate Bayesian approach relies only on the observations. The Fisher Matrix bounds method, that uses the z-table, does not always yield the best confidence intervals, and the proposed approach often performs better.

Key words: Estimation, loss functions, Monte Carlo simulation, statistical analysis.

Introduction

There is a significant amount of research in Bayesian analysis and modeling which has been published the last thirty-five years Harris B. 1976, Higgins J. J. Tsokos 1976, Shafer R. E. 1973. A Bayesian analysis implies the exploitation of suitable prior information and the choice of a loss function in association with Bayes' Theorem. It rests on the notion that a parameter within a model is not merely an unknown quantity, but rather behaves as a random variable, which follows some distribution. In the area of life testing, it is indeed realistic to assume that a life parameter is stochastically dynamic. This assertion is supported by the fact that the complexity of electronic and structural systems is likely to

cause undetected component interactions resulting in an unpredictable fluctuation of the life parameter. Drake (1966) provided an account for the use of Bayesian statistics in reliability problems. He stated,

He [a Bayesian] realizes... that his selection of a prior (distribution) to express his present state of knowledge will necessarily be somewhat arbitrary. But he greatly appreciates this opportunity to make his entire assumptive structure clear to the world... Why should an engineer not use his engineering judgment and prior knowledge about a parameter in the classical distribution he has picked? For example, if it is the mean time between failures (MTBF) of an exponential distribution that must be evaluated from some tests, he undoubtedly has some idea of what the value will turn out to be". (315-320)

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Consider the exponential underlying model characterized by

$$f(x) = \theta e^{-\theta x}; x \geq 0, \theta > 0 \quad (1)$$

It is well known that once the underlying model is found to have an exponential distribution,

Fisher Matrix bounds method (Nelson, 1982) uses the Z-table and considers the following confidence interval [] for θ .

$$L_{\theta} = \frac{\Lambda}{e^{\frac{K_{\alpha} \sqrt{\text{Var}(\hat{\theta})}}{\hat{\theta}}}}$$

and

$$U_{\theta} = \hat{\theta} e^{\frac{K_{\alpha} \sqrt{\text{Var}(\hat{\theta})}}{\hat{\theta}}}, \quad (2)$$

where K_{α} is defined by

$$\alpha = \frac{1}{\sqrt{2\pi}} \int_{K_{\alpha}}^{\infty} e^{-\frac{t^2}{2}} dt = 1 - \Phi(K_{\alpha})$$

and

$$\text{Var}(\hat{\theta}) = \left(\frac{\partial^2 \Lambda}{\partial \theta^2} \right)^{-1}$$

Λ is the log-likelihood function of the exponential distribution (1).

Fisher Matrix bounds method considers large samples to ensure the use of the Z-table.. With some studies that have been conducted with small samples it has been found that the assumption of normal approximations for estimates based on small sample sizes reduces the accuracy of confidence bounds (Hartley, 2004).

For the above model (1), approximate Bayesian confidence bounds for the parameter

θ and the population mean $\frac{1}{\theta}$ will be derived to challenge Fisher bounds method (2).

Although there is no specific analytical procedure that allows us to identify the appropriate loss function to be used, the most commonly used is the square error loss function. One of the reasons for selecting this loss function is because of its analytical tractability in Bayesian analysis. As it will be shown, selecting the square error loss does not always

lead to the best approximate Bayesian confidence intervals. However, the obtained approximate Bayesian confidence intervals corresponding to the square error and the Higgins-Tsokos loss functions will be respectively used to challenge Fisher bounds method (2). The loss functions that will be used are given below, along with a statement of their key characteristics.

Square Error Loss Function

The popular square error loss function places a small weight on estimates near the true value and proportionately more weight on extreme deviation from the true value of the parameter. Its popularity is due to its analytical tractability in Bayesian modeling. The square error loss is defined as follows:

$$L_{SE}(\hat{\theta}, \theta) = \left(\hat{\theta} - \theta \right)^2 \quad (3)$$

Higgins-Tsokos Loss Function:

The Higgins-Tsokos loss function places a heavy penalty on extreme over- or underestimation. That is, it places an exponential weight on extreme errors. The Higgins-Tsokos loss function is defined as follows:

$$L_{HT}(\hat{\theta}, \theta) = \frac{f_1 e^{f_2(\hat{\theta}-\theta)} + f_2 e^{-f_1(\hat{\theta}-\theta)}}{f_1 + f_2} - 1, f_1, f_2 > 0. \quad (4)$$

Assume that θ behaves as a random variable that is being characterized by the Pareto probability density function given by

$$f_1(\theta) = \frac{a}{b} \left(\frac{b}{\theta} \right)^{a+1}; \theta \geq b > 0, a > 0. \quad (5)$$

The Pareto prior has been selected because of its mathematical tractability. Using observations from exponential distributions, the Pareto will approximate prior (5) in such a way that good approximate Bayesian estimates of θ are obtained.

Preliminaries

Let $x_1, x_2, \dots, x_n$ denote the observations of a given system that are being characterized by the exponential distribution (1). The following posterior distribution is obtained:

$$h(\theta | x) = \frac{\theta^{n-a-1} e^{-\theta \sum_{i=1}^n x_i}}{\int_b^{\infty} \theta^{n-a-1} e^{-\theta \sum_{i=1}^n x_i} d\theta}, \theta > b. \quad (6)$$

Methodology

Approximate confidence bounds for θ

With respectively the following approximate priors for the square error and the Higgins-Tsokos loss functions, good approximate Bayesian estimates of θ are obtained.

Approximate prior for the square error loss:

$$f_1(\theta) = \frac{a_0}{b_0} \left(\frac{b_0}{\theta} \right)^{a_0+1}; \theta \geq b_0 > 0, a_0 > 0. \quad (7)$$

$$a_0 = n, b_0 = \frac{n-1}{\sum_{i=1}^n x_i}$$

Approximate prior for the Higgins-Tsokos loss:

$$f_1(\theta) = \frac{a_1}{b_1} \left(\frac{b_1}{\theta} \right)^{a_1+1}; \theta \geq b_1 > 0, a_1 > 0. \quad (8)$$

$$a_1 = n, b_1 = \frac{n}{\sum_{i=1}^n x_i} - \frac{1}{f_1 + f_2} \ln \left(\frac{\sum_{i=1}^n x_i + f_2}{\sum_{i=1}^n x_i - f_1} \right)$$

with

$$f_1 < \sum_{i=1}^n x_i.$$

It's easily shown that the approximate Bayesian estimate of the parameter θ , subject to the square error loss; is the same as the Bayesian estimate of θ under the Higgins-Tsokos loss. They are equal to

$$\frac{n}{\sum_{i=1}^n x_i}.$$

Using respectively the approximate posterior distributions that correspond to (7) and (8), along with the equalities $P(\theta > L | x) = 1 - \alpha/2$ and $P(\theta > U | x) = \alpha/2$, the following lower and upper confidence bounds for θ are obtained:

Approximate Bayesian confidence bounds of θ corresponding to the square error:

$$L_{\theta(SE)} = \frac{n-1-\ln(1-\alpha/2)}{\sum_{i=1}^n x_i}$$

and

$$U_{\theta(SE)} = \frac{n-1-\ln(\alpha/2)}{\sum_{i=1}^n x_i} \quad (9)$$

Approximate Bayesian confidence bounds of θ corresponding to the Higgins-Tsokos:

$$L_{\theta(HT)} = \frac{n - \ln(1-\alpha/2)}{\sum_{i=1}^n x_i} - \frac{1}{f_1 + f_2} \ln \left(\frac{\sum_{i=1}^n x_i + f_2}{\sum_{i=1}^n x_i - f_1} \right)$$

$$U_{\theta(HT)} = \frac{n - \ln(\alpha/2)}{\sum_{i=1}^n x_i} - \frac{1}{f_1 + f_2} \ln \left(\frac{\sum_{i=1}^n x_i + f_2}{\sum_{i=1}^n x_i - f_1} \right)$$

Approximate Bayesian confidence bounds for the exponential population mean

Thus, we respectively obtain the following $100(1-\alpha)\%$ empirical Bayes confidence bounds for the mean b of the exponential failure model, when the squared error and the Higgins-Tsokos loss functions are considered:

$$L_{b(SE)} = \frac{\sum_{i=1}^n x_i}{n-1-\ln(\alpha/2)}$$

and

$$U_{b(SE)} = \frac{\sum_{i=1}^n x_i}{n-1-\ln(1-\alpha/2)}, \quad (10)$$

and

$$L_{b(HT)} = \frac{1}{\frac{n-Ln(\alpha/2)}{\sum_{i=1}^n x_i} - \frac{1}{f_1+f_2} Ln \left(\frac{\sum_{i=1}^n x_i + f_2}{\sum_{i=1}^n x_i - f_1} \right)} \quad (11)$$

$$U_{b(HT)} = \frac{1}{\frac{n-Ln(1-\alpha/2)}{\sum_{i=1}^n x_i} - \frac{1}{f_1+f_2} Ln \left(\frac{\sum_{i=1}^n x_i + f_2}{\sum_{i=1}^n x_i - f_1} \right)}.$$

Numerical Results

In order to compare the proposed approximate Bayesian approach to the Fisher Matrix bounds method, samples that have been obtained from exponentially distributed populations will be considered. For the Higgins-Tsokos loss function, consider $f_1 = 1, f_2 = 1$. The lengths of the Fisher Matrix bounds and approximate Bayesian confidence intervals are respectively denoted by l_F , l_{SE} and l_{HT} .

Example 1

Monte Carlo simulation has been used to generate the following 30 observations from the exponential distribution with mean equal to 1.

0.9549716 ,	0.09670773 ,	0.09107758,
2.6951610 ,	1.47495800 ,	0.56762340
1.2636410,	1.60653000 ,	0.94337030,
0.5499995 ,	0.64000010 ,	0.62536590
1.4492260 ,	0.78403890 ,	1.08172600,
0.3108478,	1.47283200,	0.47580980
3.1378870 ,	0.11715670 ,	0.92341850,
0.5124997	0.22012280	3.81572700
0.5791140 ,	0.50421350 ,	0.14532570 ,
0.7749708	1.07792000	1.08156300.

Table 1: Fisher Matrix Bounds and Approximate Bayesian Confidence Intervals of the Exponential Population Mean When the Population Mean is Equal to 1.

<i>Confidence level</i>	Fisher Matrix bounds	<i>Approx. Bayesian bounds</i> <i>(SE)</i>	<i>Approx. Bayesian</i> <i>bounds (HT)</i>
80%	0.7909 – 1.2621	0.9575 – 1.0298	0.9575 – 1.0298
90%	0.7392 – 1.3503	0.9368 – 1.0317	0.9368 – 1.0317
95%	0.6985 – 1.4289	0.9169 – 1.0326	0.9169 – 1.0326
99%	0.6238 – 1.6002	0.8739 – 1.0334	0.8739 – 1.0334

Confidence level	$(l_F) \div (l_{SE})$	$(l_F) \div (l_{HT})$
80%	6.5172	6.5172
90%	6.4394	6.4394
95%	6.3128	6.3128
99%	6.1216	6.1216

Example 2

Monte Carlo simulation has been used to generate the following 30 observations from the exponential distribution with mean equal to 9

2.0270,	4.0103,	30.0421,	0.1189,	2.7558.
13.7441,	13.3840,	27.0930,	7.3750,	3.7323,
23.4171,	0.06310.	5.6839,	8.7473,	10.2778,
25.2331,	10.1903,	0.3761,	3.3068,	3.4954,
6.9136,	1.8234,	16.3160,	2.4359,	19.9108,
2.5285,	3.9314,	3.4645,	6.9229,	10.4509.

Table 2: Fisher Matrix Bounds and Approximate Bayesian Confidence Intervals of the Exponential Population Mean When the Population Mean is Equal to 9.

Confidence level	Fisher Matrix bounds	Approx.Bayesian bounds (SE)	Approx.Bayesian bounds (HT)
80%	7.1184 – 11.3598	8.6182 – 9.2688	8.6182 – 9.2688
90%	6.6534 – 12.1537	8.4315 – 9.2861	8.4315 – 9.2861
95%	6.2873 – 12.8614	8.2527 – 9.2944	8.2527 – 9.2944
99%	5.6144 – 14.4028	7.8655 – 9.3009	7.8655 – 9.3009

Confidence level	$(l_F) \div (l_{SE})$	$(l_F) \div (l_{HT})$
80%	6.5192	6.5192
90%	6.4361	6.4361
95%	6.3109	6.3109
99%	6.1226	6.1226

Example 3

Monte Carlo simulation has been used to generate the following 40 observations from the exponential distribution with mean equal to 20

4.5046,	8.9119,	66.7603,	0.2643,	6.1241,
30.5425,	29.7423,	60.2067,	16.3891,	8.2941,
52.0380,	0.1402,	12.6309,	19.4385,	22.8395,
52.3378,	3.4389,	19.3268,	8.2350,	3.4737,
56.0736,	22.6451,	0.8359,	7.3484,	7.7675,
15.3635,	4.05222,	36.2578,	5.6189,	8.7365,
7.6990,	15.3844,	23.2242,	11.8542,	63.6975,
14.8772,	32.9585,	2.2127,	5.4132,	44.2462

Table 3: Fisher Matrix Bounds and Approximate Bayesian Confidence Intervals of the Exponential Population Mean When the Population Mean is Equal to 20.

Confidence level	Fisher Matrix bounds	Approx.Bayesian bounds (SE)	Approx.Bayesian bounds (HT)
80%	16.5786 – 24.8507	19.6574 – 20.7619	19.6574 – 20.7619
90%	15.6366 – 26.3479	19.3330 – 20.7907	19.3330 – 20.7907
95%	14.8886 – 27.6715	19.0191 – 20.8045	19.0191 – 20.8045
99%	13.4983 – 30.5216	18.3281 – 20.8153	18.3281 – 20.8153

Confidence level	$(l_F) \div (l_{SE})$	$(l_F) \div (l_{HT})$
80%	7.4894	7.4894
90%	7.3480	7.3480
95%	7.1596	7.1596
99%	6.8443	6.8443

Example 4

The following exponential data and results were obtained by Washington State

Department of Ecology while conducting research on the amount of lead concentration in certain types of fish found in the Spokane River.

Lead (Pb) Concentrations in 1999 Spokane River Fish Source: WA State Dept. of Ecology report concentrations in parts per million (ppm)			
Filets	trout	whitefish	sucker
	0.480	0.020	0.088
	0.071	0.020	0.210
	0.110	0.020	0.280
	0.320	0.020	0.030
	0.120	0.020	0.036
	0.220	0.065	0.047
	0.055	0.020	0.077
	0.320	0.037	0.069
	0.077	0.020	0.160
	0.081	0.036	0.088
	0.170		0.120
	0.130		0.054
	0.110		0.080
	0.081		0.059
	0.098		0.094
	0.180		0.059
	0.230		0.068
	0.082		0.020
	0.210		0.090
	0.200		0.046
	0.025		
	0.038		
Mean	0.155	0.028	0.089
std dev	0.110	0.015	0.063

Table 4: Fisher Matrix Bounds and Approximate Bayesian Confidence Intervals of the Mean Lead Concentration in Trout.

Confidence level	Fisher Matrix bounds	Approx. Bayesian bounds (SE)	Approx. Bayesian bounds (HT)
80%	0.11791 - 0.20351	0.15280 – 0.169507	0.15301 – 0.16976
90%	0.10896 – 0.22021	0.14820 – 0.16996	0.14839 – 0.17022
95%	0.10199 – 0.23526	0.14386 – 0.17018	0.14404 – 0.17044
99%	0.08936 – 0.26851	0.13471 – 0.17035	0.13487 – 0.17061

Confidence level	$(l_F) \div (l_{SE})$	$(l_F) \div (l_{HT})$
80%	5.1236	5.1104
90%	5.1125	5.0961
95%	5.0634	5.0481
99%	5.0266	5.0125

Table 5. Fisher Matrix Bounds and Approximate Bayesian Confidence Intervals of the Mean Lead Concentration in Whitefish.

Confidence level	Fisher Matrix bounds	Approx.Bayesian bounds (SE)	Approx.Bayesian bounds (HT)
80%	0.01854 – 0.04167	0.02698 - 0.03429	0.02556 – 0.03204
90%	0.01649 – 0.04684	0.02528 – 0.03452	0.02403 – 0.03224
95%	0.01495 – 0.05166	0.02378 – 0.03464	0.02267 – 0.03234
99%	0.01229 – 0.06285	0.02090 – 0.03472	0.02004 - 0.03241

Confidence level	$(l_F) \div (l_{SE})$	$(l_F) \div (l_{HT})$
80%	3.1641	3.5694
90%	3.2846	3.6967
95%	3.3802	3.7962
99%	3.6584	4.0873

Table 6. Fisher Matrix Bounds and Approximate Bayesian Confidence Intervals of the Mean Lead Concentration in Sucker.

Confidence level	Fisher Matrix bounds	Approx.Bayesian bounds (SE)	Approx.Bayesian bounds (HT)
80%	0.06666 – 0.11816	0.08742 – 0.09803	0.08799 – 0.09875
90%	0.06136 – 0.12835	0.08454 – 0.09833	0.08507 – 0.09905
95%	0.05725 – 0.13756	0.08183 – 0.09847	0.08234 – 0.09919
99%	0.04984 – 0.15802	0.07618 – 0.09858	0.07662 – 0.09931

Confidence level	$(l_F) \div (l_{SE})$	$(l_F) \div (l_{HT})$
80%	4.8539	4.7862
90%	4.8578	4.7918
95%	4.8263	4.7661
99%	4.8294	4.7677

Example 5

The following exponential data represent a random sample of cycles to failure in ten-thousands for twenty heater switches subject to an overload voltage.

0.01,	0.034,	0.194,	0.567,	0.601,
0.712,	1.291,	1.367,	1.949,	2.37,
2.411,	2.875,	3.162,	3.28,	3.491,
3.686,	3.854,	4.211,	4.397,	6.473.

Elfessi and Raineke (2001) conducted some studies on the above data and obtained the following the following maximum likelihood estimate and 95% confidence interval for the parameter θ : 0.4261 and (0.2603, 0.6322).

Table 1, Table 2 and Table 3 show that, in the first three examples, the proposed approximate Bayesian confidence intervals perform better than confidence interval obtained with Fisher Matrix bounds method. All seven Tables show that the proposed approximate Bayesian confidences intervals perform well.

Conclusion

Approximate Bayesian confidence intervals for parameters of exponential populations under two different loss functions have been derived. The loss functions that are employed are the square error and the Higgins-Tsokos loss functions. Based on the above numerical results, the following may be concluded:

Table 7: Fisher Matrix Bounds and Approximate Bayesian Confidence Intervals of θ

Confidence level	Fisher Matrix bounds	Approx.Bayesian bounds (SE)	Approx.Bayesian bounds (HT)
80%	0.32005 – 0.56732	0.38575 – 0.43256	0.38575 – 0.43256
90%	0.29464 – 0.61626	0.38460 – 0.44733	0.38459 – 0.44733
95%	0.27491 – 0.66049	0.38404 – 0.46210	0.38404 – 0.46210
99%	0.23932 – 0.75871	0.38361 – 0.49639	0.38361 – 0.49639

Confidence level	$(l_F) \div (l_{SE})$	$(l_F) \div (l_{HT})$
80%	5.2824	5.2824
90%	5.1270	5.1262
95%	4.9353	4.9395
99%	4.6053	4.6053

1. When representative samples are considered, the Fisher Matrix bounds method used to construct confidence intervals for exponential parameters does not always yield the best coverage accuracy.
2. The Fisher Matrix bounds method used to construct confidence intervals for the mean of an exponential population does not always yield the best coverage accuracy. In fact, in Table 1, Table 2 and Table 3, each of the obtained approximate Bayesian confidence intervals contains the population mean and is strictly included in the corresponding confidence interval obtained with Fisher Matrix bounds method.
3. Contrary to Fisher Matrix bounds method that uses the Z-table, the proposed approach relies only on the observations.
4. With the proposed approach, approximate Bayesian confidence intervals for exponential population means are easily computed for any level of significance.
5. Bayesian analysis contributes to reinforcing well-known statistical theories such as the estimation theory.

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Better Binomial Confidence Intervals

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The construction of a confidence interval for a binomial parameter is a basic analysis in statistical inference. Most introductory statistics textbook authors present the binomial confidence interval based on the asymptotic normality of the sample proportion and estimating the standard error - the Wald method. For the one sample binomial confidence interval the Clopper-Pearson exact method has been regarded as definitive as it eliminates both overshoot and zero width intervals. The Clopper-Pearson exact method is the most conservative and is unquestionably a better alternative to the Wald method. Other viable alternatives include Wilson's Score, the Agresti-Coull method, and the Borkowf SAIFS-z.

Key words: Binomial distribution, confidence intervals, coverage probability, Wald method, Clopper-Pearson Method, Score Method, Agresti-Coull method.

Introduction

The International Committee of Medical Journal editors indicated that confidence intervals are preferred over simple point estimates and p-values. This applies to over 300 international medical/scientific journals. Most introductory statistics textbook authors present the binomial confidence interval based on the asymptotic normality of the sample proportion and estimating the standard error. This approximate method is referred to as the Wald interval. In order to avoid approximation, some advanced statistics textbooks recommend the Clopper-Pearson exact binomial confidence interval. Other methods, asymptotic as well as exact, have been proposed and appear sporadically in introductory textbooks. There is a rather large

set of articles, primarily in the statistics literature, about these and other less common methods of constructing binomial confidence intervals.

The purpose of this article is to provide a review of alternatives to the Wald method for computing a binomial confidence interval and provide a set of tractable and better methods of constructing binomial confidence intervals for a single proportion.

Methodology

When a binomial confidence interval is reported, the computational method is rarely given. This may imply that there is only one standard method for computing a binomial confidence interval - the Wald method (W). The W binomial confidence interval, either with or without a continuity correction, is found in every introductory statistics text. Typically, a warning or rule of thumb for determining when not to use W is included, but usually ignored. Occasionally, the Wald with a continuity correction (WCC) is included. For a single proportion the W and WCC lower bound (LB) and upper bound (UB) are defined as:

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$$\begin{aligned}
W \text{ LB} &= p - z_{\alpha/2} \sqrt{[pq/n]} \\
W \text{ UB} &= p + z_{\alpha/2} \sqrt{[pq/n]}, \\
WCC \text{ LB} &= p - (z_{\alpha/2} \sqrt{[pq/n]} + 1/(2n)) \\
WCC \text{ UB} &= p + (z_{\alpha/2} \sqrt{[pq/n]} + 1/(2n))
\end{aligned}$$

where $p = r/n$, $q = 1-p$, r =number of successes, and n is the total sample size.

Even though these two confidence interval methods are similar to large-sample formulas for means, both the W and WCC confidence intervals behave poorly in terms of zero width intervals and overshoot (Beal, 1987; Vollset, 1993; Newcombe, 1998; Pires, 2002; Rieczigel, 2003; Agresti, 2003). For instance, when $r=0$ or n , W and WCC have zero width or degenerate confidence intervals. Despite the known poor performance of the W and WCC confidence intervals, they continue to dominate in statistics textbooks, typically accompanied by warnings that when np is small, usually less than 5 or 10, exact or score methods should be used. A slightly different version of the rule of thumb requires that npq should be greater than or equal to 5. A better rule is to not compute confidence bounds for a proportion using the W method but rather to use one of the better methods. For small proportions the calculated lower bound can be below zero. Conversely, when a proportion approaches one, such as in the sensitivity and specificity of diagnostic or screening tests, and the upper bound may exceed one. This overshoot is avoided by truncating the interval to lie within $[0, 1]$. Overshoot and zero width confidence intervals may be avoided by a variety of better methods.

One of the standard measures of binomial confidence interval performance is the coverage probability, $C(\pi|n, \alpha)$. Given $X=k, n$, and α , let $\delta(\pi|k, n, \alpha)=1$ if $\pi \in [LB(k, n, \alpha), UB(k, n, \alpha)]$, and $\delta(\pi|k, n, \alpha)=0$ otherwise. Then, $C(\pi|n, \alpha)$ for a given π is:

$$C(\pi|n, \alpha) = \sum P(X=k|n, \pi) \delta(\pi|k, n, \alpha)$$

Figure 1 shows the 95% confidence interval coverage probability of the standard Wald methods $\{W, WCC\}$ as a function of π , $\pi \in [0, 1]$, for $n=20$. The coverage probability curves demonstrate the subnomial coverage for values of π near 0 and 1.

The Clopper-Pearson (CP) binomial confidence interval is the best-known exact method for interval estimation and is considered by most to be the gold standard (Clopper & Pearson, 1934). The CP confidence interval eliminates overshoot and zero width intervals and is strictly conservative. The CP lower and upper limits are defined by inverting the exact binomial tests with equal-tailed acceptance regions.

$$CP \quad LB=0 \text{ if } x=0, (\alpha/2)^{1/n} \text{ if } x=n.$$

$$LB=[1+(n-r+1)/(r \times F_{2r, 2(n-r+1), 1-\alpha/2})]^{-1}$$

$$CP \quad UB=1-(\alpha/2)^{1/n} \text{ if } x=0, 1 \text{ if } x=n.$$

$$UB=[1+(n-r)/(r \times F_{2(r+1), 2(n-r), \alpha/2})]^{-1}$$

Fleiss (1981) preferred a more computationally intense binomial confidence interval with a continuity correction (SCC) attributed to Wilson (Wilson, 1927). For a single proportion, Wilson's Score (S) and Wilson's Score with continuity correction (SCC) LB and UB are defined as:

$$S \text{ LB}=(2np+z^2-z\sqrt{\{z^2+4npq\}})/2(n+z^2)$$

$$S \text{ UB}=(2np+z^2+z\sqrt{\{z^2+4npq\}})/2(n+z^2)$$

$$SCC \text{ LB} = [2np+z^2-1-z\sqrt{\{z^2-2-1/n+4p(nq+1)\}}]/(2n+2z^2)$$

$$SCC \text{ UB} = [2np+z^2+1+z\sqrt{\{z^2+2-1/n+4p(nq-1)\}}]/(2n+2z^2)$$

Blyth and Still (1983) investigated the performance of W , WCC , CP , Sterne's binomial confidence interval method (Sterne, 1954), and Pratt's (P) approximate confidence interval method (Pratt, 1968). Their results demonstrate the need for a continuity correction even when n is large. Blythe and Still then suggested a modification to W (WBS). While the WBS was an improvement over W and WCC , they concluded that it still was not

Figure 1. Coverage Probabilities ($n=20$) for the Wald and Wald CC Binomial Confidence Interval Methods.

satisfactory. The LB and UB for WBS are defined as:

$$LB = p - [z/\sqrt{(n-z^2-2z/\sqrt{n-1/n})}][\sqrt{(pq)+1/2n}],$$

except $LB=0$ when $r=0$.

$$UB = p + [z/\sqrt{(n-z^2-2z/\sqrt{n-1/n})}][\sqrt{(pq)+1/2n}],$$

except $UB=1$ for $r=n$.

Vollset (Vollset, 1993) compared thirteen methods for computing binomial

confidence intervals using evaluative criteria of $C(P)$, interval width, and errors relative to limits. Vollset proposed a mean Pratt (MP), a modification of P that is a closed form approximation to the mid- P exact interval. Define the UB of P as:

$$P \text{ UB} = [1 + (r+1)/(n-r)]^2 ((A-b)/c)^3]^{-1},$$

with

$$A = 81(r+1)(n-r) - 9n - 8,$$

$$B = 3z\sqrt{[9(r+1)(n-r)(9n+5z^2)+n+1]},$$

and

$$C=81(r+1)2-9(r+1)(2+z^2)+1.$$

For P LB, replace r with $r-1$ and z with $-z$.

The Vollset MP lower and upper bound are then defined as:

$$\begin{aligned} \text{MP LB} &= \{P_l(r) + P_l(r+1)\}/2, \\ \text{MP UB} &= \{P_u(r) + P_u(r-1)\}/2 \end{aligned}$$

Vollset argued that W and WCC were unsatisfactory and the Clopper-Pearson, Pratt's approximation, SCC, MP, S and SCC are methods that may be safely used in all applications.

Newcombe (1998) compared seven methods for constructing two-sided binomial confidence intervals (W, WCC, S, SCC, Clopper-Pearson, mid-P and a likelihood-based method). The W and WCC were quickly judged as being inadequate, highly anti-conservative, asymmetrical in coverage, and incurred a higher risk of unacceptable boundary limits. Newcombe argued that neither W nor WCC should be acceptable methods for the scientific literature since other methods are tractable and all perform much better. Newcombe further argued that the use of the simple asymptotic standard error of a proportion should be restricted to sample size planning and introductory teaching purposes. Newcombe preferred three methods: the Clopper-Pearson method, the Score method and mid-P binomial based method.

Agresti and Coull, in noting the poor performance of the Wald interval and conservativeness of the Clopper-Pearson interval, proposed a straightforward adjustment - the add 4 to Wald. They suggested that by simply adding two successes and two failures and then use the Wald formula. Alternatively, one could add $z^2/2$ successes and $z^2/2$ failures before computing the Wald confidence interval.

The latter is preferred. The Agresti-Coull adjusted Wald (AC) lower and upper bounds are:

$$\begin{aligned} \text{LB} &= p' - z\sqrt{p'q'/n'}, \\ \text{UB} &= p' + z\sqrt{p'q'/n'}, \text{ where} \\ p' &= (2r+z^2)/(2n+z^2), \text{ and } n' = n+z^2 \end{aligned}$$

Pires (2002) compared twelve methods for constructing confidence intervals for a binomial proportion and concluded that a clear classification of conservative methods included the Clopper-Pearson, the Score, and two arcsine transformation methods. A second tier of recommended confidence interval construction methods included a Bayesian method and the SCC.

Agresti (2003) argued for reducing the effects of discreteness in binomial confidence intervals by inverting two-sided tests rather than two one-sided tests. In most statistical practice, for interval estimation of a proportion or a difference or ratio of proportions, the inversion of the asymptotic score test is the best choice. If one wants to be a bit more conservative, mid-P adaptations or the Clopper-Pearson are recommended. For teaching purposes, the Wald-type interval plus and minus a normal-score multiple of a standard error is simplest.

Reiczigel compared four methods for constructing binomial confidence intervals: Wilson's Score, Agresti and Coull Adjusted Wald, the Clopper-Pearson, the mid-P, and Sterne's interval (Reiczigel, 2003). Unique to this study is the recommendation of using the Sterne interval and the Agresti-Coull adjusted Wald interval for binomial confidence intervals.

Tobi et al. (2005) compared the performance of seven approximate methods and the exact Clopper-Pearson exact confidence intervals for small proportions. Three criteria were used to evaluate the performance of confidence intervals; coverage, confidence interval width, and aberrant confidence intervals. They concluded that: (1) one should

compute confidence intervals for small proportions even when the number of events equals zero, (2) report what method has been used for confidence interval calculation, (3) the W method should be discarded, and (4) the Clopper-Pearson and the SCC are the best choices to calculate confidence intervals for small proportions.

Borkowf (2005) argued that even though the Agresti-Coull method binomial confidence intervals are substantially better than the Wald method, it can yield sub nominal coverage for some values of π for moderate sample sizes. A binomial confidence interval, which results in near nominal coverage and is easy to calculate by first augmenting the original data with a single imaginary failure to compute the lower confidence bound and a single imaginary success to compute the upper confidence bound is proposed - a single augmentation with an imaginary failure or success (SAIFS) method. The lower and upper SAIFS confidence bounds are then:

$$\text{SAIFS LB} = p_1 - \xi_{1-\alpha/2} \sqrt{[p_1 q_1/n]}$$

and

$$\text{UB} = p_2 + \xi_{1-\alpha/2} \sqrt{[p_2 q_2/n]},$$

with

$$p_1 = (r + 0)/(n+1) \text{ and } p_2 = (r+1)/(n+1)$$

Borkowf (2005) evaluated two forms of the SAIFS. The first uses the z-quantiles ($\xi_{1-\alpha/2}$) and the second used the t-quantiles ($\tau_{n-1, 1-\alpha/2}$). Compared to the Clopper-Pearson method, the SAIFS method using either the z or t quantiles results in confidence intervals with mean widths that are narrower for proportion parameters near 0 or 1 and whose coverage probabilities are marginally better over all values of π . The SAIFS-Z is preferred.

Figure 2 shows the 95% confidence interval coverage probability as a function of π , $\pi \in [0,1]$, for $n=20$ for CP, WBS, S, SCC, AC, and SAIFS-Z. Note that the sawtooth appearance of the coverage functions is due to the discontinuities for values of p corresponding to any lower or upper limits in the set of $n+1$ confidence intervals. The Clopper-Pearson and Borkowf SAIFS-z methods give at least nominal coverage for all values of $\pi \in [0,1]$, with severe over coverage near 0 and 1. The Score CC method gives at least nominal coverage for all values of $\pi \in [0,1]$ and avoids the over coverage of either the Clopper-Pearson or Score methods. The Score and Agresti-Coull methods yield nearly nominal coverage for all values of $\pi \in [0,1]$.

Conclusion

For the one sample binomial confidence interval, a new generation of introductory and medical statistics textbooks should emphasize the poor performance properties of W, WCC and include better binomial confidence methods. At least one from the set of Clopper-Pearson, S, SCC, Agresti-Coull, or the SAIFS-z methods should be mentioned. With the widespread use of laptop computers and access to computing resources on the internet, the complexity of computing binomial confidence intervals should not be an issue. The question remains as to which method to use. The Clopper-Pearson exact method has been regarded as definitive as it eliminates both overshoot and zero width intervals. The Clopper-Pearson exact method is the most conservative and is unquestionably a better alternative to the W when constructing and reporting binomial confidence intervals. In terms of programming ease, the Clopper-Pearson is easily programmed as are the Blythe & Still, Wilson's Score, Score with a continuity correction, the Agresti-Coull method, and the Borkowf SAIFS-z.

Figure 2. Coverage Probabilities ($n=20$) for the Clopper-Pearson, Score, Score CC, Agresti-Coull, and Borkowf SAIFS-z Binomial Confidence Interval Methods.

Figure 2 (Continued). Coverage Probabilities ($n=20$) for the Clopper-Pearson, Score, Score CC, Agresti-Coull, and Borkowf SAIFS-z Binomial Confidence Interval Methods.

Table 1. Methods for Calculation of Confidence Intervals for a Single Proportion

Method		Formula
Clopper-Pearson	CP	$LB=0 \text{ if } x=0, (\alpha/2)^{1/n} \text{ if } x=n.$ $LB=[1+(n-r+1)/(r \times F_{2r, 2(n-r+1), 1-\alpha/2})]^{-1}$ $UB=1-(\alpha/2)^{1/n} \text{ if } x=0, 1 \text{ if } x=n.$ $UB=[1+(n-r)/(r \times F_{2(r+1), 2(n-r), \alpha/2})]^{-1}$
Score (Wilson)	S	$LB=(2np+z^2-z\sqrt{\{z^2+4npq\}})/2(n+z^2)$ $UB=(2np+z^2+z\sqrt{\{z^2+4npq\}})/2(n+z^2)$
Score (w/CC)	SCC	$LB=[2np+z^2-1-z\sqrt{\{z^2-2-1/n+4p(nq+1)\}}]/(2n+2z^2)$ $UB=[2np+z^2+1+z\sqrt{\{z^2+2-1/n+4p(nq-1)\}}]/(2n+2z^2)$
Agresti-Coull	AC	$LB=p'-z\sqrt{[p'q'/n']}$ $UB=p'+z\sqrt{[p'q'/n]}, \text{ where}$ $p'=(2r+z^2)/(2n+z^2), \text{ and } n'=n+z^2.$
Borkowf	SAIFS	$LB = p_1 - \xi_{1-\alpha/2} \sqrt{[p_1 q_1 / n]}$ $UB = p_2 + \xi_{1-\alpha/2} \sqrt{[p_2 q_2 / n]}, \text{ with}$ $p_1=(r+0)/(n+1) \text{ and } p_2=(r+1)/(n+1), \text{ where}$ $\xi_{1-\alpha/2} \text{ are z-quantiles or } \tau_{n-1, 1-\alpha/2} \text{ the t-quantiles}$

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A Comparison of Eight Shrinkage Formulas under Extreme Conditions

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The performance of various shrinkage formulas for estimating the population squared multiple correlation coefficient (ρ^2) were compared under extreme conditions often found in educational research with small sample sizes of 10, 15, 20, 25, 30 and regressor variates ranging from 2 to 4. A new formula for estimating ρ^2 , Adj R^2_{DW} , was examined in terms of its performance under various conditions of N , p , ρ^2 , along with its bias properties and standard error estimates. The two shrinkage formulas that performed most consistently were the Claudy (Adj R^2_C) and Walker (Adj R^2_{DW}).

Key Words: Adjusted R^2 , shrinkage, population squared multiple correlation

Introduction

Various shrinkage formulas for estimating the population squared multiple correlation coefficient (ρ^2) has been the topic of interest (cf. Carter, 1979; Claudy, 1978; Huberty & Mourad, 1980; Lucke & Embretson, 1984). The purpose of this article is to compare the performance of eight shrinkage formulas for estimating the population multiple correlation coefficient with small sample sizes of 10, 15, 20, 25, 30 and with regressor variates ranging from 2 to 4. Small sample sizes were used because in applied research fields, such as educational research, these sample conditions often are encountered (Claudy, 1972; Huberty & Mourad, 1980). Also, regressor variates were chosen to be between 2 and 4 for the same reason cited formerly with sample size; typicality of conditions frequently encountered in educational research.

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The sample squared multiple correlation coefficient, or R^2 , indicates the percentage of variance in the dependent variable explained by the linear combination of the independent variables. R^2 has been found to overestimate the population multiple correlation (ρ^2) and, hence, is seen as an upwardly biased approximation of ρ^2 with limited accuracy (Agresti & Finlay, 1997; Pedhazur, 1997). This overestimation has been linked to the problem of error, often either measurement or sampling error, connected to the variability found in random independent variables (Claudy, 1972), related to sample size, and associated with the number of X variables in a model (Huberty & Mourad, 1980; Shumacker, Mount, & Monahan, 2002). The population multiple correlation can be expressed as (Browne, 1975):

$$\rho^2 = \text{corr}^2\{Y, \sim Y(X|\beta_0, \beta)\} \quad (1)$$

where,

Y = Dependent variable

X = Set of regressors

β = Population regression weights

Due to amending for this overestimation, the adjusted R^2 (adj R^2) has been used as a more accurate method than R^2 for estimating ρ^2 . That is, the adj R^2 is more exact than R^2 due to its correction for shrinkage and its ability to produce an accurate estimate of the population value for ρ^2 . Adjusted R^2 can be

expressed as (Agresti & Finlay, 1997):

$$R^2_{adj} = R^2 - \frac{p-1}{N-p} * (1 - R^2) \quad (2)$$

Other shrinkage formulas for estimating the population multiple correlation coefficient have been presented with the goal of reducing the positive bias of R^2 . As noted by Carter (1979), many of the subsequent formulas are decidedly related algebraically and/or are hybrids of one another.

Formulas 3 to 6 and 9 are reproduced in Huberty and Mourad (1980). According to Huberty and Mourad, Smith proposed, but presented by Ezekiel (1929), the first adjusted R^2 shrinkage formula, R^2_s , where:

$$R^2_s = 1 - \frac{N}{N-p-1} * (1 - R^2) \quad (3)$$

Ezekiel (1930) proposed R^2_E , where:

$$R^2_E = 1 - \frac{N-1}{N-p-1} * (1 - R^2) \quad (4)$$

Wherry (1931) proposed R^2_W , where:

$$R^2_W = 1 - \frac{N-1}{N-p} * (1 - R^2) \quad (5)$$

Olkin and Pratt (1958) proposed R^2_{OP} , where:

$$R^2_{OP} = 1 - \frac{N-3}{N-p-1} * (1 - R^2) - \frac{2(N-3)}{(N-p-1)(N-p+1)} * (1 - R^2)^2 \quad (6)$$

Pratt (1964 as cited in Claudy, 1978) proposed R^2_P , where:

$$R^2_P = 1 - \frac{(N-3) * (1 - R^2)}{N-p-1} * 1 + \frac{2(1 - R^2)}{(N-p-2.3)} \quad (7)$$

Herzberg (1969 as cited in Claudy, 1978)

proposed R^2_H , where:

$$R^2_H = 1 - \frac{(N-3) * (1 - R^2)}{N-p-1} * 1 + \frac{2(1 - R^2)}{(N-p+1)} \quad (8)$$

Claudy (1978) proposed R^2_C , where:

$$R^2_C = 1 - \frac{N-4}{N-p-1} * (1 - R^2) - \frac{2(N-4)}{(N-p-1)(N-p+1)} * (1 - R^2)^2 \quad (9)$$

Walker (2006) proposed R^2_{DW} , which is an algebraic alteration of R^2_C and, hence, $N - 4.15$ was a more optimal empirical modification of $N - 4$ than $N - 5$, where:

$$R^2_{DW} = 1 - \frac{N-4.15}{N-p-1} * (1 - R^2) - \frac{2(N-4.15)}{(N-p-1)(N-p+1)} * (1 - R^2)^2 \quad (10)$$

where,

N = Sample size

p = Number of X variables

R^2 = Multiple correlation coefficient

Methodology

Via a simulation program written in SPSS (Statistical Package for the Social Sciences) v. 12.0, the following study reviewed the shrinkage performance of the eight multiple correlation estimators noted previously when ρ^2 is known at .15, .30, .45, .60, .75, .90, $N = 10, 15, 20, 25, 30$, $p = 2, 3, 4$, under normal distributional assumptions, and where the number of iterations within the simulation was 500.

Results

Overall, the study's findings indicated that all of the eight shrinkage formulas utilized under the research's specified conditions did succumb to bias, as was expected, either via under or overestimation of the population multiple

correlation. Table 1 indicates that the two most consistently accurate formulas were Claudy and Walker. When looking at small sample sizes with few predictors with a $\rho^2 \leq .45$, Table 1 shows that the Smith, Ezekiel, Wherry, and Olkin and Pratt formulas typically underestimated, often times greatly, ρ^2 in

comparison to the Pratt, Herzberg, Claudy, and Walker formulas. However, the Pratt and Herzberg formulas tended to overestimate the population multiple correlation at .60, .75, and .90, respectively, regardless of the sample size and especially when $p = 2$ and 3. The Claudy and Walker formulas were consistently accurate in these same conditions, with only a small portion of overestimation when $p = 2$.

Table 1. Values for Eight Shrinkage Formulas when $N = 10$ to 30, $p = 2$ to 4

$N = 10, p = 2$

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.214	-.093	.044	-.011	.134	.199	.181	.155
.300	.000	.100	.213	.191	.307	.389	.357	.324
.450	.214	.293	.381	.383	.471	.572	.528	.484
.600	.429	.486	.550	.564	.627	.747	.693	.636
.750	.643	.679	.719	.736	.774	.914	.854	.779
.900	.857	.871	.888	.898	.912	1.000	1.000	.915

$N = 15, p = 2$

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.063	.008	.085	.047	.126	.176	.170	.138
.300	.125	.183	.246	.230	.294	.348	.336	.304
.450	.313	.358	.408	.407	.456	.515	.500	.464
.600	.500	.533	.569	.577	.612	.679	.660	.618
.750	.688	.708	.731	.741	.763	.838	.817	.766
.900	.875	.883	.892	.899	.907	.993	.971	.908

$N = 20, p = 2$

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	.000	.050	.103	.074	.128	.168	.165	.137
.300	.176	.218	.261	.248	.293	.332	.327	.299
.450	.353	.385	.419	.418	.452	.494	.487	.458
.600	.529	.553	.578	.583	.608	.654	.644	.611
.750	.706	.721	.736	.743	.759	.810	.799	.761
.900	.882	.888	.894	.899	.905	.963	.952	.906

$N = 25, p = 2$

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	.034	.073	.113	.090	.131	.163	.162	.137
.300	.205	.236	.270	.259	.293	.325	.321	.298
.450	.375	.400	.426	.425	.451	.484	.479	.455
.600	.545	.564	.583	.587	.605	.641	.635	.608
.750	.716	.727	.739	.745	.756	.795	.789	.758
.900	.886	.891	.896	.899	.904	.948	.941	.904

Table 1. Continued

N = 30, p = 2

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	.056	.087	.120	.100	.133	.161	.160	.138
.300	.222	.248	.275	.266	.293	.320	.318	.297
.450	.389	.409	.430	.429	.450	.477	.474	.453
.600	.556	.570	.586	.589	.604	.633	.629	.606
.750	.722	.731	.741	.746	.755	.786	.782	.757
.900	.889	.893	.896	.899	.903	.939	.934	.904

N = 10, p = 3

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.417	-.275	-.093	-.202	-.031	.012	.010	-.005
.300	-.167	-.050	.100	.040	.178	.250	.222	.198
.450	.083	.175	.293	.270	.374	.477	.428	.390
.600	.333	.400	.486	.487	.560	.692	.627	.571
.750	.583	.625	.679	.690	.734	.897	.819	.741
.900	.833	.850	.871	.880	.898	1.000	1.000	.900

N = 15, p = 3

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.159	-.082	.008	-.049	.039	.087	.083	.052
.300	.045	.109	.183	.154	.225	.278	.267	.235
.450	.250	.300	.358	.349	.403	.464	.448	.412
.600	.455	.491	.533	.537	.575	.645	.624	.581
.750	.659	.682	.708	.717	.740	.821	.797	.744
.900	.864	.873	.883	.889	.898	.992	.966	.900

N = 20, p = 3

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.063	-.009	.050	.012	.070	.109	.107	.078
.300	.125	.169	.218	.198	.246	.286	.280	.253
.450	.313	.347	.385	.380	.416	.459	.451	.422
.600	.500	.525	.553	.556	.582	.630	.620	.586
.750	.688	.703	.721	.727	.743	.797	.785	.745
.900	.875	.881	.888	.893	.899	.961	.948	.900

N = 25, p = 3

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.012	.029	.073	.044	.087	.120	.118	.094
.300	.167	.200	.236	.222	.257	.290	.286	.263
.450	.345	.371	.400	.396	.424	.457	.452	.428
.600	.524	.543	.564	.566	.586	.622	.616	.589
.750	.702	.714	.727	.732	.745	.785	.778	.746
.900	.881	.886	.891	.894	.899	.945	.938	.900

Table 1. Continued

N = 30, p = 3

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	.019	.052	.087	.064	.098	.126	.125	.104
.300	.192	.219	.248	.237	.265	.292	.290	.269
.450	.365	.387	.409	.406	.428	.456	.453	.432
.600	.538	.554	.570	.573	.589	.618	.614	.591
.750	.712	.721	.731	.736	.746	.778	.773	.747
.900	.885	.888	.893	.895	.899	.936	.931	.900

N = 10, p = 4

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.700	-.530	-.275	-.479	-.268	-.285	-.240	-.236
.300	-.400	-.260	-.050	-.176	-.008	.029	.025	.017
.450	-.100	.010	.175	.109	.236	.326	.281	.255
.600	.200	.280	.400	.376	.465	.606	.528	.479
.750	.500	.550	.625	.625	.679	.870	.766	.687
.900	.800	.820	.850	.856	.877	1.000	.995	.880

N = 15, p = 4

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.275	-.190	-.082	-.165	-.067	-.024	-.023	-.053
.300	-.050	.020	.109	.062	.140	.191	.183	.152
.450	.175	.230	.300	.279	.340	.401	.384	.349
.600	.400	.440	.491	.488	.531	.604	.581	.537
.750	.625	.650	.682	.688	.714	.801	.773	.717
.900	.850	.860	.873	.878	.888	.991	.961	.890

N = 20, p = 4

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.133	-.077	-.009	-.060	.003	.042	.041	.012
.300	.067	.113	.169	.141	.192	.232	.227	.199
.450	.267	.303	.347	.336	.375	.419	.411	.381
.600	.467	.493	.525	.525	.553	.603	.592	.557
.750	.667	.683	.703	.708	.725	.782	.769	.728
.900	.867	.873	.881	.885	.892	.958	.944	.893

N = 25, p = 4

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.063	-.020	.029	-.007	.039	.071	.070	.045
.300	.125	.160	.200	.181	.218	.251	.248	.224
.450	.313	.340	.371	.365	.394	.428	.423	.398
.600	.500	.520	.543	.544	.565	.602	.596	.568
.750	.688	.700	.714	.719	.732	.773	.766	.733
.900	.875	.880	.886	.889	.894	.942	.935	.895

Table 1. Continued

N = 30, p = 4

ρ^2	Smith	Ezekiel	Wherry	Olkin-Pratt	Claudy	Pratt	Herzberg	Walker
.150	-.020	.014	.052	.024	.060	.088	.088	.066
.300	.160	.188	.219	.205	.234	.262	.259	.239
.450	.340	.362	.387	.382	.405	.433	.429	.408
.600	.520	.536	.554	.555	.572	.602	.597	.574
.750	.700	.710	.721	.725	.735	.769	.764	.737
.900	.880	.884	.888	.891	.895	.933	.928	.896

Table 2 depicts adjusted R^2 Walker's bias properties or the error that results when estimating ρ^2 . Because Walker has similar properties as the Olkin and Pratt formula, the following bias formula presented by Lucke and Embretson (1984) was modified:

$$\text{Bias } R^2_{\text{DW}} = 1 - \frac{N - 4.15}{N + 1} * R^2 *$$

$$\frac{2(1 - R^2)}{(N - 1)} \quad (11)$$

The bias properties for this shrinkage formula show that it is a function of sample size. As would be anticipated, when the sample increases, the bias in this estimator decreases. This formula's bias properties are similar in comparison to other estimators found by Lucke and Embretson (1984).

Table 2. Bias Properties for Adjusted R^2 Walker, $N = 10$ to 30

ρ^2	N	Bias
.150	10	.174
.300	10	.131
.450	10	.093
.600	10	.061
.750	10	.033
.900	10	.012
.150	15	.109
.300	15	.080
.450	15	.055
.600	15	.034
.750	15	.018
.900	15	.006
.150	20	.079
.300	20	.057
.450	20	.038
.600	20	.023
.750	20	.011
.900	20	.003
.150	25	.062
.300	25	.044
.450	25	.029
.600	25	.017
.750	25	.008
.900	25	.002
.150	30	.051
.300	30	.036
.450	30	.024
.600	30	.014
.750	30	.006
.900	30	.002

Table 3 illustrates Walker's accurateness via standard error estimates for every situation presented in the research. A bootstrapping program conducted 500 resamples to derive the standard error estimate terms presented. Replications of 500 were chosen because the standard error estimates converged quickly at this level and there were relatively no precision differences above this value. As would be expected, bias was greatest under conditions of small N , specifically when $N = 10$

and 15, where error ranged from 1% to 1.5% in these two situations regardless of p . When $N = 20, 25$, and 30 , standard errors were all $< 1\%$. For instance, Figure 1 shows that the Walker formula produced almost no bias under the extreme case of $N = 10$, $p = 2$, and $\rho^2 = .15$, and became more accurate in this same situation when the sample size increased to $N = 15$. Further, Figure 2 illustrates this same small bias propensity with the Walker formula, and also the Claudy formula, when $p = 2$ and $\rho^2 = .45$, and shows that both the Pratt and Herzberg formulas in this same situation produced overestimations of the ρ^2 value.

Table 3. Standard Error Estimates for Adj. R^2 Walker

p = 2

N	SE	SE Range (Min/Max)
10	.015	(.000, .026)
15	.010	(.000, .017)
20	.008	(.000, .013)
25	.006	(.000, .011)
30	.005	(.000, .009)

p = 3

N	SE	SE Range (Min/Max)
10	.014	(.000, .024)
15	.010	(.000, .017)
20	.007	(.000, .013)
25	.006	(.000, .011)
30	.005	(.000, .009)

p = 4

N	SE	SE Range (Min/Max)
10	.015	(.000, .026)
15	.010	(.000, .016)
20	.007	(.000, .013)
25	.006	(.000, .011)
30	.005	(.000, .009)

Figure 1. A Comparison of Shrinkage Formulas when $\rho^2 = .15$, $p = 2$

Figure 2. A Comparison of Shrinkage Formulas when $\rho^2 = .45$, $p = 2$ Figure 3. A Comparison of Shrinkage Formulas when $\rho^2 = .75$, $p = 3$

Figure 4. A Comparison of Shrinkage Formulas when $\rho^2 = .90$, $p = 4$

Considering data depicted in Figures 3 and 4, it is recommended that when $N = 10$ to 30 with either $p = 3$ or 4 , use the Walker formula, which was more accurate in every instance than Claudy, and the majority of the time more exact than either Pratt or Herzberg due to their overestimations typically at ρ^2 values of .60, .75, and .90. When $N = 10$ to 30 and $p = 2$, the Claudy formula was more accurate than Walker, except in the case where $\rho^2 = .15$. It is not recommended, however, to use either Smith or Ezekiel in any of the presented situations when $\rho^2 \leq .60$. Wherry and Olkin and Pratt may be regarded in some instances when $\rho^2 = .60$, but tend to be more accurate in all cases at the .75 and .90 levels.

Lastly, extreme research situations can produce adjusted R^2 values that are nonsensical. For example, the negative values depicted in Table 1 and Figure 1 have been noted before in previous research associated with shrinkage

formulas by Huberty and Mourad (1980), where it was found that, "Negative values will result from using a small R^2 value and/or a small N/p ratio" (p. 108). Thus, these negative figures should be considered to take on the value of zero.

Conclusion

When estimating the population multiple correlation coefficient, reducing the positive bias found in R^2 , the coefficient of determination, is approached via an unbiased estimator called the adjusted R^2 . However, a caveat with adjusted R^2 is that not all unbiased estimators of ρ^2 function the same under varying research situations. The goal of this research was to look at this issue and determine which of the eight estimators chosen performed the most consistently under biased research conditions often found within the field of educational research, where N was small and the number of X variables ranged from 2 to 4.

The results of this study yielded no definitive answers pertaining to the best estimators in every situation examined, but it did ascertain that the two most consistently accurate formulas in the many conditions studied were Claudy and Walker. The tabled data derived from this research should provide researchers and students with information to understand when to use various adjusted R^2 estimators pertaining to a given research situation. Also, this research introduced a new shrinkage formula, Adj. R^2_{DW} , and provided a complete error profile and comparison analysis under extreme research conditions for the user's consideration. Future research affiliated with shrinkage formulas should include the performance of these eight estimators under the same extreme conditions, but when operating in very biased distributional situations such as with outlier data points and/or under non-normal conditions of various skew.

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Beta-Weibull Distribution: Some Properties and Applications to Censored Data

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Some properties of a four-parameter beta-Weibull distribution are discussed. The beta-Weibull distribution is shown to have bathtub, unimodal, increasing, and decreasing hazard functions. The distribution is applied to censored data sets on bus-motor failures and a censored data set on head-and-neck-cancer clinical trial. A simulation is conducted to compare the beta-Weibull distribution with the exponentiated Weibull distribution.

Key words: Bathtub, unimodal, censored data, bootstrap.

Introduction

Let $F(x)$ be the cumulative distribution function of a Weibull random variable X . Famoye, Lee, and Olumolade (2005) defined the cumulative distribution function for beta-Weibull random variable as

$$G(x) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \int_0^{F(x)} t^{\alpha-1} (1-t)^{\beta-1} dt, \quad 0 < \alpha, \beta < \infty. \quad (1)$$

From (1), the corresponding probability density function for the beta-Weibull distribution is given by

$$g(x) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \frac{c}{\gamma} \left(\frac{x}{\gamma}\right)^{c-1} \left[1 - e^{-(x/\gamma)^c}\right]^{\alpha-1} e^{-\beta(x/\gamma)^c} \quad (2)$$

for $x > 0$, $\alpha, \beta, c, \gamma > 0$. One may introduce a location parameter ξ in the density in (2) by replacing x with $x - \xi$ where $-\infty < \xi < \infty$. In the rest of this article, take ξ to be zero.

The Weibull distribution has wide applications in many disciplines. See, e.g., Hallinan (1993), Johnson, Kotz, and Balakrishnan (1994). Various extensions have appeared in the literature. For instance, Zacks (1984) introduced the Weibull-exponential distribution. Mudholkar and Kollia (1994) defined a generalized Weibull distribution by introducing an additional shape parameter. Mudholkar, Srivastava, and Kollia (1996) applied the generalized Weibull distribution to model survival data. They showed that the distribution has increasing, decreasing, bathtub, and unimodal hazard functions.

Mudholkar, Srivastava, and Freimer (1995), Mudholkar and Hutson (1996) and Nassar and Eissa (2003) studied various properties of the exponentiated Weibull distribution. Mudholkar et al. (1995) applied exponentiated Weibull distribution to model failure data. Mudholkar and Hutson (1996) applied exponentiated Weibull distribution to extreme value data. They showed that exponentiated Weibull distribution has increasing, decreasing, bathtub, and unimodal hazard rates. The exponentiated exponential distribution proposed by Gupta and Kundu (1999, 2001) is a special case of the exponentiated Weibull family.

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Recently, Famoye et al. (2005) introduced a four-parameter beta-Weibull distribution. They showed that the beta-Weibull distribution is unimodal and obtained some results on the non-central moments. The maximum likelihood technique was used for parameter estimation and a likelihood ratio test was derived for the beta-Weibull distribution. The exponentiated Weibull distribution, Rayleigh distribution (Johnson et al., 1994, p. 686), the Type 2 extreme value distribution (Johnson, Kotz and Balakrishnan, 1995, p. 3), Burr Type (X) distribution (Johnson et al., 1994, p. 54), and the distribution of the order statistic from a Weibull population are special cases of the beta-Weibull distribution (Famoye et al., 2005).

In this article, the hazard function and entropy of the beta-Weibull distribution is examined. It is applied to several failure rate data and survival data. Some properties of the beta-Weibull model are discussed and the shapes of the hazard function are provided. Application of the beta-Weibull distribution to censored data sets is presented. Finally, the results of a simulation study are presented. The simulation study compares the beta-Weibull distribution with the exponentiated Weibull distribution.

Some Properties of Beta-Weibull Distribution

The survival function is given by $S(x) = 1 - G(x)$. The hazard function (or failure rate) of beta-Weibull distribution is given by

$$h(x) = \frac{g(x)}{1 - G(x)} = \frac{g(x)}{S(x)}, \quad (3)$$

where $G(x)$ and $g(x)$ are given by (1) and (2) respectively and $S(x)$ is the survival function.

Theorem 1: The limit of beta-Weibull hazard function as $x \rightarrow 0$ is

$$\lim_{x \rightarrow 0} h(x) = \begin{cases} \infty, & \text{when } \alpha c < 1 \\ \frac{c\Gamma(\alpha + \beta)}{\gamma\Gamma(\alpha)\Gamma(\beta)}, & \text{when } \alpha c = 1 \\ 0, & \text{when } \alpha c > 1. \end{cases} \quad (4)$$

and the limit of beta-Weibull hazard function as $x \rightarrow \infty$ is given by

$$\lim_{x \rightarrow \infty} h(x) = \begin{cases} \infty, & \text{when } c > 1 \\ \frac{\beta}{\gamma}, & \text{when } c = 1 \\ 0, & \text{when } c < 1. \end{cases} \quad (5)$$

Proof: When $x \rightarrow 0$, the limit of $h(x)$ is the same as the limit of $g(x)$. Famoye et al. (2005) obtained the limit in (4) for $g(x)$. When $x \rightarrow \infty$, the beta-Weibull hazard function in (3) is indeterminate as both numerator and denominator become 0. By using L'Hôpital's rule, the limit of $h(x)$ as $x \rightarrow \infty$ is given by (5). This completes the proof.

Theorem 2: The beta-Weibull distribution has

- a constant ($= \beta/\gamma$) failure rate when $\alpha c = 1$,
- a decreasing failure rate when $\alpha c \leq 1$ and $c \leq 1$,
- an increasing failure rate when $\alpha c \geq 1$ and $c \geq 1$,
- a bathtub failure rate when $\alpha c < 1$ and $c > 1$, and
- upside down bathtub (or unimodal) failure rate when $\alpha c > 1$ and $c < 1$.

Proof: It follows from Theorem 1.

Glaser (1980) gave sufficient conditions to characterize a given failure rate distribution as being bathtub shaped (BT), increasing failure rate (IFR), upside-down bathtub (UBT), or decreasing failure rate (DFR). Glaser defined the quantity $\eta(t) = -g'(t)/g(t)$ where $g(t)$ is the probability density function and gave a list of conditions to characterize a given failure rate based on $\eta'(t)$. It is not difficult to show that the beta-Weibull distribution satisfies all the conditions given by Glasser (1980). In Figure 1, the various shapes for the beta-Weibull hazard functions are provided.

Figure 1: Beta-Weibull hazard functions for $\beta=2.0$, $\gamma=4.0$ and various values of $\alpha=a$ and c

Entropies

Entropy has been used in various situations in science and engineering. Numerous entropy measures have been studied and compared in the literature. See the recent work of Nadarajah and Zografos (2005) and the references therein. Nadarajah and Zografos (2003) derived formulas for Renyi and Shannon entropies for 26 continuous univariate distributions.

The entropy of a random variable X with density $g(x)$ is a measure of variation of the uncertainty. Renyi entropy is defined by

$$I_R(\rho) = \frac{1}{1-\rho} \log \left\{ \int g^\rho(x) dx \right\}, \quad (6)$$

where $\rho > 0$ and $\rho \neq 1$, Renyi (1961). For the beta-Weibull density see equation 7. By using the substitution $t = (x/\gamma)^c$ and simplifying the resulting quantity, equation 8 is obtained. Hence,

$$\int_0^\infty g^\rho(x)dx = \left[\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \frac{c}{\gamma} \right]^\rho \int_0^\infty (x/\gamma)^{\rho(c-1)} [1 - \exp[-(x/\gamma)^c]]^{\rho(\alpha-1)} \exp[-\rho\beta(x/\gamma)^c] dx \quad (7)$$

$$\int_0^\infty g^\rho(x)dx = \left[\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \right]^\rho \left(\frac{c}{\gamma} \right)^{\rho-1} \sum_{k=0}^\infty \frac{(-1)^k \Gamma(\rho(\alpha-1)+1) \Gamma(\rho(1-1/c)+1/c)}{k! \Gamma(\rho(\alpha-1)-k+1) (k+\beta\rho)^{\rho(1-1/c)+1/c}} \quad (8)$$

$$I_R(\rho) = -\log(c/\gamma) + \frac{\rho}{1-\rho} \log \left(\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \right) + \frac{1}{1-\rho} \log \left\{ \sum_{k=0}^\infty \frac{(-1)^k \Gamma(\rho(\alpha-1)+1) \Gamma(\rho(1-1/c)+1/c)}{k! \Gamma(\rho(\alpha-1)-k+1) (k+\beta\rho)^{\rho(1-1/c)+1/c}} \right\} \quad (9)$$

$$\begin{aligned} E[-\log(g(x))] &= -\log \left(\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \right) - [(\alpha-1)\psi(\alpha) + (1-1/c)\Gamma'(1)] \\ &+ \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \sum_{k=0}^\infty \binom{\alpha-1}{k} \frac{(-1)^k}{k+\beta} [(\alpha-1)\psi(\alpha-k) + (1-1/c)\log(k+\beta) + \beta/(k+\beta)] \end{aligned} \quad (10)$$

Renyi entropy for the beta-Weibull density is given by equation 9.

The Shannon's (1948) entropy is defined as $E[-\log(g(x))]$. This is a special case of (6) when $\rho \rightarrow 1$. Hence, the Shannon entropy is obtained by taking the limit of (9) as $\rho \rightarrow 1$. On taking the limit of (9) as $\rho \rightarrow 1$, $0/0$ is obtained and hence, the L'Hopital's rule is applied. After using this rule and simplifying, equation 10 is obtained, where $\psi(\cdot)$ is the digamma function and $\Gamma'(\cdot)$ is the derivative of the gamma function.

Applications of beta-Weibull distribution to censored data

In survival analysis, the data may be in grouped form or in ungrouped form and quite often, the data involve censoring. In the case of grouped data, the right censoring is in the form of a last open interval as provided in Tables 1 and 2. Suppose a grouped data consisting of k intervals and the j^{th} interval (I_{j-1}, I_j) contains n_j observations for $j = 1, 2, 3, \dots, k-1$. The boundary I_0 is equal to 0 and the k^{th} interval

(I_{j-1}, ∞) has n_k observations. The total number of observations is $n = \sum_{j=1}^k n_j$. By using the result in Lawless (1982), the log-likelihood function for the grouped data is

$$\begin{aligned} \ell(\alpha, \beta, c, \gamma) &= \sum_{j=1}^{k-1} n_j \log[S(I_{j-1}) - S(I_j)] \\ &+ n_k \log[S(I_{k-1})] \end{aligned} \quad (11)$$

where $S(\cdot)$ is the beta-Weibull survival function. Estimates of the parameters are obtained by maximizing (11), the logarithm of the censored likelihood function.

The log-likelihood function for the ungrouped data $x_j, j = 1, 2, 3, \dots, n$ is given by

$$\ell(\alpha, \beta, c, \gamma) = \sum_u \log[h(x_j)] + \sum_{j=1}^n \log[S(x_j)], \quad (12)$$

where $h(\cdot)$ is the beta-Weibull hazard function given by (3) and $\sum_u$ denotes the summation over the uncensored observations. Estimates of the parameters are obtained by maximizing (12), the log-likelihood function. Both the log-likelihood functions in (11) and (12) are maximized directly by using *nlminb*, an SPLUS non-linear optimization routine with bounds. Taking the first and second partial derivatives of (11) and (12) with respect to the model parameters are quite involving. Hence, the Bootstrap method is used, Efron (1981), to estimate the standard errors of the parameter estimates for the beta-Weibull distribution.

Mudholkar et al. (1995) re-analyzed the classical bus-motor-failure data, first considered by Davis (1952), for a fleet of 191 buses. Mudholkar et al. (1995) re-analyzed the first, second, third, fourth, and fifth motor failures. They found that only the exponentiated Weibull provides a good fit to the first two data sets. However, the exponential, the Weibull, and the exponentiated Weibull provide good fits to the last three data sets. In this article, the beta Weibull is applied to all data sets and it provides excellent fits to all. However, the result for the first and the second motor failures are presented in Tables 1 and 2.

The beta-Weibull parameter estimates (standard errors in parentheses) in Table 1 are as follows: $\hat{\alpha} = 0.3707(0.0610)$, $\hat{\beta} = 0.1256(0.0189)$, $\hat{c} = 4.5753(1.853)$, $\hat{\gamma} = 76.2155(1.5219)$. The beta-Weibull model has an increasing hazard rate for these parameter estimates because $\hat{\alpha}\hat{c} > 1$ and $\hat{c} > 1$.

The beta-Weibull maximum likelihood estimates (standard errors in parentheses) in Table 2 are as follows: $\hat{\alpha} = 0.1479(0.0634)$, $\hat{\beta} = 0.1757(0.0821)$, $\hat{c} = 5.5104(1.3385)$, $\hat{\gamma} = 81.4003(5.6775)$. The beta-Weibull model has a bathtub hazard rate for these parameter estimates because $\hat{\alpha}\hat{c} < 1$ and $\hat{c} > 1$.

The exponentiated Weibull and beta-Weibull distributions provided adequate fits to the two data sets, but the fit from beta-Weibull distribution is better by using the chi-square goodness of fit measure. Also, the expected frequencies from the beta-Weibull model are much closer to the observed frequencies than the corresponding results from exponentiated Weibull model. In particular, it is noticed that only Beta-Weibull identifies that the failure rate has a bathtub shape, which logically fits the failure rate of motors well as shown in the above data. The last class (120,000 miles and up) had lower occurrence because the data is right-censored.

Table 1. Re-analysis of the First Bus-Motor Failure

Class interval (1,000 miles)	Observed frequency	Expected frequency		Beta Weibull
		Weibull	Exponentiated Weibull	
0 – 20	6	1.4066	3.8965	5.2925
20 – 40	11	8.9031	11.7722	11.8987
40 – 60	16	21.2228	19.6848	17.4895
60 – 80	25	33.5374	27.4955	24.2573
80 – 100	34	39.8566	34.5251	34.1451
100 – 120	46	36.7799	38.3690	42.5039
120 – 140	33	26.3822	33.8352	35.5682
140 – 160	16	14.5357	18.0184	16.2516
160 – up	4	8.3757	3.4034	3.5932
Total	191	191.0	191.0	191.0
Pearson χ^2		26.218	3.979	0.836
df		6	5	4
p-value		0.0002	0.5524	0.9336
Log-likelihood		-389.936	-381.811	-380.335

Table 2. Re-analysis of the Second Bus-Motor Failure

Class interval (1,000 miles)	Observed frequency	Expected frequency		Beta Weibull
		Weibull	Exponentiated Weibull	
0 – 20	19	13.3474	16.7866	18.6316
20 – 40	13	19.4117	15.8037	14.1624
40 – 60	13	18.7796	15.4234	13.0820
60 – 80	15	15.7765	15.1924	13.4357
80 – 100	15	12.1399	15.0160	16.0268
100 – 120	18	8.7520	14.6341	17.5898
120 – up	11	15.7929	11.1438	11.0717
Total	104	104.0	104.0	104.0
Pearson χ^2		18.2291	1.9485	0.3611
df		4	3	2
p-value		0.0011	0.5832	0.8348
Log-likelihood		-208.872	-201.707	-200.918

Mudholkar et al. (1995) applied the exponentiated Weibull distribution to model Efron's (1988) Arm A data on the survival times of 51 head-and-neck cancer patients given in Table 3. The beta-Weibull model was applied to fit the data in Table 3 and the result were grouped into 13 classes as in Table 12 of Mudholkar et al. (1995). For more details about the data, see Mudholkar et al. (1995). The results of the analysis and that of Mudholkar et al.

(1995) are presented in Table 4. The fits from both exponentiated Weibull and beta-Weibull distributions are very similar for the data. It appears the exponentiated Weibull distribution is slightly better because it has only three parameters compared to the beta-Weibull distribution with four parameters. A likelihood ratio test can be applied to test the adequacy of beta-Weibull distribution against a reduced special case (Famoye et al. 2005).

Table 3. Survival Times (in days) for the Patients in Arm A of the Head-and-Neck-Cancer Trial

7, 34, 42, 63, 64, 74+, 83, 84, 91, 108, 112, 129, 133, 133, 139, 140, 140, 146, 149, 154, 157, 160, 160, 165, 173, 176, 185+, 218, 225, 241, 248, 273, 277, 279+, 297, 319+, 405, 417, 420, 440, 523, 523+, 583, 594, 1101, 1116+, 1146, 1226+, 1349+, 1412+, 1417.

Note. Data is from Efron (1988); + indicates observations lost to follow-up.

Table 4. Re-analysis of Arm A of the Head-and-Neck-Cancer Trial

j^{th} class interval (in months)	N_j	S_j	Expected Deaths (E_j)		
			Weibull	Exponentiated Weibull	Beta Weibull
0 – 1	51	1	4.2739	1.8814	1.8374
1 – 2	50	2	3.8787	4.2669	4.2335
2 – 3	48	5	3.5922	4.6938	4.6845
3 – 4	42	2	3.0697	4.1702	4.1676
4 – 6	72	15	5.1380	6.8828	6.8742
6 – 8	49	3	4.4120	4.3158	4.3023
8 – 11	56	4	3.8190	4.4572	4.4353
11 – 14	45	3	3.0079	3.1773	3.1583
14 – 18	45	2	2.9567	2.8248	2.8091
18 – 24	46	2	2.9666	2.5099	2.5019
24 – 31	49	0	3.0988	2.2784	2.2833
31 – 38	47	2	2.9258	1.9072	1.9241
38 – 47	28	1	1.7189	1.0029	1.0197
$\sum_{j=1}^{13} R_j^2$			27.930	17.490	17.410
Approx. df			11	10	9
p -value			0.0033	0.0642	0.0427

Note. $R_j = \sqrt{2} \text{sign}(S_j - E_j) \left[S_j \log(S_j / E_j) + (N_j - S_j) \log \left(\frac{N_j - S_j}{N_j - E_j} \right) \right]^{1/2}$.

The parameter estimates (standard errors in parentheses) from beta-Weibull model are as follows: $\hat{\alpha} = 11.2139(3.3705)$, $\hat{\beta} = 0.5874(0.1791)$, $\hat{c} = 0.3859(0.0622)$, $\hat{\gamma} = 0.2947(0.1451)$. The estimates show that the model has a unimodal hazard function because $\hat{\alpha}\hat{c} > 1$ and $\hat{c} < 1$.

Comparison between beta-Weibull and exponentiated Weibull distributions

In the previous section, the fits from both beta-Weibull and exponentiated Weibull distributions are very close. In this section, a simulation is conducted to compare these two distributions. The parameters are estimated by the method of maximum likelihood. Samples of sizes $n = 250, 500$, and 1000 were generated from beta-Weibull and exponentiated Weibull distributions. The parameter sets for which the beta-Weibull hazard function is bathtub (Table 5), unimodal (Table 6), increasing (Table 7), and decreasing (Table 8) are simulated. For each simulated sample, the likelihood ratio test proposed by Famoye et al. (2005) is applied to compare the beta-Weibull and exponentiated Weibull distributions. In each case, there is no significance difference between the two models. The biases were examined (actual parameter value minus the estimated value) and the standard errors of the maximum likelihood estimates. These biases and the standard errors tell a different story.

For each sample size, 100 different samples were generated in order to obtain 100 parameter estimates which are used to compute the biases and the standard errors. The biases and the standard errors of the maximum likelihood estimates (mle) are reported in Tables 5 through 8. When the parameter $\beta = 1$, the simulated data is considered to be from the exponentiated Weibull distribution. The following are some observations from the simulation study.

a. For the parameter set of a bathtub hazard function (Table 5):

a.1 When $\beta < 1$, the biases of the mle from beta-Weibull estimates are smaller than the corresponding biases from the exponentiated

Weibull distribution. The standard errors of the mle of α and c for the two distributions are comparable, while the standard errors of the mle of γ are larger for beta-Weibull distribution.

a.2 When $\beta = 1$, the biases and standard errors of the mle of α and c for the two distributions are comparable. When comparing the mle of γ , the beta-Weibull distribution seems to have larger bias and standard error.

a.3 When $\beta > 1$, the biases and standard errors of the mle for beta-Weibull distribution seem to be larger than the biases and standard errors of the mle for exponentiated Weibull distribution.

b. For the parameter set of a unimodal hazard function (Table 6):

b.1 When $\beta < 1$, similar results as in (a.1) are observed.

b.2 When $\beta = 1$, similar results as in (a.2) are observed.

b.3 When $\beta > 1$, the biases of the mle of α and c are larger for beta-Weibull, while the standard errors of the mle of α and c for the two distributions are comparable. The mle of γ have comparable biases for the two distributions. The mle of γ have larger standard errors for the beta-Weibull distribution.

c. For the parameter set of an increasing hazard function (Table 7):

c.1 When $\beta < 1$, similar results as in (a.1) are observed.

c.2 When $\beta = 1$, the biases and standard errors of the mle of α for beta-Weibull are smaller than the biases and standard errors of the mle from exponentiated Weibull. The biases of the mle of c are larger for beta-Weibull but the standard errors are comparable for the two distributions. Both biases and standard errors of the mle of γ are larger for beta-Weibull.

c.3 When $\beta > 1$, the biases and standard errors of the mle of α for the two distributions are

comparable. The biases of the mle of c are slightly larger for beta-Weibull but the standard errors are comparable for the two distributions. The estimates of γ have larger biases and standard errors for the beta-Weibull.

d. For the parameter set of a decreasing hazard function (Table 8):

d.1 When $\beta < 1$, both biases and standard errors of the mle of α , c and γ are smaller for beta-Weibull.

d.2 When $\beta = 1$, similar results as in (c.2) are observed.

d.3 When $\beta > 1$, the biases and standard errors of the mle of α and c for the two distributions are comparable. The estimates of γ have comparable biases with larger standard errors for the beta-Weibull.

Conclusion

The biases of the mle from beta-Weibull distribution are smaller than the biases of the mle from exponentiated Weibull model with comparable standard errors when $\beta < 1$. The biases and standard errors are, in general, smaller for the exponentiated Weibull distribution when $\beta \geq 1$. In all the three examples in previous section, the estimates for parameter β are less than 1.0 and thus, this simulation study supports the use of the beta-Weibull distribution for describing the data sets. In addition, another implication of the simulation results is that one can take the advantage of the Beta-Weibull distribution and the exponentiated Weibull distribution by using the Beta-Weibull distribution and setting up the upper bound of parameter estimate of β to be one.

Table 5: Bias (standard error) of parameter estimate for $\alpha = 0.5$, $c = 1.5$ and various values of β and γ (bathtub hazard function)

Actual values			Exponentiated Weibull distribution			
β	γ	n	$\hat{\alpha}$	$\hat{c}$	$\hat{\gamma}$	
0.5	2	250	.006 (.097)	-.093 (.224)	-1.457 (0.397)	
		500	.036 (.067)	-.151 (.164)	-1.577 (0.262)	
		1000	.036 (.048)	-.143 (.118)	-1.597 (0.217)	
	4	250	.005 (.097)	-.093 (.224)	-2.909 (0.793)	
		500	.037 (.067)	-.155 (.168)	-3.158 (0.528)	
		1000	.036 (.047)	-.144 (.119)	-3.192 (0.431)	
1.0	2	250	-.030 (.147)	-.036 (.317)	.021 (0.364)	
		500	-.009 (.105)	-.035 (.229)	-.003 (0.270)	
		1000	.000 (.058)	-.023 (.133)	-.010 (0.157)	
	4	250	-.031 (.147)	-.038 (.318)	.046 (0.722)	
		500	-.011 (.105)	-.030 (.228)	.004 (0.537)	
		1000	.000 (.058)	-.023 (.133)	-.021 (0.314)	
2.0	2	250	-.017 (.137)	-.024 (.289)	.821 (0.200)	
		500	-.012 (.101)	.000 (.200)	.815 (0.149)	
		1000	-.023 (.070)	.042 (.133)	.839 (0.102)	
	4	250	-.020 (.134)	-.016 (.278)	1.658 (0.378)	
		500	-.012 (.100)	.001 (.198)	1.631 (0.294)	
		1000	-.023 (.070)	.042 (.133)	1.677 (0.204)	
Actual values			Beta-Weibull distribution			
β	γ	n	$\hat{\alpha}$	$\hat{\beta}$	$\hat{c}$	$\hat{\gamma}$
0.5	2	250	-.030 (.094)	-.104 (.253)	.032(.210)	-.171 (0.897)
		500	-.005 (.068)	-.066 (.237)	-.002 (.163)	-.143 (0.853)
		1000	-.013 (.051)	-.018 (.232)	.026 (.123)	.024 (0.825)
	4	250	-.030 (.094)	-.106 (.250)	.030 (.210)	-.360 (1.778)
		500	-.004 (.069)	-.069 (.239)	-.007 (.170)	.311 (1.728)
		1000	-.013 (.052)	-.018 (.231)	.025 (.123)	.041 (1.641)
1.0	2	250	-.049 (.145)	.185 (.395)	.033 (.291)	.392 (0.731)
		500	-.035 (.107)	.261 (.385)	.053 (.227)	.508 (0.749)
		1000	-.027 (.065)	.245 (.378)	.061 (.157)	.489 (0.710)
	4	250	-.049 (.143)	.163 (.409)	.028 (.292)	.717 (1.481)
		500	-.037 (.106)	.253 (.405)	.058 (.224)	1.003 (1.539)
		1000	-.027 (.065)	.245 (.378)	.061 (.157)	.977 (1.421)
2.0	2	250	-.036 (.132)	1.126 (.497)	.047 (.255)	.999 (0.496)
		500	-.040 (.100)	1.261 (.384)	.086 (.198)	1.127 (0.429)
		1000	-.051 (.075)	1.203 (.509)	.119 (.154)	1.098 (0.516)
	4	250	-.038 (.133)	1.124 (.490)	.047 (.259)	1.994 (0.992)
		500	-.039 (.099)	1.240 (.415)	.085 (.197)	2.217 (0.902)
		1000	-.052 (.073)	1.224 (.486)	.123 (.148)	2.237 (0.990)

Table 6: Bias (standard error) of parameter estimate for $\alpha = 1.5$, $c = 0.75$ and various values of β and γ (unimodal hazard function)

Actual values			Exponentiated Weibull distribution			
β	γ	n	$\hat{\alpha}$	$\hat{c}$	$\hat{\gamma}$	
0.5	2	250	-.562 (.449)	.119 (.056)	-1.080 (0.399)	
		500	-.450 (.303)	.103 (.043)	-1.277 (0.555)	
		1000	-.343 (.197)	.090 (.029)	-1.496 (0.402)	
0.5	4	250	-.594 (.511)	.121 (.059)	-2.090 (1.457)	
		500	-.446 (.303)	.103 (.043)	-2.572 (1.110)	
		1000	-.337 (.198)	.089 (.029)	-3.016 (0.800)	
1.0	2	250	-.052 (.458)	-.022 (.120)	-.077 (0.680)	
		500	-.028 (.367)	-.010 (.088)	-.046 (0.509)	
		1000	-.045 (.266)	.002 (.066)	.019 (0.388)	
1.0	4	250	-.018 (.431)	-.028 (.116)	-.243 (1.310)	
		500	-.022 (.363)	-.012 (.087)	-.108 (1.006)	
		1000	-.022 (.250)	-.003 (.064)	-.018 (0.747)	
2.0	2	250	-.058 (.532)	-.035 (.137)	1.085 (0.328)	
		500	.004 (.338)	-.032 (.099)	1.090 (0.238)	
		1000	.061 (.213)	-.035 (.066)	1.077 (0.159)	
2.0	4	250	-.055 (.523)	-.030 (.131)	2.172 (0.633)	
		500	.015 (.335)	-.035 (.098)	2.164 (0.472)	
		1000	.061 (.204)	-.035 (.065)	2.151 (0.308)	
Actual values			Beta-Weibull distribution			
β	γ	n	$\hat{\alpha}$	$\hat{\beta}$	$\hat{c}$	$\hat{\gamma}$
0.5	2	250	-.412 (.399)	-.107 (.221)	.072 (.065)	.153 (0.765)
		500	-.305 (.269)	-.071 (.225)	-.052 (.052)	.147 (0.791)
		1000	-.209 (.177)	-.047 (.222)	.039 (.042)	.116 (0.782)
0.5	4	250	-.439 (.436)	-.115 (.216)	.075 (.066)	.291 (1.519)
		500	-.306 (.268)	-.086 (.221)	.055 (.051)	.191 (1.562)
		1000	-.207 (.180)	-.056 (.222)	.040 (.043)	.168 (1.565)
1.0	2	250	-.019 (.439)	.147 (.395)	-.038 (.116)	.227 (0.940)
		500	-.001 (.373)	.156 (.388)	-.026 (.088)	.281 (0.877)
		1000	-.006 (.247)	.163 (.409)	-.018 (.066)	.320 (0.887)
1.0	4	250	.005 (.426)	.139 (.393)	-.041 (.115)	.392 (1.833)
		500	.004 (.373)	.162 (.394)	-.027 (.089)	.580 (1.769)
		1000	.009 (.244)	.148 (.402)	-.020 (.067)	.561 (1.744)
2.0	2	250	-.041 (.558)	1.013 (.553)	-.047 (.135)	1.074 (0.644)
		500	.024 (.342)	.975 (.678)	-.045 (.098)	1.027 (0.749)
		1000	.071 (.224)	.995 (.531)	-.043 (.070)	1.055 (0.522)
2.0	4	250	-.048 (.575)	1.011 (.623)	-.041 (.133)	2.179 (1.321)
		500	.032 (.343)	.974 (.678)	-.047 (.099)	2.046 (1.495)
		1000	.076 (.214)	1.025 (.538)	-.046 (.068)	2.159 (1.066)

Table 7: Bias (standard error) of parameter estimate for $\alpha = 1.5$, $c = 1.5$ and various values of β and γ (increasing hazard function)

Actual values			Exponentiated Weibull distribution			
β	γ	n	$\hat{\alpha}$	$\hat{c}$	$\hat{\gamma}$	
0.5	2	250	-.149 (.451)	.042 (.219)	-.926 (0.494)	
		500	-.146 (.449)	.067 (.190)	-.908 (0.444)	
		1000	-.120 (.274)	.076 (.120)	-.897 (0.293)	
	4	250	-.160 (.507)	.039 (.225)	-1.861 (1.037)	
		500	-.087 (.421)	.038 (.185)	-1.942 (0.849)	
		1000	-.083 (.261)	.063 (.114)	-1.861 (0.562)	
1.0	2	250	-.054 (.621)	-.064 (.284)	-.034 (0.386)	
		500	-.046 (.401)	-.017 (.187)	.003 (0.274)	
		1000	-.034 (.274)	-.005 (.137)	.009 (0.206)	
	4	250	-.047 (.620)	-.068 (.284)	-.081 (0.770)	
		500	-.007 (.375)	-.037 (.181)	-.047 (0.521)	
		1000	-.006 (.261)	-.017 (.134)	-.024 (0.396)	
2.0	2	250	-.054 (.530)	-.065 (.266)	.667 (0.243)	
		500	.011 (.330)	-.066 (.194)	.659 (0.170)	
		1000	.058 (.206)	-.068 (.130)	.646 (0.112)	
	4	250	-.038 (.526)	-.074 (.271)	1.321 (0.488)	
		500	.026 (.330)	-.074 (.194)	1.303 (0.343)	
		1000	.068 (.208)	-.075 (.130)	1.281 (0.226)	
Actual values			Beta-Weibull distribution			
β	γ	n	$\hat{\alpha}$	$\hat{\beta}$	$\hat{c}$	$\hat{\gamma}$
0.5	2	250	-.056 (.385)	-.066 (.220)	-.031(.197)	-.125 (0.542)
		500	-.045 (.378)	-.030 (.214)	-.013 (.165)	-.032 (0.506)
		1000	-.029 (.229)	-.081 (.224)	-.002 (.103)	-.145 (0.507)
	4	250	-.055 (.413)	-.045 (.222)	-.038 (.196)	-.178 (1.129)
		500	-.002 (.368)	-.031 (.215)	-.035 (.168)	-.135 (0.983)
		1000	-.001 (.228)	-.072 (.235)	-.013 (.107)	-.265 (1.028)
1.0	2	250	-.013 (.514)	.113 (.415)	-.090 (.266)	.127 (0.577)
		500	-.012 (.386)	.141 (.408)	-.049 (.179)	.197 (0.518)
		1000	.003 (.251)	.126 (.437)	-.041 (.135)	.184 (0.564)
	4	250	-.009 (.515)	.114 (.416)	-.092 (.267)	.250 (1.150)
		500	.013 (.381)	.108 (.387)	-.059 (.181)	.272 (0.956)
		1000	.013 (.253)	.056 (.415)	-.037 (.139)	.170 (1.038)
2.0	2	250	-.036 (.558)	1.012 (.588)	-.091 (.262)	.714 (0.473)
		500	.030 (.337)	.983 (.683)	-.092 (.194)	.695 (0.482)
		1000	.078 (.207)	1.053 (.531)	-.094 (.132)	.721 (0.398)
	4	250	-.037 (.581)	.962 (.624)	-.091 (.275)	1.356 (0.921)
		500	.038 (.342)	.948 (.671)	-.093 (.197)	1.321 (0.940)
		1000	.075 (.221)	.977 (.523)	-.089 (.139)	1.317 (0.739)

Table 8: Bias (standard error) of parameter estimate for $\alpha = 1.5$, $c = 0.5$ and various values of β and γ (decreasing hazard function)

Actual values			Exponentiated Weibull distribution			
β	γ	n	$\hat{\alpha}$	$\hat{c}$	$\hat{\gamma}$	
0.5	2	250	-1.018 (.627)	.111 (.035)	-.644 (0.914)	
		500	-.742 (.270)	.097 (.022)	-1.145 (0.634)	
		1000	-.633 (.180)	.090 (.016)	-1.433 (0.469)	
	4	250	-1.017 (.627)	.112 (.035)	-1.286 (1.829)	
		500	-.746 (.272)	.097 (.022)	-2.280 (1.269)	
		1000	-.633 (.180)	.090 (.016)	-2.867 (0.937)	
1.0	2	250	-.114 (.478)	-.002 (.071)	-.028 (0.896)	
		500	-.043 (.363)	-.004 (.056)	-.067 (0.723)	
		1000	.034 (.248)	.001 (.042)	-.004 (0.540)	
	4	250	-.095 (.467)	-.005 (.072)	-.130 (1.794)	
		500	-.043 (.364)	-.004 (.056)	-.136 (1.446)	
		1000	-.029 (.246)	-.000 (.042)	-.028 (1.076)	
2.0	2	250	-.065 (.524)	-.020 (.089)	1.361 (0.333)	
		500	.005 (.326)	-.020 (.062)	1.374 (0.232)	
		1000	.063 (.206)	-.024 (.043)	1.366 (0.161)	
	4	250	-.054 (.522)	-.022 (.090)	2.711 (0.667)	
		500	.019 (.318)	-.022 (.060)	2.737 (0.455)	
		1000	.061 (.204)	-.023 (.043)	2.729 (0.320)	
Actual values			Beta-Weibull distribution			
β	γ	n	$\hat{\alpha}$	$\hat{\beta}$	$\hat{c}$	$\hat{\gamma}$
0.5	2	250	-.777 (.482)	-.125 (.226)	.076(.039)	.564 (0.883)
		500	-.549 (.247)	-.093 (.203)	-.061 (.030)	.473 (0.795)
		1000	-.472 (.165)	-.122 (.207)	.059 (.024)	.226 (0.879)
	4	250	-.773 (.481)	-.120 (.227)	.076 (.039)	1.154 (1.774)
		500	-.555 (.251)	-.097 (.205)	.062 (.031)	.924 (1.598)
		1000	-.472 (.165)	-.122 (.207)	.059 (.024)	.452 (1.758)
1.0	2	250	-.086 (.483)	.164 (.370)	-.012 (.072)	.420 (1.088)
		500	-.008 (.368)	.205 (.357)	-.017 (.057)	.467 (1.055)
		1000	-.000 (.241)	.166 (.400)	-.012 (.044)	.345 (1.142)
	4	250	-.071 (.478)	-.159 (.368)	-.015 (.073)	.772 (2.178)
		500	-.009 (.369)	.205 (.356)	-.017 (.057)	.933 (2.108)
		1000	.001 (.243)	.155 (.402)	-.011 (.045)	.633 (2.287)
2.0	2	250	-.047 (.552)	1.061 (.529)	-.029 (.088)	1.366 (0.607)
		500	.029 (.330)	1.059 (.563)	-.030 (.062)	1.342 (0.636)
		1000	.078 (.215)	1.028 (.541)	-.031 (.046)	1.302 (0.595)
	4	250	-.051 (.576)	1.023 (.578)	-.028 (.091)	2.682 (1.236)
		500	.037 (.329)	1.040 (.566)	-.030 (.061)	2.631 (1.313)
		1000	.075 (.214)	1.023 (.536)	-.030 (.045)	2.597 (1.185)

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On the Properties of Beta-Gamma Distribution

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A class of generalized gamma distribution called the beta-gamma distribution is proposed. Some of its properties are examined. Its shape can be reversed J-shaped, unimodal, or bimodal. Reliability and hazard functions are also derived, and applications are discussed.

Key words: Gamma distribution, Beta distribution, reliability function, hazard function, MLE, application.

Introduction

Let $f(\cdot)$ and $F(\cdot)$ be the probability density function and the cumulative distribution function (cdf) of a random variable, respectively. Eugene, Lee, and Famoye (2002) first introduced a generalized distribution based on the logit of the beta random variable with a cumulative distribution function given by

$$G(x) = \frac{1}{B(\alpha, \beta)} \int_0^{F(x)} t^{\alpha-1} (1-t)^{\beta-1} dt, \quad 0 < \alpha, \beta < \infty,$$

and the corresponding probability density function is

$$g(x) = \frac{1}{B(\alpha, \beta)} F(x)^{\alpha-1} [1-F(x)]^{\beta-1} f(x), \quad 0 < \alpha, \beta < \infty$$

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Eugene, et al. (2002) studied properties of $g(x)$ when $F(\cdot)$ is the cdf of a normal distribution. Maynard (2003) examined the case when $F(\cdot)$ is the cdf of an exponential distribution.

Gamma distribution and its generalized distributions (e.g. McDonald, 1984) have been applied widely to the analyses of income distributions, life testing, and many physical and economical phenomena (e.g. Farewell, 1977, Lawless, 1980). In this article, the case when $F(\cdot)$ is the cdf of the gamma distribution is studied.

A random variable X is said to have a beta-gamma distribution, $BG(\alpha, \beta, \rho, \lambda)$, if its probability density function is given by

$$g(x) = \frac{x^{\rho-1} e^{-x/\lambda}}{B(\alpha, \beta) \Gamma(\rho) \lambda^\rho} F(x)^{\alpha-1} [1-F(x)]^{\beta-1}, \quad (1)$$

$$0 < \alpha, \beta, \rho, \lambda < \infty, \quad x > 0,$$

where $F(x)$ is the cdf of the gamma distribution with parameters ρ and λ . One can also introduce a location parameter ξ in the density in (1) by replacing x with $x - \xi$ where $-\infty < \xi < \infty$. In the rest of this article, it is assumed that ξ is zero. When both α and β are integers with $\alpha + \beta$ being a bounded integer, the beta-gamma density function in (1) is the marginal probability density function of

the α^{th} order statistic in a random sample of size $\alpha + \beta$ from the gamma distribution with parameters ρ and λ . When $\alpha = \beta = 1$, the beta-gamma distribution yields the gamma distribution. When $\rho = 1$, the beta-gamma distribution is beta-exponential distribution introduced in Maynard (2003).

Properties

The limit of $g(x)$ as x goes to 0 and the mode of the probability density function $g(x)$ in (1) is given in Lemma 1. The modes for cases when $\rho\alpha \leq 1$ and $\rho\alpha > 1$ are studied respectively. Although some cases can be shown mathematically, plotting the function $g(x)$ using Maple computer programs are employed to examine shapes and modalities for other cases. Illustrative graphs of $g(x)$ based on observations from numerous plots are presented. Numerical percentiles are presented in Table 7 to Table 9.

Limits

Lemma 1: The limit as x goes to 0 of the beta-gamma probability density function $g(x)$ in (1) is

$$\lim_{x \rightarrow 0} g(x) = \begin{cases} \infty & \text{if } \alpha\rho < 1 \\ \frac{1}{\Gamma^\alpha(\rho)B(\alpha, \beta)\rho^{\alpha-1}\lambda} & \text{if } \alpha\rho = 1 \\ 0 & \text{if } \alpha\rho > 1 \end{cases} \quad (2)$$

The proof is given in Appendix.

Modes of $g(x)$ When $\alpha\rho \leq 1$

Note that the derivative $df/dx = f(\rho - 1 - x/\lambda)/x$. The first derivative of the logarithm of the probability density function $g(x)$ is given by

$$\frac{\rho - 1 - x/\lambda}{x} + \frac{\alpha - 1}{F} f + \frac{1 - \beta}{1 - F} f. \quad (3)$$

The mode(s) x_m of $g(x)$ if exists is the solution to the equation by setting (3) to be zero.

It is shown below that $g(x)$ has a reversed-J shape when $\rho\alpha \leq 1$ and $\beta \geq 1$. The derivative in (3) is equal to

$$(1 - \beta) \frac{f}{1 - F} + \frac{1}{xF} [(\alpha - 1)xf + (\rho - 1 - x/\lambda)F]. \quad (4)$$

When $\beta \geq 1$, the first term in (4) is less or equal to 0. Also,

$$\begin{aligned} & \frac{d}{dx} [(\alpha - 1)xf + (\rho - 1 - x/\lambda)F] \\ &= (\alpha - 1)f + (\alpha - 1)xf \frac{\rho - 1 - x/\lambda}{x} \\ & \quad - F/\lambda + (\rho - 1 - x/\lambda)f \\ &= (\alpha\rho - 1)f - \alpha xf/\lambda - F/\lambda \end{aligned}$$

which is negative when $\alpha\rho \leq 1$. This implies that $(\alpha - 1)xf + (\rho - 1 - x/\lambda)F$ is a decreasing function. Because $(\alpha - 1)xf + (\rho - 1 - x/\lambda)F = 0$ when $x = 0$, the second term in (4) is therefore negative. That is, $g'(x)$ is negative. By (2) and the fact that $\lim_{x \rightarrow \infty} g(x) = 0$, $g(x)$ has a reversed-J shape for the cases when $\rho\alpha \leq 1$ and $\beta \geq 1$ with maximum occurring at $x = 0$.

When $\alpha \leq 1$ and $\rho \leq 1$ regardless of β , one can see that $g(x)$ has a reversed-J shape by rewriting $g(x)$ as

$$g(x) = \frac{1}{B(\alpha, \beta)} \frac{f(x)}{1 - F(x)} F(x)^{\alpha-1} [1 - F(x)]^\beta.$$

Because the cdf F is an increasing function and the hazard function $f/(1 - F)$ of the gamma distribution function is a decreasing function when $\rho \leq 1$, $g(x)$ is therefore a decreasing function with $\lim_{x \rightarrow 0} g(x) = \infty$ when $\alpha \leq 1$ and $\rho \leq 1$.

(2.3)

Figure 1. Plot of the density function $g(x)$ when $\rho\alpha = 1$, and $\beta = 0.25, 0.5, 2, 4$

Next, graphical results are shown to examine the cases when $\beta < 1$ and $\alpha\rho \leq 1$ with α or ρ greater than 1. Figure 1 represents

cases when $\alpha\rho = 1$. Figure 2 contains cases when $\alpha\rho < 1$. Note that $a = \alpha$, $b = \beta$, and $p = \rho$ in all figures in this article.

Figure 2. Plot of the density function $g(x)$ when $\rho\alpha < 1$, and $\beta=0.25, 0.5, 2, 4$

When $\rho\alpha = 1$ and $\beta \geq 1$, the beta-gamma distribution appears to have a reversed-J shape. Figure 1 also shows that when $\alpha = 2$ and $\rho = 0.5$, it has a non-zero mode for β values of 0.25 and 0.5.

When $\rho\alpha < 1$ and $\beta < 1$, it is found that $g(x)$ is not necessarily a reverse J-shape, it can be bimodal (with one mode at 0). Figure 3 shows two such cases. The top two are for $\rho = 0.25$, $\alpha = 3.9$, and $\beta = 0.5$; the bottom

graph is for $\rho = 2$, $\alpha = 0.49$, and $\beta = 0.01$. Note that the horizontal axis of the first plot ranges from 0 to 0.01 and the one of the second plot ranges from 0.01 to 2. Tables 1 – 4 give the 2nd non-zero mode in addition to the mode at $x = 0$ for some examples when $\alpha\rho < 1$ and $\rho < 1$. The empty cells are cases where $g(x)$ is reverse J-shaped and the only mode is at $x = 0$.

Figure 3. Graphs of $BG(\alpha, \beta, \rho, 1)$

Table 1. Nonzero 2nd mode of $BG(\alpha, \beta, \rho, 1)$ with $\rho = 1/2$.

	$\beta = 0.01$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$\alpha = 1.8$	1.04									
1.9	1.31	.529	.234							
1.95	1.42	.616	.319	.167	.074					
1.99	1.50	.678	.374	.219	.013	.071	.035	.012		

Table 2(a). Nonzero 2nd mode of $BG(\alpha, \beta, \rho, 1)$ with $\rho = 1/4$.

	$\beta = 0.01$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$\alpha = 3.01$										
3.02	.365									
3.1	.571									
3.2	.714									
3.3	.826	.274								
3.4	.923	.382								
3.5	1.01	.460	.193							
3.6	1.09	.526	.266	.103						
3.7	1.16	.585	.323	.173	.064					
3.8	1.22	.638	.373	.222	.124	.052				
3.9	1.29	.687	.417	.264	.165	.097	.049			

Table 2(b). Nonzero 2nd mode of $BG(\alpha, \beta, \rho, 1)$ with $\rho = 1/4$.

	$\beta = 0.91$	0.92	0.93	0.94	0.95	0.96	0.97	0.98	0.99
$\alpha = 3.99$	.004	.003	.001						
3.995	.005	.004	.003	.002	.001				

Table 3. Nonzero 2nd mode of $BG(\alpha, \beta, \rho, 1)$ with $\rho = 1/6$

	$\beta = .01$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$\alpha = 5.8$	1.21	.67	.41	.27	.17	.10	.05			
5.9	1.24	.69	.44	.29	.19	.12	.07	.036	.020	
5.99	1.27	.72	.48	.31	.21	.14	.09	.052	.026	.008

Table 4. Nonzero 2nd mode of $BG(\alpha, \beta, \rho, 1)$ with $\rho = 2$

	$\beta = 0.01$	0.015	0.1	0.2	0.3	0.4
$\alpha = 0.48$						
0.49	9.85					
0.499	9.86	7.656				

Note that, for example, when $\alpha = 0.48$, $\beta = 0.01$, and $\rho = 2$, $g(x)$ has an inversed-J shape and therefore does not have a nonzero mode. The range of β where $g(x)$ is bimodal appears to widen as α increases. When bimodality occurs, the nonzero mode increases as the parameter α increases and decreases as the parameter β increases. The bimodality property of beta-gamma distribution is not independent of the gamma parameters (α, ρ) . The bimodality property also exists for beta-normal (Famoye, Lee, & Eugene, 2004).

Modes when $\alpha\rho > 1$

The second derivative of the logarithm of $g(x)$ is given by

$$\frac{\rho-1-x/\lambda}{x} \left[\frac{(\alpha-1)f}{F} + \frac{(1-\beta)f}{1-F} + \frac{\rho-1-x/\lambda}{x} \right] - \left[\frac{(\rho-1-x/\lambda)^2}{x^2} + \frac{(\alpha-1)f^2}{F^2} - \frac{(1-\beta)f^2}{(1-F)^2} + \frac{\rho-1}{x^2} \right]$$

The first term equals to 0 at the mode x_m .

Hence, when $x = x_m$,

$$\frac{d^2 \ln g}{dx^2} = - \left[\frac{(\rho-1-x)^2}{x^2} + \frac{(\alpha-1)f^2}{F^2} + \frac{(\beta-1)f^2}{(1-F)^2} + \frac{\rho-1}{x^2} \right]. \quad (5)$$

When $\beta \geq 1, \alpha \geq 1$, and $\rho \geq 1$, (5) is less than 0 at $x = x_m$. In this case, since there must be a minimum between any two maxima and that $\lim_{x \rightarrow 0} g(x) = 0$ and $\lim_{x \rightarrow \infty} g(x) = 0$, it is concluded that $g(x)$ is unimodal with a concave shape.

When $\beta \geq 1$ and $\alpha\rho > 1$ with $\alpha < 1$ or $\rho < 1$, though not being shown mathematically, graphs of such cases indicate that beta-gamma density function $g(x)$ is also unimodal with a concave shape. Based on numerous graphs, the density functions $g(x)$ is unimodal when $\alpha\rho > 1$ regardless the value of β . The following illustrates some examples when $\alpha\rho > 1$.

Figure 4. Plot of the density function $g(x)$ when $\rho\alpha > 1$, and $\beta=0.5, 1.5$

In this case $g(x)$ is unimodal with a concave shape and the mode is nonzero. Tables 5 and 6 tabulate modes for $BG(\alpha, \beta, 2, 1)$ and $BG(\alpha, \beta, 1/2, 1)$ when $\rho\alpha > 1$.

The results indicate that when $\rho\alpha > 1$ the mode increases as α increases and that the mode decreases as β increases for both $BG(\alpha, \beta, 2, 1)$ and $BG(\alpha, \beta, 1/2, 1)$; see

also Figure 4. For other cases when $\alpha\rho > 1$, this pattern holds for other values of parameters ρ and λ though the computation results are not reported here.

Percentiles of $g(x)$

The 50th, 75th, 90th, and 95th percentiles of $BG(\alpha, \beta, \rho, 1)$ are computed and tabulated in the following Tables 7-9.

Table 5. Modes for $BG(\alpha, \beta, 2, 1)$ when $\rho\alpha > 1$

	$\beta=0.2$	0.5	1	1.5	2	2.5	5	10
$\alpha=1$	2.236	1.414	1.000	.8165	.7071	.6325	.4472	.3162
$\alpha=1.5$	3.206	2.162	1.555	1.270	1.097	.9775	.6815	.4744
$\alpha=2$	3.729	2.628	1.938	1.598	1.386	1.238	.8644	.5994
$\alpha=2.5$	4.087	2.963	2.229	1.856	1.618	1.451	1.018	.7063
$\alpha=5$	5.055	3.915	3.111	2.672	2.379	2.163	1.570	1.107
$\alpha=10$	5.913	4.787	3.964	3.498	3.176	3.947	2.228	1.626

Table 6. Modes for $BG(\alpha, \beta, 1/2, 1)$ when $\rho\alpha > 1$.

	$\beta=0.2$	0.5	1	1.5	2	2.5	5	10
$\alpha=2.5$	0.832	.3919	.1692	.0903	.0545	.0359	.0291	.0154
$\alpha=5$	1.788	1.129	.7150	.5137	.3923	.3114	.1337	.0735
$\alpha=10$	2.653	1.798	1.286	1.016	.8411	.7155	.3925	.1812

Table 7. Percentiles of $BG(\alpha, \beta, \rho, 1)$ with $\rho = 1/2$

α	β	50th	75th	90th	95th
0.25	0.25	.2275	2.011	5.260	7.855
	0.5	.0235	.4372	1.684	2.846
	1	.0031	.0831	.4479	.8765
	2	.0005	.0169	.1116	.2445
	4	.0001	.0038	.0277	.0654
0.5	0.25	.9346	3.194	6.550	9.171
	0.5	.2275	1.054	2.530	3.716
	1	.0508	.3014	.8588	1.358
	2	.0115	.0802	.2632	.4522
	4	.0027	.0207	.0752	.1370
1	0.25	1.735	4.163	7.568	10.21
	0.5	.6617	1.735	3.317	4.570
	1	.2275	.6617	1.353	1.921
	2	.0706	.2275	.5022	.7405
	4	.0202	.0706	.1678	.2576
2	0.25	2.473	4.979	8.413	11.06
	0.5	1.205	2.405	4.044	5.316
	1	.5531	1.123	1.899	2.501
	2	.2275	.4817	.8367	1.115
	4	.0816	.1824	.3306	.4504
4	0.25	3.160	5.710	9.166	11.82
	0.5	1.787	3.057	4.731	6.016
	1	.9914	1.649	2.478	3.102
	2	.5073	.8444	1.261	1.570
	4	.2275	.3872	.5869	.7351

Table 8. Percentiles of $BG(\alpha, \beta, \rho, 1)$ with $\rho = 1$

α	β	50th	75th	90th	95th
0.25	0.25	.6939	3.106	6.752	9.535
	0.5	.1882	1.050	2.710	4.070
	1	.0645	.3804	1.067	1.685
	2	.0265	.1577	.4517	.7249
	4	.0120	.0718	.2065	.3330
0.5	0.25	1.763	4.466	8.125	10.90
	0.5	.6925	1.919	3.704	5.077
	1	.2877	.8267	1.661	2.328
	2	.1285	.3729	.7592	1.075
	4	.0512	.1758	.3588	.5086
1	0.25	2.773	5.545	9.210	11.98
	0.5	1.386	2.773	4.605	5.991
	1	.6931	1.386	2.303	2.996
	2	.3466	.6931	1.151	1.498
	4	.1733	.3466	.5756	.7489
2	0.25	3.644	6.436	10.10	12.88
	0.5	2.115	3.565	5.366	6.720
	1	1.228	2.010	2.970	3.676
	2	.6931	1.120	1.631	2.000
	4	.3766	.6055	.8768	1.071
4	0.25	4.428	7.229	10.90	13.68
	0.5	2.836	4.312	6.167	7.556
	1	1.838	2.668	3.650	4.363
	2	1.159	1.641	2.187	2.571
	4	.6931	.9706	1.278	1.490

Table 9. Percentiles of $BG(\alpha, \beta, \rho, 1)$ with $\rho = 2$

α	β	50th	75th	90th	95th
0.25	0.25	1.678	4.874	9.049	12.09
	0.5	.7450	2.220	4.397	6.021
	1	.4035	1.142	2.244	3.094
	2	.2482	.6713	1.273	1.729
	4	.1631	.4277	.7860	1.050
0.5	0.25	3.197	6.479	10.58	13.58
	0.5	1.678	3.404	5.597	7.194
	1	.9613	1.887	3.063	3.922
	2	.5961	1.128	1.782	2.254
	4	.3893	.7157	1.102	1.374
1	0.25	4.472	7.710	11.76	14.74
	0.5	2.693	4.472	6.638	8.212
	1	1.678	2.693	3.890	4.744
	2	1.078	1.678	2.365	2.845
	4	.7095	1.078	1.487	1.767
2	0.25	5.519	8.710	12.72	15.69
	0.5	3.653	5.425	7.560	9.116
	1	2.473	3.518	4.712	5.557
	2	1.678	2.320	3.023	3.505
	4	1.135	1.536	1.963	2.250
4	0.25	6.434	9.587	13.57	16.53
	0.5	4.549	6.299	8.408	9.949
	1	3.296	4.344	5.526	6.359
	2	2.376	3.036	3.744	4.225
	4	1.678	2.103	2.543	2.834

The percentiles increase as α increases and decrease as β increases with fixed ρ , which is consistent with the results of modes. As seen in all figures, the beta-gamma distribution is skewed to the right, one would expect that the mode to be less than the median.

Moments

The closed form solutions of moments for $BG(\alpha, \beta, \rho, \lambda)$ exist only when α and β are integers. The closed form solution for the n th

moment of $BG(\alpha, \beta, \rho, \lambda)$ is derived in Theorem 1 for the cases when α and β are integers in this section. The first four moments are also numerically computed for various parameters.

Theorem 1: When α, β are integers, the n th moment of the beta-gamma random variable $BG(\alpha, \beta, \rho, \lambda)$ is given by

$$\frac{1}{B(\alpha, \beta)} \sum_{j=0}^{\beta-1} (-1)^j \binom{\beta-1}{j} \left\{ \sum_{k=0}^{\alpha+j-1} (-1)^k \binom{\alpha+j-1}{k} I_{n,k} \right\} \quad (6)$$

where

$$I_{n,k} = \int_0^{\infty} x^n f(x) (1-F)^k dx.$$

The proof is given in Appendix. The follow Corollary gives $E(X)$ and $E(X^2)$ that are used to obtain variance.

Corollary 1: When $\alpha = 2, \beta = 1$ and ρ is an integer, $E(X)$ and $E(X^2)$ are given by:

$$\begin{aligned} E(X) &= 2\lambda\rho - \sum_{i=0}^{\rho-1} \frac{\lambda(\rho+i)!}{2^{\rho+i}(\rho-1)!i!} \\ &= 2\lambda\rho - \rho\lambda \sum_{i=0}^{\rho-1} \frac{\binom{\rho+i}{\rho}}{2^{\rho+i}}; \end{aligned} \quad (7)$$

$$\begin{aligned} E(X^2) &= 2\lambda^2(\rho+1)\rho \\ &= \rho(\rho+1)\lambda^2 \left[2 - \sum_{i=0}^{\rho-1} \frac{\binom{\rho+i+1}{\rho+1}}{2^{\rho+i+1}} \right] \end{aligned} \quad (8)$$

The proof is given in Appendix.

Applying (6), the first four moments of $BG(\alpha, \beta, \rho, 1)$ for a certain combinations of the parameters are evaluated and given in Tables 10 and 11.

Table 10. The mean, std, skewness and kurtosis of $BG(\alpha, \beta, \rho, 1)$ with $\rho = 2$.

α	β	mean	std	skewness	kurtosis
1	1	2.000	1.414	1.415	6.005
	2	1.250	.8292	1.261	5.329
	4	.8047	.5048	1.120	4.768
	10	.4660	.2757	.9672	4.220
2	1	2.750	1.479	1.207	5.347
	2	1.824	.8975	1.010	4.588
	4	1.215	.5585	.8693	4.117
	10	.7150	.3063	.7319	3.736
4	1	3.547	1.494	1.106	5.094
	2	2.503	.9356	.8595	4.238
	4	1.747	.5987	.7038	3.779
	10	1.062	.3345	.5752	3.481
10	1	4.623	1.500	1.057	5.007
	2	3.503	.9505	.7650	4.063
	4	2.618	.6278	.5759	3.577
	10	1.705	.3654	.4363	3.302

Table 11. The mean, std, skewness and kurtosis of $BG(\alpha, \beta, \rho, 1)$ with $\rho = 1/2$

α	β	mean	std	skewness	kurtosis
1	1	.5000	.7071	2.829	15.00
	2	.1814	.2828	3.287	18.66
	4	.0604	.1038	3.834	26.22
	10	.0124	.0237	4.688	39.71
2	1	.8180	.8468	2.172	10.28
	2	.3523	.3830	2.290	11.11
	4	.1356	.1586	2.544	13.14
	10	.0319	.0413	3.032	17.96
4	1	1.235	.9584	1.762	8.011
	2	.6280	.4830	1.669	7.422
	4	.2868	.2289	1.718	7.614
	10	.0820	.0712	1.955	9.080
10	1	1.900	1.057	1.468	6.683
	2	1.154	.5878	1.218	5.491
	4	.6508	.3228	1.097	4.941
	10	.2505	.1290	1.119	4.968

Based on the numerical results, the mean and standard deviation appear to increase with α for a fixed β ; and skewness and kurtosis appear to decrease as α increases for a fixed β in both cases when $\rho = 2$ and $\rho = 1/2$. Based on Figure 4, the density function has a heavier right tail as α increases. The mean and standard deviation decrease as β decreases for a fixed α . Although the skewness and kurtosis decrease with β when $\rho = 2$ as shown in Table 10, the skewness and kurtosis increase with β when $\rho = 1/2$ and $\alpha\rho \leq 1$, as shown in Table 11. However, no clear pattern is noticed when $\alpha\rho > 1$.

Reliability and Hazard Functions

The reliability and hazard functions of the beta-gamma distribution are derived in this

section. The reliability function, $R(x) = 1 - P[X \leq x]$, at time x defined to be the probability that a unit X survives beyond time x . For a beta-gamma random variable, it is given by

$$1 - \frac{1}{B(\alpha, \beta)} \int_0^x F^{\alpha-1} (1-F)^{\beta-1} dF(t) \\ = 1 - \frac{1}{B(\alpha, \beta)} \int_0^{F(x)} t^{\alpha-1} (1-t)^{\beta-1} dt$$

where f and F are the density function and cdf of the gamma random variable with parameters ρ and λ , respectively. The hazard function defined to be a instantaneous measure of failure at time x given survival to time x is equal to

$$H(x) = \frac{g(x)}{R(x)} = \frac{\frac{1}{B(\alpha, \beta)} F^{\alpha-1} (1-F)^{\beta-1} f(x)}{1 - \frac{1}{B(\alpha, \beta)} \int_0^x F^{\alpha-1} (1-F)^{\beta-1} f(x) dx}.$$

Lemma 2:

- (a) $\lim_{x \rightarrow 0} H(x) = \lim_{x \rightarrow 0} g(x)$
- (b) $\lim_{x \rightarrow \infty} H(x) = \beta / \lambda$

The proof is given in Appendix.

The hazard functions of $BG(\alpha, \beta, \rho, 1)$ are plotted. Cases with $\alpha\rho < 1$ are presented in Figure 5 and cases with $\alpha\rho \geq 1$ are given in Figure 6. The graphs in the first column represent the cases $\alpha\rho = 1$ with $\beta = 1/2, 1$, and 2 ; and those in the second column represent the cases when $\alpha\rho > 1$ with $\beta = 1/2, 1$, and 2 in Figure 6.

Figure 5. Hazard Function of $BG(\alpha, \beta, \rho, 1)$ when $\alpha\rho < 1$

Figure 6. Hazard Function of $BG(\alpha, \beta, \rho, 1)$ when $\alpha\rho \geq 1$

As stated in Lemma 2, the curves of the hazard functions start at the values given in Lemma 1 and go to the value of β as x goes to ∞ regardless the values of other parameters. When $\alpha\rho < 1$ and $\beta \geq 1$ (see also Figure 2), $g(x)$ has a reversed J shape and the trends of hazard functions for $\beta = 1$ and $\beta = 2$ (both $\beta > 1$) are similar (Figure 5). When $\alpha\rho = 1$ and $\beta = 1/2$, the hazard function has a nonzero maximum or minimum. The hazard function is constant when $\alpha = \rho = \beta = 1$, since $g(x)$ is the exponential distribution. Within each plot, a larger α value seems to result in a larger value of the hazard function. When $\alpha\rho > 1$, $g(x)$ has a nonzero mode (see also Figure 4) and the corresponding hazard function is non-decreasing.

When $\alpha = \beta = 1$, it is Gamma function. $\lim_{x \rightarrow \infty} = 1/\lambda$, which is different from that of beta-gamma. Also, the hazard function of the beta-gamma can handle bathtub cases where gamma can not. Therefore, the beta-gamma distribution is more flexible. This is especially important when the beta parameter is not near one.

Parameter Estimation Using Maximum Likelihood Method

Let $x_1, x_2, \dots, x_n$ be a random sample of size n from a beta-gamma distribution defined in (1.1), the log-likelihood function $l(\alpha, \beta, \rho, \lambda)$ is then given by

$$n \log \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} + (\alpha - 1) \sum_{i=1}^n \log F(x_i) \\ + (\beta - 1) \sum_{i=1}^n \log(1 - F(x_i)) + \sum_{i=1}^n \log f(x_i),$$

where $f(x)$ and $F(x)$ are the pdf and cdf of the gamma distribution with parameters ρ and

λ , respectively. Let $\psi(z) = d\Gamma(z)/dz$ be the digamma function. The equations for solving the maximum likelihood estimates of α, β, ρ and λ are given in Appendix.

The example in the next section, initial estimates of ρ and λ is first computed by assuming the data set follows gamma distribution with $\alpha = 1$ and $\beta = 1$, the results from MLE of (ρ, λ) along with $\alpha = 1$ and $\beta = 1$ then are used as the initial values for solving the equations (A.3) to (A.6).

Applications of the Beta-Gamma Distribution

An application of the proposed distribution is presented using the data sets given in Park, Leslie, and Mertz (1964), Park (1954), Moffa and Costantino (1977). Costantino and Desharnais (1981) established a gamma-state probability distribution for adult numbers in continuously growing populations of the flour beetle *Tribolium*. The hypothesis that the data set is from a beta-gamma distributed population is tested using the observed frequency distributions of adult numbers for *Tribolium castaneum* and *Tribolium Confusum*.

The beta-gamma distribution is fitted to the ten data sets discussed above, and the results are compared to those from gamma distribution and beta-normal distribution proposed by Eugene (2001) where the maximum likelihood method was used. Table 12 tabulates the resulting chi-square values from the goodness-of-fit test for the 10 data sets, and for illustration of the computations Tables 13 and 14 contains results for two of the ten data sets (Data set # 6 and #10). The expected numbers are calculated using the respective distribution with the parameters set at their maximum likelihood estimates. The chi-square goodness-of-fit test is then employed to make a comparison between the observed and expected number of observations under each distribution. Note that a class interval with an expected number less than 5 is combined with the adjacent class to avoid inflating the chi-square test statistic.

Table 12. The resulting χ^2 values (p-value, d.f.) from the goodness-of-fit tests for the 10 data sets.

Data set	Gamma	Beta-Normal	Beta-Gamma
#1	24.03 (0.0043, 9)	5.04 (0.6545, 7)	7.88 (0.3433, 7)
#2	48.16 (0, 12)	27.02 (0.0026, 10)	20.50 (0.0249, 10)
#3	129.18 (0, 17)	74.85 (0, 15)	72.63 (0, 15)
#4	78.07 (0, 11)	25.39 (0.0030, 9)	28.36 (0.0008, 9)
#5	23.62 (0.0144, 11)	19.99 (0.0180, 9)	17.89 (0.0365, 9)
#6	10.72 (0.3793, 10)	7.42 (0.4913, 8)	7.05 (0.5312, 8)
#7	21.67 (0.0169, 10)	10.56 (0.2280, 8)	12.89 (0.1157, 8)
#8	55.71 (0, 9)	25.05 (0.0007, 7)	22.28 (0.0023, 7)
#9	25.02 (0.2463, 21)	16.85 (0.6001, 19)	16.54 (0.6210, 19)
#10	17.19 (0.3076, 15)	17.07 (0.1959, 13)	15.01 (0.3067, 13)

It is of no surprise that the proposed beta-gamma distribution fits better than the gamma distribution for all the data sets. Seven of the ten data sets, the beta-gamma distribution fits better than the beta-normal distribution

based on the chi-squares values. Note that, for example, the data set in Table 14 appears to have a long right tail, it is reasonable that beta-gamma distribution performed the best.

Table 13. Observed and Expected Frequencies for Tribolium Confusum Strain # 4(b)

$x - value$	observed	Expected		
		Gamma	Beta-Normal	Beta-Gamma
37.5 } 42.5 }	5 } 5 } 10	2.36 } 6.42 } 8.78	2.85 } 7.78 } 10.63	4.01 } 8.11 } 12.12
47.5	14	15.37	16.45	16.90
52.5	33	28.26	27.43	28.59
57.5	40	41.74	37.79	40.48
62.5	49	51.32	45.59	49.06
67.5	44	53.98	50.12	51.78
72.5	52	49.66	50.31	48.48
77.5	44	40.67	44.99	41.02
82.5	28	30.07	34.99	31.64
87.5	29	20.31	23.48	22.07
92.5	13	12.66	13.62	13.62
97.5	9	7.34	6.87	7.24
102.5 } 107.5 } 112.5 }	1 } 1 } 3 1 }	3.99 } 2.05 } 7.84 1.80 }	3.02 } 1.16 } 5.73 1.55 }	3.25 } 1.23 } 5.01 0.53 }
Total	368	368	368	368
$\hat{\alpha}$			0.45	0.17
$\hat{\beta}$			0.23	0.69
$\hat{\mu}$			62.79	
$\hat{\sigma}$			6.74	
$\hat{\rho}$		25.61		111.58
$\hat{\lambda}$		2.71		0.74
χ^2		10.72	7.42	7.05
p-value		0.3793	0.4913	0.5312
degree of freedom		10	8	8

Table 14. Observed and Expected Frequencies for *Tribolium Castaneum* at 24° C (b)

$x - \text{value}$	observed	Expected		
		Gamma	Beta-Normal	Beta-Gamma
25	0	0.02	0.12	0.03
35	0	0.44	0.75	0.46
45	3	2.97	3.38	3.20
55	9	11.51	11.18	12.30
65	39	29.71	28.07	31.23
75	53	57.05	55.08	58.77
85	77	87.54	87.09	88.39
95	105	112.64	114.43	111.90
105	135	125.81	128.66	123.66
115	114	125.09	127.23	122.40
125	113	112.87	113.37	110.58
135	92	93.80	92.91	92.45
145	59	72.63	71.18	72.29
155	54	52.89	51.60	53.29
165	38	36.51	35.72	37.27
175	22	24.03	23.75	24.87
185	17	15.17	15.22	15.91
195	6	9.22	9.43	9.80
205	10	5.42	5.65	5.83
215	3	3.09	3.28	3.36
225	2	1.71	1.85	1.88
235	0	0.92	1.01	1.03
245	1	0.49	0.53	0.55
255	0	0.25	0.27	0.29
265	0	0.22	0.24	0.22
$\hat{\alpha}$			12.34	0.82
$\hat{\beta}$			0.68	0.79
$\hat{\mu}$			27.33	
$\hat{\sigma}$			47.01	
$\hat{\rho}$		13.86		17.23
$\hat{\lambda}$		8.50		6.74
χ^2		17.19	17.07	15.01
p-value		0.3076	0.1959	0.3067
degree of freedom		15	13	13

Conclusion

A beta-gamma distribution is proposed that include the gamma, exponential, and beta-exponential distributions as its special cases. When $\alpha\rho > 1$, it is unimodal with a concave shape. When $\alpha\rho \leq 1$ and $\beta \geq 1$, it has a reversed-J shape. When $\alpha < 1$ and $\rho < 1$, it also has a reversed-J shape. When $\alpha\rho = 1$ and $\beta < 1$, it can be reverse J-shaped or unimodal with a concave shape. When $\alpha\rho < 1$ and $\beta < 1$, $g(x)$ has a reversed-J shape except when $\alpha\rho$ is close to 1 with $\alpha > 1$ or $\rho > 1$ for a range of β values of less than one, in which it is bimodal with a mode of zero and a nonzero mode.

Note that the beta-normal distribution in Eugene, *et al* (2002) can be bimodal with two nonzero modes; the beta-gamma can be bimodal with a mode of zero and a nonzero mode. Closed forms of moments are derived when parameters are integers. The mean and standard deviation increase with α and decrease with β .

The hazard function of the proposed beta-gamma distribution appears to be versatile in the sense it could be constant, nondecreasing, nonincreasing, concave, and convex. This property is potentially useful in real word problems. The estimation of the parameters can be computed via maximum likelihood method. The proposed beta-gamma distribution is a generalization of the widely used gamma distribution and is at least as efficient as the beta-normal if not better.

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Appendix

Proof of Lemma 1

Using the Taylor's expansions of $e^{-x/\lambda}$, the gamma density function is

$$\begin{aligned} f(x) &= \frac{x^{\rho-1}}{\lambda^\rho \Gamma(\rho)} e^{-x/\lambda} \\ &= \frac{x^{\rho-1}}{\lambda^\rho \Gamma(\rho)} \left[1 - \frac{x}{\lambda} + \frac{x^2}{2! \lambda^2} + \cdots + \frac{(-1)^n x^n}{n! \lambda^n} + O(x^{n+1}) \right] = \frac{x^{\rho-1}}{\lambda^\rho \Gamma(\rho)} + O(x^\rho), \end{aligned} \quad (\text{A.1})$$

and $F(x) = \int_0^x f(x) dx = \frac{x^\rho}{\rho \lambda^\rho \Gamma(\rho)} + O(x^{\rho+1})$. For simplicity of presentation, let $f = f(x)$, $g = g(x)$, $F = F(x)$ and $F^c = [F(x)]^c$. Using (A.1), the density function $g(x)$ in (1) becomes

$$\begin{aligned} & \frac{x^{\rho-1} e^{-x/\lambda}}{\lambda^\rho \Gamma(\rho) B(\alpha, \beta)} \left[\frac{x^\rho}{\rho \lambda^\rho \Gamma(\rho)} + O(x^{\rho+1}) \right]^{\alpha-1} (1-F)^{\beta-1} \\ &= \frac{x^{\rho-1+\rho(\alpha-1)} e^{-x/\lambda}}{\Gamma^\alpha(\rho) B(\alpha, \beta) \rho^{\alpha-1} \lambda^{\rho\alpha}} [1 + O(x)]^{\alpha-1} (1-F)^{\beta-1} \\ &= \frac{x^{\rho\alpha-1} e^{-x/\lambda}}{\Gamma^\alpha(\rho) B(\alpha, \beta) \rho^{\alpha-1} \lambda^{\rho\alpha}} [1 + O(x)]^{\alpha-1} (1-F)^{\beta-1}. \end{aligned}$$

Lemma 1 can now be readily seen because F is a cdf and $\lim_{x \rightarrow 0} F(x) = 0$.

Proof of Theorem 1

When α and β are integers, the n th moment of the beta-gamma random variable with density function in (1) is

$$\begin{aligned}
 E(X^n) &= \int_0^\infty x^n \frac{1}{B(\alpha, \beta)} F(x)^{\alpha-1} [1-F(x)]^{\beta-1} f(x) dx \\
 &= \frac{1}{B(\alpha, \beta)} \sum_{j=0}^{\beta-1} (-1)^j \binom{\beta-1}{j} \int_0^\infty x^n F^{\alpha-1} F^j f(x) dx \\
 &= \frac{1}{B(\alpha, \beta)} \sum_{j=0}^{\beta-1} (-1)^j \binom{\beta-1}{j} \int_0^\infty x^n F^{\alpha+j-1} f(x) dx . \\
 &= \frac{1}{B(\alpha, \beta)} \sum_{j=0}^{\beta-1} (-1)^j \binom{\beta-1}{j} \int_0^\infty x^n [1-(1-F)]^{\alpha+j-1} f(x) dx \\
 &= \frac{1}{B(\alpha, \beta)} \sum_{j=0}^{\beta-1} (-1)^j \binom{\beta-1}{j} \left\{ \sum_{k=0}^{\alpha+j-1} (-1)^k \binom{\alpha+j-1}{k} I_{n,k} \right\} ,
 \end{aligned}$$

where

$$I_{n,k} = \int_0^\infty x^n f(x) (1-F)^k dx .$$

Proof: of Corollary 1

When $\alpha = 2, \beta = 1$,

$$E(X^n) = \frac{1}{B(2,1)} \sum_{k=0}^1 (-1)^k \binom{1}{k} I_{n,k} = \frac{1}{B(2,1)} [I_{n,0} - I_{n,1}] = 2I_{n,0} - 2I_{n,1} . \quad (\text{A.2})$$

The first term $I_{n,0}$ is given by

$$\int_0^{\infty} \frac{x^{n+\rho-1}}{\lambda^\rho \Gamma(\rho)} e^{-x/\lambda} dx = \int_0^{\infty} \frac{\lambda^{n+\rho} (\frac{x}{\lambda})^{n+\rho-1}}{\lambda^\rho \Gamma(\rho)} e^{-x/\lambda} d(\frac{x}{\lambda}) = \int_0^{\infty} \frac{\lambda^{n+\rho} t^{n+\rho-1}}{\lambda^\rho \Gamma(\rho)} e^{-t} d(t) = \frac{\lambda^n \Gamma(n+\rho)}{\Gamma(\rho)},$$

and $I_{n,1} = \int_0^{\infty} x^n f(x)(1-F)dx$ is

$$\begin{aligned} & \int_0^{\infty} \frac{x^{\rho-1}}{\lambda^\rho \Gamma(\rho)} x^n e^{-x/\lambda} [e^{-x/\lambda} + (x/\lambda)e^{-x/\lambda} + \dots + \frac{(x/\lambda)^{\rho-1} e^{-x/\lambda}}{\Gamma(\rho)}] dx \\ &= \int_0^{\infty} \frac{(2x/\lambda)^{n+\rho-1} (\lambda/2)^{n+\rho-1}}{\lambda^\rho \Gamma(\rho)} e^{-2x/\lambda} [1 + x/\lambda + \dots + \frac{(x/\lambda)^{\rho-1}}{\Gamma(\rho)}] d(2x/\lambda)(\lambda/2) \\ &= \frac{\lambda^n}{2^{n+\rho} \Gamma(\rho)} \int_0^{\infty} t^{n+\rho-1} e^{-t} [1 + t/2 + \dots + \frac{(t/2)^{\rho-1}}{\Gamma(\rho)}] d(t) \\ &= \frac{\lambda^n}{2^{n+\rho} \Gamma(\rho)} \left[\int_0^{\infty} t^{n+\rho-1} e^{-t} dt + \int_0^{\infty} t^{n+\rho-1} e^{-t} (t/2) dt + \dots + \int_0^{\infty} t^{n+\rho-1} e^{-t} (t/2)^{\rho-1} / \Gamma(\rho) dt \right] \\ &= \frac{\lambda^n \Gamma(n+\rho)}{2^{n+\rho} \Gamma(\rho)} + \frac{\lambda^n \Gamma(n+\rho+1)}{2^{n+\rho+1} \Gamma(\rho)} + \dots + \frac{\lambda^n \Gamma(n+2\rho-1)}{2^{n+2\rho-1} \Gamma^2(\rho)} \\ &= \sum_{i=0}^{\rho-1} \frac{\lambda^n \Gamma(n+\rho+i)}{2^{n+\rho+i} \Gamma(\rho) \Gamma(i+1)}. \end{aligned}$$

When ρ is an integer, $I_{n,0} = \lambda^n (n+\rho-1) \cdots (\rho+1)\rho$ and $I_{n,1} = \sum_{i=0}^{\rho-1} \frac{\lambda^n (n+\rho+i-1)!}{2^{n+\rho+i} (\rho-1)! i!}$.

Substituting $I_{n,0}$ and $I_{n,1}$ into (A.2), the results of (7) and (8) are obtained.

Proof of Lemma 2:

(a) As x goes 0, $\lim_{x \rightarrow 0} H(x)$ is

$$\lim_{x \rightarrow 0} \frac{\frac{1}{B(\alpha, \beta)} F^{\alpha-1} (1-F)^{\beta-1} f(x)}{1 - \frac{1}{B(\alpha, \beta)} \int_0^x F^{\alpha-1} (1-F)^{\beta-1} f(x) dx} = \lim_{x \rightarrow 0} g(x),$$

which is given in Lemma 1.

Proof: (b) As x goes to ∞ , by *L'Hospital Rule*, $\lim_{x \rightarrow \infty} H(x)$ is

$$\begin{aligned} & \lim_{x \rightarrow \infty} \frac{(\alpha-1)F^{\alpha-2} f(x)(1-F)^{\beta-1} f(x) + F^{\alpha-1}(\beta-1)(1-F)^{\beta-2}(-f^2) + F^{\alpha-1}(1-F)^{\beta-1} f'}{-F^{\alpha-1}(1-F)^{\beta-1} f} \\ &= \lim_{x \rightarrow \infty} \left[\frac{(1-\alpha)f(x)}{F(x)} + \frac{(\beta-1)f(x)}{1-F(x)} - \frac{f'(x)}{f(x)} \right] \\ &= \frac{0}{1} + (\beta-1) \lim_{x \rightarrow \infty} \frac{f'(x)}{-f(x)} - \lim_{x \rightarrow \infty} \frac{f'(x)}{f(x)} \\ &= -\beta \lim_{x \rightarrow \infty} \frac{f'(x)}{f(x)} = -\beta \lim_{x \rightarrow \infty} \frac{\frac{-x^{\rho-1} e^{-\frac{x}{\lambda}}}{\lambda} + (\rho-1)x^{\rho-2} e^{-\frac{x}{\lambda}}}{x^{\rho-1} e^{-\frac{x}{\lambda}}} \\ &= -\beta \lim_{x \rightarrow \infty} \left(-\frac{1}{\lambda} + \frac{\rho-1}{x} \right) = \frac{\beta}{\lambda}. \end{aligned}$$

Note that unlike $\lim_{x \rightarrow 0} H(x)$, the limit $\lim_{x \rightarrow \infty} H(x) = \beta / \lambda$ does not depend on α and ρ . In other word, the instantaneous failure rate will not depend on α and ρ in the long run.

The Equations for Solving the Maximum Likelihood Estimates:

$$0 = \frac{\partial l}{\partial \alpha} = n\psi(\alpha + \beta) - n\psi(\alpha) + \sum_{i=1}^n \log F(x_i). \quad (\text{A.3})$$

$$0 = \frac{\partial l}{\partial \beta} = n\psi(\alpha + \beta) - n\psi(\beta) + \sum_{i=1}^n \log(1 - F(x_i)). \quad (\text{A.4})$$

$$0 = \frac{\partial l}{\partial \rho} = (\alpha - 1) \sum_{i=1}^n \frac{1}{F(x_i)} \frac{\partial F(x_i)}{\partial \rho} - (\beta - 1) \sum_{i=1}^n \frac{1}{1 - F(x_i)} \frac{\partial F(x_i)}{\partial \rho} + \sum_{i=1}^n \frac{1}{f(x_i)} \frac{\partial f(x_i)}{\partial \rho}, \quad (\text{A.5})$$

$$\begin{aligned} \frac{\partial f}{\partial \rho} &= \frac{e^{-x/\lambda} [x^{\rho-1} (\log x) \lambda^\rho \Gamma(\rho) - x^{\rho-1} (\lambda^\rho \Gamma'(\rho) + \lambda^\rho (\log \lambda) \Gamma(\rho))]}{\lambda^{2\rho} \Gamma^2(\rho)} \\ &= f(x) \frac{(\log x) \lambda^\rho \Gamma(\rho) - \lambda^\rho \Gamma'(\rho) - \lambda^\rho (\log \lambda) \Gamma(\rho)}{\lambda^\rho \Gamma(\rho)} = f(x) [\log x - \psi(\rho) - \log \lambda], \end{aligned}$$

$$\frac{\partial F}{\partial \rho} = \int_0^x f(x) [\log x - \psi(\rho) - \log \lambda] dx.$$

$$0 = \frac{\partial l}{\partial \lambda} = (\alpha - 1) \sum_{i=1}^n \frac{1}{F(x_i)} \frac{\partial F(x_i)}{\partial \lambda} - (\beta - 1) \sum_{i=1}^n \frac{1}{1 - F(x_i)} \frac{\partial F(x_i)}{\partial \lambda} + \sum_{i=1}^n \frac{1}{f(x_i)} \frac{\partial f(x_i)}{\partial \lambda}, \quad (\text{A.6})$$

$$\frac{\partial f}{\partial \lambda} = \frac{x^{\rho-1}}{\Gamma(\rho)} \frac{\frac{x}{\lambda^2} e^{-x/\lambda} \lambda^\rho - e^{-x/\lambda} \rho \lambda^{\rho-1}}{\lambda^{2\rho}} = f(x) (x/\lambda^2 - \rho/\lambda); \quad \frac{\partial F}{\partial \lambda} = \int_0^x f(x) (x/\lambda^2 - \rho/\lambda) dx.$$

The SAS IML optimization methods can be employed to solve the loglikelihood equations (A.3) – (A.6) iteratively. The lengthy and tedious second derivatives required in the algorithm are not presented here, but are available upon request.

On the Product of Maxwell and Rice Random Variables

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The distributions of the product of independent random variables arise in many applied problems. These have been extensively studied by many researchers. In this paper, the exact distributions of the product $|XY|$ have been derived when X and Y are Maxwell and Rice random variables respectively, and are distributed independently of each other. The associated cdfs, pdfs, and k th moments have been given.

Key words: Maxwellll distribution, products, Rice distribution.

Introduction

The distributions of the product $|XY|$, when X and Y are independent random variables, arise in many applied problems of biology, economics, engineering, genetics, hydrology, medicine, number theory, order statistics, physics, psychology, etc. (see, for example, Cigizoglu & Bayazit (2000), Galambos & Simonelli (2005), Grubel (1968), Ladekarl, et al. (1997), and Rokeach & Kliejunas (1972), among others, and references therein). The distributions of the product $|XY|$, when X and Y are independent random variables and come from the same family, have been extensively studied by many researchers, (see, for example, Bhargava & Khatri (1981), Malik & Trudel (1986), Rathie & Rohrer (1987), Springer & Thompson (1970), Stuart (1962), and Wallgren (1980), among others,). In recent years, there has been a great interest in the study of the above

kind when X and Y belong to different families, (see, for example, Nadarajah (2005), and Nadarajah & Kotz (2005), among others). In this paper, the distributions of the product $|XY|$, when X and Y are independent random variables having Maxwell and Rice distributions respectively, have been investigated.

The derivation of the cdf, pdf, and k th moment of $Z = |XY|$ involve some special functions, which are defined as follows, (see, for example, Abramowitz & Stegun, 1970, Gradshteyn & Ryzhik, 2000, and Prudnikov, et al., 1986, among others, for details). The series

$${}_pF_q(\alpha_1, \alpha_2, \dots, \alpha_p; \beta_1, \beta_2, \dots, \beta_q; z) = \sum_{k=0}^{\infty} \left\{ \frac{(\alpha_1)_k (\alpha_2)_k \dots (\alpha_p)_k}{(\beta_1)_k (\beta_2)_k \dots (\beta_q)_k} \frac{z^k}{k!} \right\},$$

is called a generalized hypergeometric series of order (p, q) , where $(\alpha)_k$ and $(\beta)_k$ represent Pochhammer symbols. For $p=1$ and $q=2$, we have generalized hypergeometric function ${}_1F_2$ of order $(1, 2)$, given by

$${}_1F_2(\alpha_1; \beta_1, \beta_2; z) = \sum_{k=0}^{\infty} \left\{ \frac{(\alpha_1)_k}{(\beta_1)_k (\beta_2)_k} \frac{z^k}{k!} \right\}.$$

The integral

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$$\Gamma(\alpha) = \int_0^{\infty} t^{\alpha-1} e^{-t} dt, \alpha > 0,$$

is defined as a (complete) gamma function, whereas the integrals

$$\gamma(\alpha, x) = \int_0^x t^{\alpha-1} e^{-t} dt, \alpha > 0,$$

and

$$\Gamma(\alpha, x) = \int_x^{\infty} t^{\alpha-1} e^{-t} dt, \alpha > 0,$$

are respectively known as incomplete gamma and complementary incomplete gamma functions. For negative values, gamma function can be defined as

$$\Gamma\left(-n + \frac{1}{2}\right) = \frac{(-1)^n 2^n \sqrt{\pi}}{1.3.5. \dots (2n-1)}, \text{ where } n \geq 0$$

is an integer (e.g., Andrews, et al., 1999, and Bohr & Mollerup, 1922). The error function is defined by

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2} du,$$

whereas the complementary error, $\operatorname{erfc}(x)$, is defined as

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-u^2} du = 1 - \operatorname{erf}(x).$$

The modified Bessel function of first kind, $I_{\nu}(x)$, for a real number ν , is defined by

$$I_{\nu}(x) = \left(\frac{1}{2}x\right)^{\nu} \sum_{k=0}^{\infty} \frac{\left(\frac{1}{4}x^2\right)^k}{(k!) \Gamma(\nu + k + 1)},$$

where $\Gamma(\cdot)$ denotes gamma function. Also,

$$I_{\nu}(x) = \frac{1}{\Gamma(\nu+1)} \left(\frac{x}{2}\right)^{\nu} e^{-x} {}_1F_1\left(\frac{1}{2} + \nu, 1 + 2\nu; 2x\right),$$

where ${}_1F_1$ denotes the confluent hypergeometric function. When $\nu = 0$, modified Bessel function of first kind, $I_0(x)$, of order 0 is obtained as follows:

$$I_0(x) = \sum_{k=0}^{\infty} \frac{\left(\frac{1}{4}x^2\right)^k}{(k!)^2} \dots \quad (1)$$

For

$$\operatorname{Re}\left(\nu + \frac{1}{2}\right) > 0, |\arg(z)| < \frac{\pi}{2};$$

or

$$\operatorname{Re}(z) = 0$$

and

$$\nu = 0,$$

the modified Bessel function of second kind of order ν is given by

$$K_{\nu}(x) = \frac{\left(\frac{z}{2}\right)^{\nu} \Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\nu + \frac{1}{2}\right)} \int_1^{\infty} e^{-zt} (t^2 - 1)^{\nu - \frac{1}{2}} dt.$$

For

$$|\arg(z)| < \frac{\pi}{2}, \operatorname{Re}(z^2),$$

one would have

$$K_{\nu}(x) = \frac{1}{2} \left(\frac{z}{2}\right)^{\nu} \int_0^{\infty} \frac{e^{-t - \frac{z^2}{4t}}}{(t)^{\nu+1}} dt.$$

For non-integer ν ,

$$K_{\nu}(x) = \frac{\pi \{I_{-\nu}(x) - I_{\nu}(x)\}}{2 \sin(\nu \pi)}.$$

The following Lemmas will also be needed in our calculations.

LEMMA 1 (Gradshteyn & Ryzhik (2000), Equation (3.381.4), Page 317). For $\operatorname{Re}(\mu) > 0$, and $\operatorname{Re}(\nu) > 0$,

$$\int_0^{\infty} t^{\nu-1} e^{-\mu t} dt = \frac{1}{\mu^{\nu}} \Gamma(\nu).$$

LEMMA 2 (Prudnikov et al. (1986), Volume 2, Equation (2.8.5.15), Page 106). For $a > 0$,

$$\begin{aligned} & \int_0^{\infty} t^{\alpha-1} e^{-p/t^2} \operatorname{erf}(ct) dt \\ &= \frac{c p^{(\alpha+1)/2}}{\sqrt{\pi}} \Gamma\left(-\frac{\alpha+1}{2}\right) {}_1F_2\left(\frac{1}{2}; \frac{3}{2}, \frac{3+\alpha}{2}; c^2 p\right) \\ & - \frac{1}{\sqrt{\pi} \alpha c^{\alpha}} \Gamma\left(\frac{\alpha+1}{2}\right) {}_1F_2\left(-\frac{\alpha}{2}; 1-\frac{\alpha}{2}, \frac{1-\alpha}{2}; c^2 p\right) \end{aligned}$$

LEMMA 3 (Prudnikov et al., 1986, Volume 2, Equations 2.10.3.14, Page 151). For $\operatorname{Re}(\alpha) < 0$, $\operatorname{Re}(p) > 0$, $\operatorname{Re}(\nu) > 0$, and $\operatorname{Re}(c) > 0$,

$$\begin{aligned} & \int_0^{\infty} x^{\alpha-1} e^{-p/x} \gamma(\nu, cx) dx \\ &= \frac{c^{\nu} (p)^{\alpha+\nu}}{\nu} \Gamma(-\alpha-\nu) {}_1F_2(\nu; \nu+1, 1+\alpha+\nu; cp) \\ & - \frac{\Gamma(\alpha+\nu)}{\alpha c^{\alpha}} {}_1F_2(-\alpha; 1-\alpha, 1-\alpha-\nu; cp) \end{aligned}$$

where ${}_1F_2$ denotes generalized hypergeometric function of order $(1, 2)$, (see definition above).

LEMMA 4 (Gradshteyn & Ryzhik (2000), Equation (3.471.9), Page 340). For $\operatorname{Re}(\beta) > 0$, $\operatorname{Re}(\gamma) > 0$,

$$\int_0^{\infty} x^{\nu-1} e^{-\frac{\beta}{x} - \gamma x} dx = 2 \left(\frac{\beta}{\gamma}\right)^{\frac{\nu}{2}} K_{\nu}(2\sqrt{\beta\gamma})$$

where $K_{\nu}(\cdot)$ denotes modified Bessel function of the second kind, (see definition above).

Distribution of the Product $|XY|$

Let X and Y be Maxwell and Rice random variables respectively, distributed independently of each other and defined as follows.

Maxwell Distribution:

A continuous random variable X is said to have a Maxwell distribution if its pdf $f_X(x)$ and cdf $F_X(x)$ are, respectively, given by

$$f_X(y) = \sqrt{\frac{2}{\pi}} a^{3/2} x^2 e^{-a x^2/2}, x > 0, a > 0 \dots \quad (2)$$

and

$$F_X(x) = \frac{2\gamma\left(\frac{3}{2}, \frac{1}{2} a x^2\right)}{\sqrt{\pi}} \dots (3)$$

$$= \operatorname{erf}\left(\sqrt{\frac{a}{2}} x\right) - \sqrt{\frac{2a}{\pi}} x e^{-a x^2/2}$$

where $\gamma(a, x)$ and $\operatorname{erf}(x)$ denote incomplete gamma and error functions respectively, (see definition above).

Rice Distribution: A continuous random variable Y is said to have a Rice distribution if its pdf $f_Y(y)$ is given by

$$f_Y(y) = \frac{y}{\sigma^2} e^{-(y^2 + \nu^2)/2\sigma^2} I_0\left(\frac{y\nu}{\sigma^2}\right), y > 0, \sigma > 0, \nu \geq 0 \dots \quad (4)$$

where $I_0(y)$ denotes the modified Bessel function of the first kind, (see definition above).

For $|v|=0$, the expression (4) reduces to a Rayleigh distribution. In what follows, we consider the derivation of the distribution of the product $|XY|$, when X and Y are Maxwell and Rice random variables respectively, distributed independently of each other and defined as above. An explicit expression for the cdf of $|XY|$ in terms of hypergeometric function has been derived in Theorem 1. In Theorem 2, another explicit expression for the cdf of $|XY|$ in terms of hypergeometric function and modified Bessel function of the second kind $K_\nu(x)$ has been derived.

Theorem 1

Suppose X is a Maxwell random variable with pdf $f_X(x)$ as given in (2) and cdf $F_X(x) = P(X \leq x)$ given by (3) in terms of the incomplete gamma function. Also, suppose Y is a Rice random variable with pdf $f_Y(y)$ given by (4) in terms of the modified Bessel function of the first kind $I_0(y)$. Then the cdf of $Z = |XY|$ can be expressed as

$$F(z) = \left[\frac{e^{-v^2/2\sigma^2}}{\sqrt{\pi}\sigma^2} \sum_{k=0}^{\infty} \frac{v^{2k}}{2^{2k} \sigma^{4k} (k!)^2} \left[\frac{\Gamma\left(k - \frac{1}{2}\right) 2^{k-1} a^{\frac{3}{2}} \sigma^{2k-1} z^3}{3} {}_1F_2\left(\frac{3}{2}; \frac{5}{2}, \frac{3}{2} - k; \frac{az^2}{4\sigma^2}\right) + \frac{\Gamma\left(\frac{1}{2} - k\right) a^{k+1} z^{2(k+1)}}{2^{k+1} (k+1)} {}_1F_2\left(k+1; k+2, k+\frac{1}{2}; \frac{az^2}{4\sigma^2}\right) \right] \right]$$

where ${}_1F_2(\cdot)$ denotes hypergeometric function of order $(1, 2)$, (see definition above).

Proof

Using the expressions (3) for cdf of Maxwell random variable X and the expression

(4) for pdf of Rice random variable Y , the cdf $F(z) = \Pr(|XY| \leq z)$ can be expressed as

$$\begin{aligned} F(z) &= \Pr\left(|X| \leq \frac{z}{|Y|}\right) \\ &= \int_0^{\infty} F_X\left(\frac{z}{y}\right) f_Y(y) dy \quad \dots \\ &= \left[\frac{2 e^{-v^2/2\sigma^2}}{\sqrt{\pi} \sigma^2} \right] \int_0^{\infty} y e^{-y^2/2\sigma^2} \gamma\left(\frac{3}{2}, \frac{ay^2}{2y^2}\right) I_0\left(\frac{vy}{\sigma^2}\right) dy \end{aligned} \quad (5)$$

where $y > 0, z > 0, a > 0, \sigma > 0, v \geq 0$. The proof of Theorem 1 easily follows by using definition (1) of modified Bessel function of first kind, $I_0(x)$, of order 0, and Lemma 3 in the integral (5) above.

Theorem 2

Suppose X is a Maxwell random variable with pdf $f_X(x)$ as given in (2) and cdf $F_X(x) = P(X \leq x)$ given by (3) in terms of the error function. Also, suppose Y is a Rice random variable with pdf $f_Y(y)$ given by (4) in terms of the modified Bessel function of the first kind $I_0(y)$. Then the cdf of $Z = |XY|$ can be expressed as

$$\begin{aligned} F(z) &= \left[\frac{\sqrt{a} e^{-v^2/2\sigma^2}}{\sqrt{\pi} \sigma^2} \sum_{k=0}^{\infty} \frac{v^{2k}}{2^{2k} \sigma^{4k} (k!)^2} \left[\Gamma\left(k + \frac{1}{2}\right) 2^k \sigma^{2k+1} z {}_1F_2\left(\frac{1}{2}; \frac{3}{2}, \frac{1}{2} - k; \frac{az^2}{4\sigma^2}\right) + \frac{\Gamma\left(-k - \frac{1}{2}\right) a^{k+\frac{1}{2}} z^{2(k+1)}}{2^{k+2} (k+1)} {}_1F_2\left(k+1; k+2, k+\frac{3}{2}; \frac{az^2}{4\sigma^2}\right) - \sqrt{2} (\sqrt{a} \sigma)^{k+\frac{1}{2}} z^{k+\frac{3}{2}} K_{k+\frac{1}{2}}\left(\frac{\sqrt{a} z}{\sigma}\right) \right] \right] \end{aligned}$$

where ${}_1F_2(\cdot)$ denotes hypergeometric function of order $(1, 2)$, and $K_k(\cdot)$ denotes the modified Bessel functions of the second kind of order k , (see definition above).

Proof

Using the expressions (3) for cdf of Maxwell random variable X and the expression (4) for pdf of Rice random variable Y , the cdf $F(z) = \Pr(|XY| \leq z)$ can be expressed as

$$\begin{aligned} F(z) &= \Pr\left(|X| \leq \frac{z}{|Y|}\right) \\ &= \int_0^\infty F_X\left(\frac{z}{y}\right) f_Y(y) dy \\ &= \left[\frac{e^{-v^2/2\sigma^2}}{\sigma^2} \right] \int_0^\infty y e^{-y^2/2\sigma^2} \left\{ \frac{\operatorname{erf}\left(\sqrt{\frac{a}{2}} \frac{z}{y}\right)}{\sqrt{\frac{2a}{\pi}} \frac{z}{y} e^{-\frac{a z^2}{2y^2}}} \right\} I_0\left(\frac{vy}{\sigma^2}\right) dy \dots \end{aligned} \quad (6)$$

where $y > 0, z > 0, a > 0, \sigma > 0, v \geq 0$. The proof of Theorem 2 easily follows by using the definition (1) of modified Bessel function of the first kind, $I_0(x)$, of order 0, substituting $y = \frac{1}{t}$ in the first term and $y^2 = u$ in the second term of the integral (6) above, and then using Lemmas 2 and 4 respectively.

PDF of the Product $Z = |XY|$, and k th Moment of RV $Z = |XY|$

In what follows, without loss of generality, for simplicity of computations, this section discusses the derivation of the pdf of the product $Z = |XY|$, when X and Y are Rice and Maxwell random variables distributed according to (4) and (2), respectively, and independently of each other. An explicit expression for the pdf of the product $Z = |XY|$

in terms of the modified Bessel function of the second kind $K_\nu(x)$ has been derived in Theorem 3. The expression for the k th moment of RV $Z = |XY|$ in terms of gamma functions has been derived in Theorem 4.

Theorem 3

Suppose X and Y are Rice and Maxwell random variables having pdf given by (4) and (2), respectively. Then the pdf of $Z = |XY|$ can be expressed as

$$\begin{aligned} f_Z(z) &= \left(\sqrt{\frac{2}{\pi}} e^{-v^2/2\sigma^2} \right) \\ &\sum_{n=0}^{\infty} \frac{v^{2n} a^{n+2}}{\sigma^{2n+1} (n!)^2} K_{n+\frac{1}{2}}\left(\frac{\sqrt{a} z}{\sigma}\right) \dots \end{aligned} \quad (7)$$

where $K_{n+\frac{1}{2}}(\cdot)$ denotes the modified Bessel functions of the second kind of order $n + \frac{1}{2}$, (see definition above).

Proof

The pdf of $Z = |XY|$ can be expressed as

$$\begin{aligned} f_Z(z) &= \int_0^\infty \frac{1}{y} f_X\left(\frac{z}{y}\right) f_Y(y) dy \\ &= \left(\sqrt{\frac{2}{\pi}} \frac{a^{\frac{3}{2}}}{\sigma^2} e^{-v^2/2\sigma^2} z \right) \\ &\int_0^\infty e^{-\frac{z^2}{2\sigma^2 y^2} - \frac{a y^2}{2}} I_0\left(\frac{v z}{\sigma^2 y}\right) dy, \dots \end{aligned} \quad (8)$$

where $y > 0, z > 0, a > 0, \sigma > 0, v \geq 0$. The proof of Theorem 3 easily follows by using the definition (1) of modified Bessel function of the

first kind, $I_0(x)$, of order 0, substituting

$y^2 = \frac{1}{t}$, and then using Lemma 4 in the integral (8) above.

Theorem 4

If Z is a random variable with pdf given by (7), then its k th moment can be expressed as

$$E(Z^k) = \left(\frac{2^{\frac{k-1}{2}} e^{-v^2/2\sigma^2}}{\sqrt{\pi}} \right) \sum_{n=0}^{\infty} \frac{v^{2n} a^{\frac{n-k}{2} + \frac{3}{2}}}{\sigma^{2n-k} (n!)^2} \Gamma\left(\frac{2k-2n+1}{4}\right) \Gamma\left(\frac{2k+2n+3}{4}\right)$$

Proof

$$E(Z^k) = \left(\sqrt{\frac{2}{\pi}} e^{-v^2/2\sigma^2} \right) \sum_{n=0}^{\infty} \frac{v^{2n} a^{n+2}}{\sigma^{2n+1} (n!)^2} \int_0^{\infty} z^k K_{n+\frac{1}{2}} \left(\frac{\sqrt{a} z}{\sigma} \right) dz \dots \quad (9)$$

By using the equation (6.621.3 / page 712) from Gradshteyn and Ryzhik (2000), in the integral (9) above, the result of Theorem 4 easily follows.

Conclusion

This article has derived the exact distributions of the product of two independent random variables X and Y , where X and Y have Maxwell and Rice distributions respectively. The pdf and k th moment of the product of two variables are also given. The distribution is obtained as a function of hypergeometric of order (1, 2), where as the pdf has been obtained as a function of Bessel of the second kind. We hope the findings of the article will be useful for the practitioners which are indicated in the introduction of the article.

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Optimal L_p -Metric for Minimizing Powered Deviations in Regression

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Minimizations by least squares or by least absolute deviations are well known criteria in regression modeling. In this work the criterion of generalized mean by powered deviations is suggested. If the parameter of the generalized mean equals one or two, the fitting corresponds to the least absolute or the least squared deviations, respectively. Varying the power parameter yields an optimum value for the objective with a minimum possible residual error. Estimation of a most favorable value of the generalized mean parameter shows that it almost does not depend on data. The optimal power always occurs to be close to 1.7, so these powered deviations should be used for a better regression fit.

Key words: Regression, absolute and squared deviations, L_p -metric, gamma-function.

Introduction

The criterion of generalized mean by powered deviations is considered for regression modeling. Usually regressions are constructed by minimization of squared deviations of the observations to a theoretical surface, although some other measures, particularly, absolute deviations are also applied in regression, multidimensional scaling, clustering, and other distance-based techniques (Armstrong & Frome, 1976; Hastie & Tibshirani, 1990; McCullagh & Nelder, 1997; Venables & Ripley, 1997). Robust regression modeling and kernel smoothing use different measures of distance for smaller and bigger deviations (Huber, 1972, 1981; Hill & Holland, 1977; Hampel et al., 1986; Ripley, 1996). Particularly, the L_p -metric, or the generalized mean, is widely used as so called M -estimator (Maximum likelihood) for robust evaluations (Ramsay, 1977; Sposito, 1982).

In other fields it is also called L_p -metric for operators spaces, vector and matrix norms, Hölder's mean, power mean, exponential mean,

Kolmogorov's mean, or Minkowski distance (Hardy, Littlewood, & Polya, 1934; Daykin & Eliezer, 1969; Borwein & Borwein, 1987; Korn & Korn, 1988; Alvarez, 1992; Rooij & Heiser, 2005). Power means are related to Box-Cox transformation often used in applied statistics aims (Weisberg, 1985; McCullagh & Nelder, 1997; Tishler & Lipovetsky, 1997, 2000; Lipovetsky & Conklin, 2000).

If the parameter of the generalized mean equals one or two, $p=1$ or $p=2$, the fitting corresponds to the least absolute L_1 or the least squared L_2 deviations, respectively. Theoretical properties of the L_p -metrics in the range from 1 to 2 were studied in works on approximation theory, Banach's conjecture, and random processes (Breiman, 1968; Fletcher et al., 1971; Kanter, 1973). It is also known due to Jensen's inequality that a generalized mean of a lower power is smaller than a generalized mean of a larger power (Beckenbach, 1946; Korn & Korn, 1988) that is true for the constant set of the averaging values. However, the estimates of the model parameters and the corresponding residual errors depend on a power parameter, so the better generalized power mean can be reached for a smaller power value. In the literature, known numerical simulations indicated that the minimal residuals correspond to the p -powered deviations close to $L_{1.5}$ or $L_{1.8}$ metrics (Gentleman, 1965; Forsythe, 1972; Ramsay, 1977).

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In the current work, trying an objective of least powered deviations in a wide range of the power parameter, it was possible to find an optimum value for the objective by minimizing the residual error. Numerical estimation of an optimum value of the generalized mean parameter indicates a remarkable outcome – this optimum value is almost a constant that does not depend on the data. Analytical derivation shows that the optimal metric parameter is defined via the gamma function of this parameter, and the optimal value occurs to be close to $p \approx 1.7$. Thus, the optimum metric for fitting any data can be suggested – it is neither the mostly used squared deviations L_2 , nor the absolute deviations L_1 , but the intermediate powered deviations of $L_{1.7}$.

Powered Deviations in Regression Modeling

Consider a multiple linear regression model of the dependent variable y by n independent variables $x_1, x_2, \dots, x_n$:

$$y_i = a_0 + a_1 x_{i1} + a_2 x_{i2} + \dots + a_n x_{in} + \varepsilon_i, \quad (1)$$

where i denotes observations ($i = 1, 2, \dots, N$), and ε_i are deviations of the empirical values y_i from the theoretical model. Least squares minimization corresponds to the objective:

$$S^2 = \frac{1}{N} \sum_{i=1}^N \varepsilon_i^2 = \frac{1}{N} \sum_{i=1}^N (y_i - a_0 - a_1 x_{i1} - \dots - a_n x_{in})^2 \quad (2)$$

This distance is equivalent to the squared Euclidean norm of the errors, or the L_2 metric. Absolute deviations minimization corresponds to the objective of the mean module:

$$S^1 = \frac{1}{N} \sum_{i=1}^N |\varepsilon_i| = \frac{1}{N} \sum_{i=1}^N |y_i - a_0 - a_1 x_{i1} - \dots - a_n x_{in}|. \quad (3)$$

It is the Hamming distance (also known as Manhattan, or taxi-driver distance), or L_1 metric.

Generalized powered mean of the deviations can be expressed as follows:

$$S^{2q} = \frac{1}{N} \sum_{i=1}^N (\varepsilon_i^2)^q = \frac{1}{N} \sum_{i=1}^N (y_i - a_0 - a_1 x_{i1} - \dots - a_n x_{in})^{2q} \quad (4)$$

In this definition, if power parameter q equals one, then the generalized mean (4) is reducing to the squared mean (2). If q equals one half, the generalized mean (4) is presented as a square root of squared deviation that coincides with absolute value of the deviations in the objective (3). The definition (4) emphasizes that only positive items are summed, and the parameter p of L_p metric equals doubled q -parameter. Then (4) can be simplified by using $2q$ parameter, and represented as the power-mean deviation itself:

$$\begin{aligned} S &= \left(\frac{1}{N} \sum_{i=1}^N \varepsilon_i^{2q} \right)^{\frac{1}{2q}} \\ &= \left(\frac{1}{N} \sum_{i=1}^N \left(y_i - \sum_{j=0}^n a_j x_{ij} \right)^{2q} \right)^{\frac{1}{2q}}. \end{aligned} \quad (5)$$

where the intercept's variable x_0 identically equals one.

For a given value of power parameter q , minimization of the objective (5) by the parameters of regressions yields a system of the first order partial derivatives:

$$\begin{aligned} U_k &= \frac{\partial S}{\partial a_k} \\ &= \left(\frac{1}{N} \sum_{i=1}^N \varepsilon_i^{2q} \right)^{\frac{1}{2q}-1} \left[\frac{-1}{N} \sum_{i=1}^N x_{ik} \varepsilon_i^{2q-1} \right] = 0 \end{aligned} \quad (6)$$

with errors defined as in (5):

$$\varepsilon_i = y_i - \sum_{j=0}^n x_{ij} a_j. \quad (7)$$

Non-linear system of equations (6) can be solved numerically by the Newton-Raphson procedure in the Iteratively Re-Weighted Least Squares (IRLS) approach (Bender, 2000; Lipovetsky & Conklin, 2005). For this algorithm the elements of Hessian, or the matrix of second derivatives, are constructed using the derivatives of (6):

$$\begin{aligned} H_{mk} &= \frac{\partial^2 S}{\partial a_m \partial a_k} \\ &= \frac{\partial U_k}{\partial a_m}, \\ &= \frac{2q-1}{N} \left(\frac{1}{N} \sum_{i=1}^N \epsilon_i^{2q} \right)^{\frac{1}{2q}-1} G_{mk} \end{aligned} \quad (8)$$

where the elements G_{mk} are defined by the expression:

$$\begin{aligned} G_{mk} &= \sum_{i=1}^N x_{im} x_{ik} \epsilon_i^{2q-2} \\ &- \left(\sum_{i=1}^N \epsilon_i^{2q} \right)^{-1} \left(\sum_{i=1}^N x_{im} \epsilon_i^{2q-1} \right) \left(\sum_{i=1}^N x_{ik} \epsilon_i^{2q-1} \right) \end{aligned} \quad (9)$$

Newton-Raphson procedure for finding vector of coefficients a (5) can be presented as:

$$a^{(t+1)} = a^{(t)} - H^{-1}U, \quad (10)$$

where t denotes iteration steps, H^{-1} is the inverted Hessian, and U is the gradient-vector with the elements (6). The round parentheses in (6) and in (8) contain the same constant that is canceled in the expression (10), and also the constant N is canceled, so (10) can be reduced to:

$$a^{(t+1)} = a^{(t)} + (2q-1)^{-1} G^{-1} X' \epsilon^{2q-1}, \quad (11)$$

where G^{-1} is the inverted matrix of elements (9), X' denotes the transposed matrix of all the

regressors in (5), and $X' \epsilon^{2q-1}$ is matrix notation for the sum in the squared parentheses (6).

It is convenient to introduce a diagonal matrix of powered errors by all observations:

$$\begin{aligned} W &= \text{diag}(\epsilon^{2q-2}) \\ &= \text{diag}(\epsilon_1^{2q-2}, \epsilon_2^{2q-2}, \dots, \epsilon_N^{2q-2}) \end{aligned} \quad (12)$$

where ϵ is the N -th order vector-column of the deviations (7). Then (9) in the matrix form is:

$$G = X'WX - \frac{1}{\epsilon'W\epsilon} (X'W\epsilon)(X'W\epsilon)'. \quad (13)$$

The subtracted outer product in (13) is arranged of the vector $X'W\epsilon$ of the weighted product of regressors and residuals. Such a product is always close to zero due to the relations of orthogonality between regressors x and residual errors ϵ . This property is exact for linear and approximate for a nonlinear regression (Lipovetsky & Conklin, 2006).

It is always advisable to keep in only the stable part of the Hessian (Becker & Le Cun, 1988), so it makes sense to reduce (13) to the main first item of the weighted second moment matrix $X'WX$. Then the solution (11) can be simplified to:

$$a^{(t+1)} = a^{(t)} + (2q-1)^{-1} (X'WX)^{-1} X'W\epsilon, \quad (14)$$

where due to (12) the equality $X' \epsilon^{2q-1} = X'W\epsilon$ is used. It is interesting to note that the exact expression (14) yields if instead of the mean deviation objective S (5) the powered-deviation S^{2q} objective (4) is minimized. With (7) in the matrix form, the expression (14) becomes:

$$\begin{aligned} a^{(t+1)} &= (X'WX)^{-1} (X'WX) a^{(t)} \\ &+ (2q-1)^{-1} (X'WX)^{-1} X'W(y - Xa^{(t)}), \\ &= (X'WX)^{-1} X'Wz^{(t)} \end{aligned} \quad (15)$$

where the working variable is denoted as:

$$\begin{aligned}
z^{(t)} &= Xa^{(t)} \\
&+ (2q-1)^{-1}(y - Xa^{(t)}) \\
&= (2q-1)^{-1}(y + (2q-2)Xa^{(t)})
\end{aligned} \quad (16)$$

The working variable (16) is a combination of the empirical dependent variable (vector y) and the predicted values of the dependent variable (vector $Xa^{(t)}$) at any t -th iteration step. The right-hand side (15) shows that the solution is presented as a weighted linear regression of the dependent variable $z^{(t)}$ by all the predictors, so (15)-(16) define the IRLS algorithm.

It is interesting to note that if $q=1$ then $z^{(t)}$ (16) is reducing to the constant vector y , and W (12) is reducing to the scalar matrix of identical ones, so the problem (5) and solution (15) coincide with a regular linear regression. For $q=0.5$ the Hessian (8) degenerates to zero, so the approach (10) does not work, and the methods of linear programming are mostly applied. The process of minimization (5)-(16) can include the power parameter q as well. However, the residuals are usually only weakly dependable on this parameter. So, it is better to find parameters of regression for each fixed q , trying q in a wide range of its values.

To explain the results on stability of the power parameter that yields the minimum residual errors in regression modeling, assume the normal distribution for the residual errors using the probability density function:

$$f(\varepsilon) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\varepsilon^2}{2\sigma^2}\right), \quad (17)$$

where ε are the residuals (7) and σ is the standard error. For a new random variable of the powered error $\delta = \varepsilon^{2q}$, its probability density function can be defined by the technique of variables transformation (Hogg & Craig, 1969), that yields:

$$f(\delta) = \frac{1}{\sqrt{2\pi}\sigma \cdot 2q} \delta^{\frac{1}{2q}-1} \exp\left(-\frac{\delta^{1/q}}{2\sigma^2}\right). \quad (18)$$

Such a distribution corresponds to a badness of fit function for M -estimates in robust regression (Huber, 1972, 1981; Ramsay, 1977). Approximation of the generalized powered mean (4) by the integral of the random variable $\delta = \varepsilon^{2q}$ (18), can be expressed as follows:

$$\begin{aligned}
S^{2q} &= \frac{1}{N} \sum_{i=1}^N (\varepsilon_i^2)^q = \frac{1}{N} \sum_{i=1}^N \delta_i \approx \int_{-\infty}^{\infty} \delta f(\delta) d\delta \\
&= \frac{1}{\sqrt{2\pi}\sigma q} \int_0^{\infty} \delta^{v-1} \exp(-\mu\delta^b) d\delta
\end{aligned} \quad (19)$$

with the parameters denoted as:

$$v = \frac{1}{2q} + 1, \quad \mu = \frac{1}{2\sigma^2}, \quad b = \frac{1}{q}. \quad (20)$$

The integral in (19) can be expressed via gamma function (Gradshteyn & Ryzhik, 1965; Gordon, 1994):

$$\int_0^{\infty} \delta^{v-1} \exp(-\mu\delta^b) d\delta = \frac{1}{|b|} \mu^{-v/b} \Gamma\left(\frac{v}{b}\right), \quad (21)$$

so (19) can be simplified to:

$$\begin{aligned}
S^{2q} &= \frac{1}{\sqrt{2\pi}\sigma q} \cdot q(2\sigma^2)^{q+1/2} \Gamma\left(q + \frac{1}{2}\right) \\
&= \frac{2^q \sigma^{2q}}{\sqrt{\pi}} \Gamma\left(q + \frac{1}{2}\right)
\end{aligned} \quad (22)$$

For the case $q=1$, when the generalized power mean (4) is reducing to the least squares, the expression (22) is simplifying to:

$$\begin{aligned}
S^2 &= \frac{2\sigma^2}{\sqrt{\pi}} \Gamma\left(1 + \frac{1}{2}\right) \\
&= \frac{2\sigma^2}{\sqrt{\pi}} \cdot \frac{1}{2} \Gamma\left(\frac{1}{2}\right), \\
&= \frac{2\sigma^2}{\sqrt{\pi}} \cdot \frac{\sqrt{\pi}}{2} \\
&= \sigma^2
\end{aligned} \quad (23)$$

where the properties $\Gamma(1+x) = x\Gamma(x)$ and $\Gamma(1/2) = \sqrt{\pi}$ of gamma function are applied (Abramowitz & Stegun, 1974). The result (23) proves that the residual mean error estimates the theoretical standard error of the distribution (17). For the case $q=1/2$, when the generalized power mean (4) reduces to the least absolute deviations, the expression (22) is:

$$S = \frac{\sqrt{2}\sigma}{\sqrt{\pi}} \Gamma(1) = \sqrt{\frac{2}{\pi}}\sigma \cong 0.8\sigma. \quad (24)$$

It is the mean absolute deviation that equals about 80% of the standard deviation (see Abraham & Ledolter, 1983, p. 133). For a positive x , gamma function reaches its minimum $\Gamma(x) = 0.886$ at the point $x=1.462$ (Abramowitz & Stegun, 1974). The q value (22) is by 0.5 less at this point, or $q = 0.962$, so $p=2q=1.924$ suggests a better powered approximation than the least squares with $p=2$. Taking the $2q$ -th root of the expression (22) shows that the generalized residual mean S is proportional to the value of the standard error σ itself. The residual mean S in the units of σ , can be presented up to a constant as the $2q$ -th root of the gamma function:

$$\frac{S}{\sigma} = \left(\Gamma\left(q + \frac{1}{2}\right) \right)^{\frac{1}{2q}}. \quad (25)$$

This function reaches its minimum at the value $q \approx 0.83$. A difference between theoretical estimate and empirical numerical trying for the best power parameter can be explained by a not exactly normal distribution of the empirical residual errors assumed in the theoretical derivation. Thus, the metric of the smallest residual deviation (4) or (22) equals $p = 2q \approx 1.7$. Although the evaluation via gamma function is a rough approximation, but it supports the empirical results that not the least-squares but a slightly-less-than-least-

squares powered deviations produce minimum residual error estimations.

Numerical Example

For an illustration of the regular numerical output the data on cars technological solutions is used. This data is given in (Chambers & Hastie, 1992), and is available in the statistical package (*S-PLUS'2000*, 1999, cu.summary file). The data contains the following variables of dimensions and mechanical specifications of 111 various cars, supplied by manufacturers or measured by Consumers Union reports: Weight (y) – pounds (considered in hundreds); Length (x_1) – inches; WheelBase (x_2) – length of wheelbase, inches; Width (x_3) – inches; Height (x_4) – height of car, inches; FrontHd (x_5) – distance between the car's head-liner and the head of a 5ft. 9in. front seat passenger, inches; RearHd (x_6) – a similar distance for the rear seat passenger, inches; FrtLegRoom (x_7) – maximum front leg room, inches; RearSeating (x_8) – rear fore-and-aft seating room, inches; FrtShld (x_9) – front shoulder room, inches; RearShld (x_{10}) – rear shoulder room, inches; Turning (x_{11}) – radius of the turning circle, feet; Disp (x_{12}) – the engine displacement, cubic inches; HP (x_{13}) – the net horsepower; Tank (x_{14}) – fuel refill capacity, gallons; HPrev (x_{15}) – the red line, or the maximum safe engine speed, rpm. The weight can be considered as an aggregate that has a strong impact on a car's cumulative characteristics, such as mileage per gallon (correlation with weight equals -0.87), and price (correlation with weight equals 0.70).

Regressions were constructed by powered deviations (5) with various values of the parameter q . Several best by the residual characteristics models are presented in Table 1. Each column of Table 1 corresponds to a particular value of q -parameter and contains the coefficients of regression (beginning from the

Table 1. Regressions by several minimized powered deviations.

q	0.83	0.84	0.85	0.86	0.87	0.88	0.89	0.9	1.0	1.1
a_0	-50.076	-48.400	-47.617	-49.880	-50.114	-50.275	-50.458	-50.641	-52.388	-54.017
a_1	0.147	0.160	0.150	0.135	0.135	0.135	0.135	0.135	0.135	0.135
a_2	0.081	0.071	0.053	0.086	0.087	0.087	0.087	0.088	0.089	0.089
a_3	0.279	0.288	0.353	0.321	0.319	0.318	0.317	0.317	0.314	0.315
a_4	0.259	0.324	0.355	0.361	0.362	0.363	0.364	0.364	0.370	0.375
a_5	-0.431	-0.098	-0.283	-0.331	-0.330	-0.327	-0.323	-0.319	-0.286	-0.256
a_6	0.708	0.238	0.091	0.098	0.092	0.088	0.083	0.079	0.042	0.011
a_7	0.348	0.305	0.137	0.169	0.170	0.170	0.171	0.172	0.181	0.190
a_8	-0.142	-0.135	-0.123	-0.129	-0.129	-0.129	-0.129	-0.129	-0.129	-0.129
a_9	0.018	-0.107	-0.105	-0.075	-0.073	-0.071	-0.069	-0.067	-0.054	-0.045
a_{10}	-0.001	0.008	0.019	0.017	0.017	0.017	0.017	0.017	0.018	0.019
a_{11}	-0.029	0.002	0.040	0.066	0.068	0.068	0.069	0.069	0.073	0.077
a_{12}	-0.013	-0.019	-0.009	-0.008	-0.008	-0.008	-0.008	-0.008	-0.008	-0.008
a_{13}	0.060	0.060	0.050	0.049	0.048	0.048	0.048	0.048	0.049	0.049
a_{14}	0.123	0.226	0.159	0.138	0.138	0.138	0.138	0.137	0.132	0.125
a_{15}	-0.001	-0.001	-0.001	-0.001	-0.001	-0.001	-0.001	-0.001	-0.001	-0.001
S^{2q}	1.845	1.430	1.280	1.266	1.279	1.292	1.305	1.319	1.468	1.646
S	1.446	1.237	1.157	1.147	1.152	1.157	1.161	1.166	1.212	1.254
$Sabs$	1.234	1.015	0.966	0.963	0.963	0.963	0.964	0.964	0.970	0.976
$Ssqr$	1.543	1.327	1.229	1.213	1.213	1.213	1.213	1.212	1.212	1.212
$Mean$	-0.733	-0.371	-0.122	0.000	0.011	0.012	0.011	0.010	0.000	-0.010
$S^{2q} \text{ cent}$	1.465	1.327	1.269	1.266	1.279	1.292	1.305	1.319	1.468	1.646
$S \text{ cent}$	1.259	1.183	1.150	1.147	1.152	1.157	1.161	1.166	1.212	1.254
$Sabs \text{ cent}$	1.043	0.965	0.966	0.963	0.963	0.964	0.964	0.965	0.970	0.975
$Ssqr \text{ cent}$	1.357	1.274	1.223	1.213	1.213	1.213	1.213	1.212	1.212	1.212

intercept a_0) that are slowly varying across the power parameter q values. Below the coefficients, several estimates for the residual errors are presented: the powered residual S^{2q} (4), the residual deviation S (5), the absolute residual $Sabs$ (3), and the residual standard error $Ssqr$ (corresponds to square root of (2) for mean square root deviation). Note that the last two estimates are obtained by the corresponding set of the regression coefficients. The three of the residual error measures – S^{2q} , S , and $Sabs$ – have minimum at the value around $q=0.86$. The residual mean square root error $Ssqr$, of course,

reaches its minimum at the point $q=1$ that corresponds the least square solution (2). Behavior of these four error measures is shown in Figure 1 in a wide range of q . After initial decreasing and oscillating for q below 0.86, the S^{2q} , S , and $Sabs$ curves reach their minima, and then with q increase they grow as well. The residual mean square root error $Ssqr$ is very flat beginning from the same threshold $q=0.86$.

The bottom section of Table 1 presents the estimate of mean value of the deviations (7), and all four residual error estimates centered by this mean value (the error estimates are denoted as $S^{2q} \text{ cent}$, $S \text{ cent}$, $Sabs \text{ cent}$, and $Ssqr \text{ cent}$). It is

interesting to see that the mean of the deviations is at first negative, than for bigger q values the mean grows and reaches zero at about $q=0.86$, then it stays positive till the next reach of zero at the value $q=1$. So, these two values of q produce minimum centered residual error estimates. The mean deviation and the four centered measures of the residual errors are shown in Figure 2 in a range of q values. The behavior of the residual mean stabilizes with q above 0.86. All centered

error measures change similarly but more flatly than those of non-centered measures from the previous graph, also with a threshold at the point of about $q=0.86$. The obtained results on the minimum of S^{2q} , S , and $Sabs$ errors in the vicinity of the parameter value about 0.83-0.87 are amazingly constant. In numerous regressions by different data sets the same power region of q is obtained for the minimum residual errors by the powered deviations.

Fig.1: Residual error estimates

Fig.2: Residual mean and centered error estimates

Conclusion

The generalized powered deviations were considered to estimate minimum possible residual error and the corresponding value of the power parameter. Numerical estimations performed in the work support the analytical result that the best optimization objective corresponds to the metric in the vicinity of $L_{1.7}$. Although change of coefficients and residuals in regressions by different power parameter is moderate, a metric close to the optimum $L_{1.7}$ can be applied for tuning the model. The objective of powered deviations can serve both to the theoretical investigation and practical application in numerous problems of regression modeling.

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LQ-Moments for Statistical Analysis of Extreme Events

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Statistical analysis of extremes is conducted for predicting large return periods events. LQ-moments that are based on linear combinations are reviewed for characterizing the upper quantiles of distributions and larger events in data. The LQ-moments method is presented based on a new quick estimator using five points quantiles and the weighted kernel estimator to estimate the parameters of the generalized extreme value (GEV) distribution. Monte Carlo methods illustrate the performance of LQ-moments in fitting the GEV distribution to both GEV and non-GEV samples. The proposed estimators of the GEV distribution were compared with conventional L-moments and LQ-moments based on linear interpolation quantiles for various sample sizes and return periods. The results indicate that the new method has generally good performance and makes it an attractive option for estimating quantiles in the GEV distribution.

Key words: LQ-moments, L-moments, quick estimator, generalized extreme value, weighted kernel.

Introduction

Statistical analysis of extremes is often interested for predicting large return period events. Thus, the more relevant analysis is the upper quantiles of the distributions and the extreme sample events (Wang, 1997). The method of classical moments (MOM) is mostly used because of its relative ease of application but it is generally not as efficient as the maximum likelihood (ML) method estimates and it is too sensitive to the upper quantiles of distributions (Vogel & Fennessey, 1993).

The ML method is the most important method because it leads to efficient parameter estimators with Gaussian asymptotic

distributions. However, this method sometimes under-estimates and so causes large bias and variance of extreme upper quantile and does not always work well in small samples (Park, 2005).

The L-moments (LMOM), certain linear functions of the expectations of order statistics, were introduced and comprehensively reviewed by Hosking (1990). Hosking (1990) presented the LMOM estimators for some common distributions and demonstrates that in some cases, the LMOM method may give even better fit than ML method. Hosking and Wallis (1997) illustrated that LMOM are efficient in estimating parameters of a wide range of distributions. In general, the bias of small sample estimates of higher-order LMOM is fairly small as compared to traditional moment estimates. This method has become a standard procedure in hydrology for estimating the parameters of certain statistical distributions. The LMOM have found wide applications in such fields of applied research as civil engineering, meteorology, hydrology, quality control and engineering (Sankarasubramanian & Srinivasan, 1999; Karvanen, 2005).

Mudolkar and Hutson (1998) extended LMOM to new moment like entitles called LQ-moments (LQMOM). The LQMOM are constructed by using functional defining the quick estimators, such as the median, trimean or Gastwirth, in places of expectations in LMOM.

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The LQMOM that are based on the quick estimators, namely the trimean and the linear interpolation quantile estimator are used to fit a GEV to observed flood frequencies. They found the LQMOM are often easier to compute than LMOM, and in general behave similarly to the LMOM.

In this article, LQMOM that are based on the trimean and the linear interpolation quantile (LIQ) estimator are reviewed for characterizing the upper part of distributions and larger events in data. The objective of this article is to revisit the LQMOM, presents the LQMOM method based on the new quick estimator using five-points quantiles and the weighted kernel estimator (WK5) to estimate the parameters of the generalized extreme value (GEV) distribution. Estimation of the GEV distribution by using LQMOM is formulated. The performance of the LQMOM based on the new estimator is compared to LMOM and LIQ methods, by using both GEV and non-GEV simulated sample data.

Definition of LQ-Moment

Let $X_1, X_2, \dots, X_n$ be a random sample from a continuous distribution function $F(\cdot)$ with quantile function $Q(u) = F^{-1}(u)$, and let $X_{1:n} \leq X_{2:n} \leq \dots \leq X_{n:n}$ denote the corresponding order statistics. Hosking (1990) defined the r th L-moment λ_r as

$$\lambda_r = \frac{1}{r} \sum_{k=0}^{r-1} (-1)^k \binom{r-1}{k} E(X_{r-k:r}), \quad r=1, 2, \dots \quad (1)$$

Mudholkar and Hutson (1998) suggested a robust modification in which the mean of the distribution of $X_{r-k:r}$ in (1) is replaced by its median or some others population location measure. In particular, they defined the r th LQ-moments ξ_r as

$$\xi_r = \frac{1}{r} \sum_{k=0}^{r-1} (-1)^k \binom{r-1}{k} \tau_{p,\alpha}(X_{r-k:r}), \quad r=1, 2, \dots \quad (2)$$

where $\tau_{p,\alpha}(X_{r-k:r})$ is a quick measure of the location of the sampling distribution of the order $X_{r-k:r}$. They introduced $\tau_{p,\alpha}$ based on a three-points quantiles of the sample calculated from the order statistics and defined as

$$\begin{aligned} & \tau_{p,\alpha}(X_{r-k:r}) \\ &= pQ_{X_{r-k:r}}(\alpha) \\ &+ (1-2p)Q_{X_{r-k:r}}(1/2) \\ &+ pQ_{X_{r-k:r}}(1-\alpha) \end{aligned} \quad (3)$$

where $0 \leq \alpha \leq 1/2, 0 \leq p \leq 1/2$. $\tau_{p,\alpha}$ is called the median for $p=0, \alpha=1$, the trimean for $p=1/4, \alpha=1/4$ and Gastwirth for $p=0.3, \alpha=1/3$.

The quick measures of location $\tau_{p,\alpha}$ for five-points quantiles is defined as

$$\begin{aligned} & \tau_{p,\alpha}(X_{r-k:r}) \\ &= pQ_{X_{r-k:r}}(\alpha) \\ &+ pQ_{X_{r-k:r}}(5\alpha) \\ &+ (1-4p)Q_{X_{r-k:r}}(1/2) \\ &+ pQ_{X_{r-k:r}}(1-5\alpha) \\ &+ pQ_{X_{r-k:r}}(1-\alpha) \end{aligned} \quad (4)$$

where $0 \leq \alpha \leq 0.1$ and $0 \leq p \leq 1/4$.

The first four LQ-moments of the random variable X are defined as

$$\xi_1 = \tau_{p,\alpha}(X), \quad (5)$$

$$\xi_2 = \frac{1}{2}[\tau_{p,\alpha}(X_{2:2}) - \tau_{p,\alpha}(X_{1:2})], \quad (6)$$

$$\xi_3 = \frac{1}{3}[\tau_{p,\alpha}(X_{3:3}) - 2\tau_{p,\alpha}(X_{2:3}) + \tau_{p,\alpha}(X_{1:3})], \quad (7)$$

$$\begin{aligned} \xi_4 = & \frac{1}{4}[\tau_{p,\alpha}(X_{4:4}) - 3\tau_{p,\alpha}(X_{3:4}) \\ & + 3\tau_{p,\alpha}(X_{2:4}) - \tau_{p,\alpha}(X_{1:4})] \end{aligned} \quad (8)$$

The skewness and kurtosis based upon the ratios of LQ-moments to be called LQ skewness and LQ kurtosis are given respectively by

$$\eta_3 = \xi_3 / \xi_2 \quad (9)$$

and

$$\eta_4 = \xi_4 / \xi_2 \quad (10)$$

Estimation of LQ-moments

For samples of size n , the r th sample LQ-moment ξ_r is given by

$$\hat{\xi}_r = \frac{1}{r} \sum_{k=0}^{r-1} (-1)^k \binom{r-1}{k} \hat{\tau}_{p,\alpha}(X_{r-k:r}), \quad r = 1, 2, \dots \quad (11)$$

where the quick estimator $\hat{\tau}_{p,\alpha}(X_{r-k:r})$ of the location of the order statistic $X_{r-k:r}$ for five-points quantiles is given by

$$\begin{aligned} & \hat{\tau}_{p,\alpha}(X_{r-k:r}) \\ &= pQ[B_{r-k:r}^{-1}(\alpha)] + pQ[B_{r-k:r}^{-1}(5\alpha)] \\ &+ (1-4p)Q[B_{r-k:r}^{-1}(1/2)] \\ &+ pQ[B_{r-k:r}^{-1}(1-5\alpha)] \\ &+ pQ[B_{r-k:r}^{-1}(1-\alpha)] \end{aligned} \quad (12)$$

where $B_{r-k:r}^{-1}(\alpha)$ is the quantile of a beta random variable with parameter $r-k$ and $k+1$, and $Q(\cdot)$ denotes the quantile estimator. The sample LQ skewness and LQ kurtosis are given respectively by

$$\hat{\eta}_3 = \hat{\xi}_3 / \hat{\xi}_2 \quad (13)$$

and

$$\hat{\eta}_4 = \hat{\xi}_4 / \hat{\xi}_2 \quad (14)$$

The Quantile Estimator

David and Nagaraja (2003), Sheather and Marron (1990), Huang and Brill (1999) and Huang (2001) discussed several quantile estimators for estimating the values of the population quantile. In this study, only the linear interpolation quantile estimator and the weighted kernel quantile estimator are presented.

The Linear Interpolation Quantile Estimator

Mudholkar and Hutson (1998) proposed the simplest quantile function estimator based on the linear interpolation (LIQ). This quantiles is used commonly in statistical packages such as MINITAB, SAS, IMSL and S-PLUS. The LIQ estimator is given by

$$\begin{aligned} Q(u) &= (1-\varepsilon)X_{[n'u]n} + \varepsilon X_{[n'u]+1:n} \\ 0 < u < 1 \end{aligned} \quad (15)$$

where

$$\varepsilon = n'u - [n'u] \text{ and } n' = n + 1.$$

The Weighted Kernel Quantile Estimator

A popular class of L quantile estimators is called kernel quantile estimators has been widely applied (Sheather & Marron, 1990; Huang & Brill, 1999; Huang, 2001). The L quantile estimators is given by

$$Q(u) = \sum_{i=1}^n \left[\int_{(i-1)/n}^{i/n} K_h(t-u) dt \right] X_{i:n} \quad (16)$$

where K is a density function symmetric about 0 and

$$K_h(\bullet) = (1/h)K(\bullet/h) \quad (17)$$

The approximation of the L quantile estimator is called as the weighted kernel quantile estimator (WKQ) is given by

$$Q(u) = \sum_{i=1}^n \left[n^{-1} K_h \left(\sum_{j=1}^i w_{j,n} - u \right) \right] X_{i:n}, \quad 0 < u < 1 \quad (18)$$

where

$$w_{i,n} = \begin{cases} \frac{1}{2} \left(1 - \frac{n-2}{\sqrt{n(n-1)}} \right), & i = 1, n, \\ \frac{1}{\sqrt{n(n-1)}}, & i = 2, 3, \dots, n-1. \end{cases} \quad (19)$$

$$h = [u(1-u)/n]^{1/2} \quad (20)$$

and $K(t) = (2\pi)^{-1/2} \exp(-1/2t^2)$ is the Gaussian Kernel.

Generalized Extreme Value

The generalized extreme value (GEV) distribution has been used widely and importantly in the modeling of extreme events in several areas including hydrology, meteorology, finance and insurance, and reliability engineering (Park, 2005). It was recommended for at-site flood frequency analysis in the United Kingdom, for rainfall frequency and for sea waves in the United States. Many studies in regional frequency have used the GEV distribution (Hosking et al., 1985b; Chowdhury et al., 1991). In practice, it has been used to model a wide variety of natural extremes, including floods, rainfall, wind speeds, and wave height. Mathematically, the GEV distribution is very attractive because its inverse has a closed form, and parameters are easily estimated by LMOM (Martin & Stedinger, 2000). The GEV distribution has cumulative distribution function (CDF)

$$\begin{aligned} F(x) &= \exp \left\{ - \left[1 - k \left(\frac{x - \mu}{\sigma} \right) \right]^{1/k} \right\} \quad k \neq 0 \\ &= \exp \left\{ - \exp \left[- \frac{(x - \mu)}{\sigma} \right] \right\} \quad k = 0 \end{aligned} \quad (21)$$

where $\mu + \sigma/k \leq x < \infty$ for $k < 0$ and $-\infty < x \leq \mu + \sigma/k$ for $k > 0$. Here, μ , σ , and k are location, scale, and shape parameters, respectively. Quantiles function of GEV distribution are given in terms of the parameters and the cumulative probability F by

$$Q(F) = \mu + \sigma Q_0(F)$$

where

$$\begin{aligned} Q_0(F) &= [1 - (-\log F)^k] / k \quad k \neq 0 \\ &= -\ln(-\ln(F)) \quad k = 0 \end{aligned} \quad (22)$$

L-Moments of GEV Distribution

The LMOM estimators for GEV distribution (Martins & Stedinger, 2000) are

$$\begin{aligned} \hat{k} &= 7.8590c + 2.9544c^2, \\ c &= 2/(3 + \hat{\tau}_3) - \log(2)/\log(3), \end{aligned} \quad (23)$$

$$\begin{aligned} \hat{\alpha} &= \frac{\hat{\lambda}_2 \hat{k}}{(1 - 2^{-\hat{k}}) \Gamma(1 + \hat{k})}, \\ \hat{\mu} &= \hat{\lambda}_1 - \frac{\hat{\alpha}}{\hat{k}} \{1 - \Gamma(1 + \hat{k})\} \end{aligned} \quad (24)$$

The $\hat{k}$ function is a very good approximation for $\hat{k}$ in the range $(-0.5, 0.5)$. The LMOM estimators $\hat{\lambda}_1, \hat{\lambda}_2, \hat{\lambda}_3$ and $\hat{\tau}_3 = \hat{\lambda}_3/\hat{\lambda}_2$ were obtained by using an unbiased estimator of the first three probability weighted moment (PWM) defined as

$$\beta_r = \mu + \frac{\alpha}{k} [1 - (r+1)^{-k} \Gamma(1+k)] / (r+1). \quad (25)$$

The unbiased estimator of β_r is

$$\begin{aligned} b_r &= \sum_{i=1}^n \frac{(i-1)(i-2)(i-3)\dots(i-r)}{n(n-1)(n-2)\dots(n-r)} X_{i:n} \\ r &= 0, 1, 2, \dots \end{aligned} \quad (26)$$

where the $X_{i:n}$ are the ordered observations from a sample of size and

$$\lambda_1 = \beta_0, \lambda_2 = 2\beta_1 - \beta_0, \text{ and } \lambda_3 = 6\beta_2 - 6\beta_1 + \beta_0. \quad (27)$$

The LQ moments of GEV Distribution

The LQ-moment estimators for the GEV distribution behave similarly to the L-moments.

From equations (5)-(9) and equation (22), the first three LQ-moments of the GEV distribution for the quick estimator based on five-points quantiles can be written as

$$\xi_1 = \mu + \sigma t_{p,\alpha}(X_{1:1}) \quad (28)$$

$$\xi_2 = \frac{1}{2} \sigma [t_{p,\alpha}(X_{2:2}) - t_{p,\alpha}(X_{1:2})] \quad (29)$$

$$\xi_3 = \frac{1}{3} \sigma [t_{p,\alpha}(X_{3:3}) - 2t_{p,\alpha}(X_{2:3}) + t_{p,\alpha}(X_{1:3})] \quad (30)$$

$$\eta_3 = \frac{\frac{1}{3} [t_{p,\alpha}(X_{3:3}) - 2t_{p,\alpha}(X_{2:3}) + t_{p,\alpha}(X_{1:3})]}{\frac{1}{2} [t_{p,\alpha}(X_{2:2}) - t_{p,\alpha}(X_{1:2})]} \quad (31)$$

where

$$\begin{aligned} & t_{p,\alpha}(X_{r-k:r}) \\ &= pQ_0[B_{r-k:r}^{-1}(\alpha)] + pQ_0[B_{r-k:r}^{-1}(5\alpha)] \\ &+ (1-4p)Q_0[B_{r-k:r}^{-1}(1/2)] \\ &+ pQ_0[B_{r-k:r}^{-1}(1-5\alpha)] + pQ_0[B_{r-k:r}^{-1}(1-\alpha)] \end{aligned} \quad (32)$$

and

$$Q_0(F) = [1 - (-\log F)^k] / k$$

The LQMOM estimators $\hat{\mu}$, $\hat{\sigma}$ and $\hat{k}$ of the parameters are the solution of (28)-(30), when ξ_r are replaced by their estimators $\hat{\xi}_r$. The relationship between η_3 and k from Eq. (31) (for example $p = 0.2$ and $\alpha = 0.05$) is shown in Figure 1. The following approximation relationships between the value of k and η_3 obtained through regression analysis

$$\begin{aligned} \hat{k} = & 0.2801 - 1.7130\hat{\eta}_3 + 0.8377\hat{\eta}_3^2 \\ & - 1.0491\hat{\eta}_3^3 + 0.6495\hat{\eta}_3^4 - 0.2934\hat{\eta}_3^5 \\ & - 0.1268\hat{\eta}_3^6 + 0.2765\hat{\eta}_3^7 - 0.0963\hat{\eta}_3^8 \end{aligned} \quad (33)$$

Figure 1: Relationship between η_3 and k for the GEV distribution.

The $\hat{k}$ function is a very good approximation for $\hat{k}$ in the range $[-1.0, 1.0]$ and $\hat{\eta}_3$ in the range $[-0.336, 0.854]$. Once the value of $\hat{k}$ is obtained, $\hat{\sigma}$ and $\hat{\mu}$ can be estimated successively from Equation (29) and (28) as

$$\hat{\sigma} = \frac{2\hat{\xi}_2}{[\hat{t}_{p,\alpha}(X_{2:2}) - \hat{t}_{p,\alpha}(X_{1:2})]} \quad (34)$$

$$\hat{\mu} = \hat{\xi}_1 - \hat{\sigma}\hat{t}_{p,\alpha}(X_{1:1}) \quad (35)$$

Monte Carlo Simulations

Monte Carlo simulations have been carried out to investigate the effect of LQ-moments based on WK5 with $p = 0.2$ and $\alpha = 0.05$ on the high quantiles estimation.

Simulation Study For Parent Distribution Function Known

It is still useful to look at how estimation is affected by various methods when the distribution function is known, although the true underlying distribution function is never known in practice. In this study, the GEV

distribution is used to generate GEV samples. Monte Carlo simulations were performed for sample sizes 15, 25, 50 and 100, and parameters of GEV are $\mu = 0$ and $\sigma = 1$ with different values of k between -0.4 and 0.4 . The samples are fitted by the GEV distribution function using the method of LMOM, LIQ, and WK5.

For each sample size, 10,000 replicates were generated, and quantile estimators of $Q(F)$, $F = 0.90, 0.98, 0.99$, and 0.999 , are examined in terms of the BIAS and root mean square error (RMSE). Results for BIAS for different quantiles show a very similar pattern. Only the result for $Q(F)$, $F = 0.99$ is presented here and is shown in Figure 2. For the extreme quantiles, the LMOM estimator consistently shows the lowest BIAS followed by WK5 and LIQ estimator for samples sizes of 25 and 50.

RMSE has been obtained for quantiles $Q(F)$, $F = 0.9, 0.98, 0.99$, and 0.999 , estimated by using LMOM, LIQ, and WK5. Results are presented in Table 1 in terms of estimation efficiency in relation to using WK5 defined as

$$\phi = \frac{\text{RMSE using WK5}}{\text{RMSE using LMOM or LIQ}} \quad (36)$$

Figure 2. Bias of $Q(F=0.99)$ Estimator Using L Moments and LQ Moments Based on WK5 and LIQ, Fitting the GEV Distribution to Generated GEV Samples For $n = 25$ and $n = 50$

Table 1: Efficiency of $Q(F)$, $F = 0.9, 0.98, 0.99$, and 0.999 Estimated By Using LMOM, LIQ, and WK5, Fitting the GEV Distribution Based on Generated GEV Samples

n	F	k									
		-0.3		-0.1		0		0.1		0.3	
		LMOM	LIQ	LMOM	LIQ	LMOM	LIQ	LMOM	LIQ	LMOM	LIQ
15	0.9	0.99	0.00	1.10	0.64	1.14	0.72	1.19	0.80	1.34	0.92
	0.98	1.15	0.00	0.87	0.18	0.83	0.26	0.81	0.29	0.79	0.30
	0.99	1.19	0.00	0.80	0.09	0.77	0.17	0.76	0.21	0.84	0.27
	0.999	1.23	0.00	0.70	0.00	0.75	0.04	0.87	0.09	1.24	0.20
25	0.9	1.22	0.71	1.10	0.73	1.13	0.77	1.17	0.82	1.28	0.89
	0.98	1.21	0.18	0.94	0.34	0.91	0.35	0.88	0.35	0.84	0.35
	0.99	1.22	0.07	0.90	0.24	0.87	0.27	0.85	0.28	0.87	0.31
	0.999	1.31	0.00	0.87	0.07	0.88	0.11	0.93	0.13	1.19	0.25
50	0.9	1.15	0.80	1.08	0.77	1.09	0.78	1.12	0.79	1.20	0.80
	0.98	1.19	0.50	1.01	0.47	0.97	0.45	0.94	0.43	0.88	0.39
	0.99	1.23	0.41	0.99	0.40	0.95	0.39	0.92	0.37	0.88	0.35
	0.999	1.53	0.14	1.01	0.22	0.97	0.24	0.95	0.25	1.02	0.31
100	0.9	0.96	0.85	1.04	0.79	1.04	0.77	1.06	0.76	1.09	0.73
	0.98	0.88	0.69	0.75	0.57	0.66	0.52	0.71	0.49	0.90	0.42
	0.99	0.91	0.67	0.72	0.53	0.62	0.48	0.67	0.44	0.89	0.38
	0.999	1.33	0.62	0.79	0.41	0.64	0.37	0.67	0.35	0.91	0.34

Values $\phi < 1$ indicated that the WK5 method is superior to the other methods. Table 1 shows the ϕ of the estimators for LMOM, and LIQ estimators compared to WK5 method for $k = -0.3, -0.1, 0, 0.1, 0.3$. For the estimation of $Q(F)$, $F > 0.9$, WK5 in many cases leads to higher efficiency especially for $k > -0.3$. The LIQ estimators lead to lower efficiency than LMOM for all n and k .

Parent Distribution Function Unknown

In practice, the true distribution function is never known. Thus, it will be even more useful to look how estimation is affected by various methods when the assumed distribution function differs from the parent distribution function. In this study Kappa distribution was used to generate the random samples data.

Hosking and Wallis (1993) used the kappa distribution to generate artificial data for assessing the goodness of fit of different distributions in their study on regional frequency

analysis. The cumulative distribution function of the Kappa distribution four-parameter is

$$F(x) = \begin{cases} \{1 - h[1 - k(x - \zeta)/\sigma]^{1/k}\}^{1/h} & \text{if } k \neq 0, h \neq 0, \\ \exp\{-[1 - k(x - \zeta)/\sigma]^{1/k}\} & \text{if } k \neq 0, h = 0, \\ \{1 - h \exp[-(x - \zeta)/\sigma]\}^{1/h} & \text{if } k = 0, h \neq 0, \\ \exp\{-\exp[-(x - \zeta)/\sigma]\} & \text{if } k = 0, h = 0. \end{cases} \quad (37)$$

where ζ is a location parameter, σ is a scale parameter, and h and k are shape parameters (Park and Park, 2002). The quantile function of the kappa distribution is

$$Q(F) = \zeta + \sigma \{1 - [(1 - F^h)/h]^k\} / k. \quad (38)$$

This distribution is a special cases of the generalized logistic (GL) ($h = -1$ and $k \neq 0$), generalized extreme-value (GEV)

Table 2: Efficiency of $Q(F)$, $F = 0.9, 0.98, 0.99$, and 0.999 Estimated By Using LMOM and WK5, Fitting the GEV Distribution Based on Generated Kappa Samples

n	F	GL		EXP		GP		Uniform	
		LMOM	WK5	LMOM	WK5	LMOM	WK5	LMOM	WK5
15	0.9	1.358	1.555	0.596	0.637	0.316	0.369	0.233	0.081
	0.98	4.322	4.444	1.335	1.212	0.589	0.446	0.169	0.123
	0.99	6.990	6.981	2.069	1.582	0.908	0.560	0.249	0.205
	0.999	33.875	32.832	9.033	4.714	3.125	1.713	0.544	0.499
25	0.9	1.051	1.178	0.465	0.505	0.250	0.301	0.208	0.093
	0.98	3.422	3.669	1.051	0.993	0.460	0.348	0.146	0.091
	0.99	5.502	5.936	1.657	1.347	0.730	0.455	0.214	0.157
	0.999	24.892	30.109	7.056	4.459	2.436	1.489	0.431	0.373
50	0.9	0.776	0.829	0.353	0.382	0.186	0.229	0.192	0.111
	0.98	2.572	2.850	0.753	0.763	0.346	0.252	0.127	0.063
	0.99	4.088	4.681	1.219	1.087	0.583	0.353	0.186	0.115
	0.999	16.568	23.406	5.321	4.072	1.965	1.253	0.351	0.264
100	0.9	0.566	0.586	0.271	0.284	0.145	0.177	0.184	0.121
	0.98	1.884	2.108	0.547	0.569	0.273	0.184	0.119	0.056
	0.99	2.989	3.461	0.939	0.874	0.496	0.303	0.174	0.103
	0.999	11.563	15.713	4.377	3.702	1.723	1.178	0.318	0.229

($h = 0$ and $k \neq 0$), generalized Pareto (GP) LMOM, and WK5 method. The WK5 almost
 ($h = 1$ and $k \neq 0$), Gumbel (EV1) always perform better than LMOM except when

($h = 0$ and $k = 0$), uniform (U) ($h = 1$ and $k = 1$)
 and exponential (EXP) ($h = 0$ and $k = 1$)
 distributions (Sing et al, 2002).

In order to evaluate the performance of the four-parameter estimation methods for GEV distribution, different parameters of kappa distribution were considered for simulation with values of the shape parameter (h, k) were set $(-1, -0.3)$ for GL, $(1, 0.3)$ for GP, $(1, 1)$ for U and $(0, 1)$ for EXP distribution. The location, ζ and scale, σ parameters were set 0 and 1, respectively. For this purpose, 10 000 random samples of $n = 15, 25, 50$, and 100 are used. The performance of the LQ-moments using WK5 are only considered to compare with LMOM because the LIQ estimator always has lower efficiency in comparison to the other estimators.

Table 2 shows the RMSE of the $F = 0.9, 0.98, 0.99$, and 0.999 quantile estimators for

the data are generated by the GL distribution for $n > 15$.

Figure 3 shows the BIAS of $Q(F)$, $F = 0.99$ estimators for $n = 25$ and 100. The results are quite similar. In term of BIAS the WK5 method is clearly superior to the LMOM method except when the data are from the GL distribution for $n = 25$.

Data Analysis

To illustrate the use of the GEV distribution for fitting data sets by various methods (LMOM, LQ moments using LIQ, and WK5), two sets of annual maximum flood series for the Feather River at Oroville and the Blackstone River at Woonsocket, were taken from Mudholkar and Hutson (1998). The parameter estimates for each data set, using various methods, are given in Table 3. Observed and computed frequency curves for the two data sets are plotted in Figure 4. The observed data values are plotted against the corresponding

EV1 reduced variates using the Cunnane plotting position.

Figure 3: Bias of $Q(F = 0.99)$ Estimator Using L-Moments and LQ-Moment Based On WK5, Fitting the GEV Distribution to Generated Kappa Samples For $n = 25$ and $n = 100$

Table 3: Estimated Values for the GEV Distribution

(a) Blackstone River Data

Parameter	L Moments Method	LQ Moment Method	
		LIQ	WK5
μ	4257.0	4495.0	4064.1
σ	1443.2	1213.4	1955.1
k	-0.479	-0.468	-0.359
10 year flood (ft^3/s)	10096.0	9335.6	10833.7
50 year flood	20764.5	18006.5	20717.1
100 year flood	28153.6	24232.2	27011.1
1000 year flood	83546.4	67657.9	63607.2

(b) Feather River Data

Parameter	L Moments Method	LQ Moment Method	
		LIQ	WK5
μ	44893.6	43537.8	46385.7
σ	37335.8	40146.3	34804.1
k	-0.094	-0.119	-0.093
10 year flood (ft^3/s)	138501.2	147176.7	146897.9
50 year flood	221017.6	243047.3	235293.5
100 year flood	259959.9	289615.9	276951.9
1000 year flood	408508.6	474246.2	435565.3

similarly to the L-moments. Results from fitting the GEV distribution function to generated GEV samples show that LQ-moments using WK5

Figure 4: Fitting the GEV Distribution To Annual Maximum Flows At Blackstone River And Feather River.

For Feather River data, the frequency curves obtained by the WK5 lie much closer to the data than LMOM and LIQ methods. For the Blackstone River data, the frequency curves of the WK5 and LMOM methods are steeper than those of LIQ method, however the fitting of these methods are in serious error, especially for the larger flows.

Conclusion

The LQ-moments are constructed by using a function that defines the quick estimators, such as the median, trimean or Gastwirth, in places of expectations in L-moments have are re-examined. The quick estimators based on five points quantiles using weighted kernel estimators are introduced for characterizing the upper quantiles of distributions and larger events in a sample. The parameters of the GEV distribution are estimated by matching LQ-moments to their sample estimates behave

almost always perform better than L-moments but has more BIAS than L-moments method. Results from fitting the GEV distribution function to samples generated from the Kappa distribution show that the WK5 lead to reduced BIAS and in many cases, higher efficiency compared to the other methods. The LIQ estimator leads to poorer estimation of high quantiles in terms of BIAS and RMSE.

This study has demonstrated that the conventional L-moment is not optimal for the estimation of GEV distribution. The new method of estimation, denoted the LQ-moments based on WK5 method, in many cases represents higher efficiency in high quantile estimation compared the L-moments method. The simplicity and generally good performance of this method make it an attractive option for estimating quantiles in the GEV distribution. Although the linear interpolation quantile estimator commonly used in most statistical software packages and in the LQ-moments

method, but it does not perform as good as the WK5 in estimating the parameters of the GEV distribution.

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A Spline-Based Lack-Of-Fit Test for Independent Variable Effect in Poisson Regression

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In regression analysis of count data, independent variables are often modeled by their linear effects under the assumption of log-linearity. In reality, the validity of such an assumption is rarely tested, and its use is at times unjustifiable. A lack-of-fit test is proposed for the adequacy of a postulated functional form of an independent variable within the framework of semiparametric Poisson regression models based on penalized splines. It offers added flexibility in accommodating the potentially non-loglinear effect of the independent variable. A likelihood ratio test is constructed for the adequacy of the postulated parametric form, for example log-linearity, of the independent variable effect. Simulations indicate that the proposed model performs well, and misspecified parametric model has much reduced power. An example is given.

Key words: B-splines, likelihood ratio test, loglinear model, penalized likelihood, Poisson regression model.

Introduction

The Poisson regression model is among the most frequently used statistical tools in event count analysis. It has been successfully used in numerous applications (e.g. McCullagh & Nelder, 1989; Cameron & Trivedi, 1998). In its parametric form, the model is constructed as follows: Let Y_i be the number of occurrences of an event of interest for the i th subject and x_i be

an independent variable, $i = 1, \dots, n$. Assuming that Y_i follows a Poisson distribution, i.e., $Y_i \sim \text{Poisson}(\mu(x_i))$ with mean $\mu(x_i)$, write the Poisson density as follows:

$$f(y_i | x_i) = \frac{\exp(-\mu(x_i)) \mu(x_i)^{y_i}}{y_i!}, \quad (1.1)$$

where $\mu(x_i) = E[Y_i | x_i]$ is the mean function, $i = 1, \dots, n$.

Under this formulation, the model depicts the dependency of the event counts on x_i via a logarithmic link function,

$$\log(\mu(x_i)) = h(x_i, \boldsymbol{\beta}), \quad (1.2)$$

where $h(\cdot; \boldsymbol{\beta})$ is a known functional form apart from the parameter vector $\boldsymbol{\beta}$. In other words, the model assumes a log parametric form for the independent variable effect. Although the theory does not restrict $h(\cdot; \boldsymbol{\beta})$ to a linear form, in practice, however, most analysts choose to use $h(x; \boldsymbol{\beta}) = \beta_0 + \beta_1 x$, which is often referred to as the loglinear model. Despite its popularity, the

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validity of this postulated loglinear form is rarely verified, possibly due to the lack of readily accessible testing procedures. In addition, the consequences of a misspecified functional form of the independent variable are not well studied.

An alternative approach is to replace the linear predictor $h(\cdot; \beta)$ with a regression spline. This approach is semiparametric in nature because it has not only a parametric component for the data distribution (Poisson in the case of counts), but also a nonparametric component involving the predictor (e.g. Ruppert et al., 2003). Such an approach is known to enhance the modeling flexibility in regression analysis. Regression spline techniques have been used frequently to estimate independent variable effects in generalized linear models (e.g., Eilers & Marx, 1996). But testing procedures based on regression splines have attracted considerably less attention.

The purpose of this article is to construct a general test for the inference concerning the adequacy of a given functional form of the independent variable effect in count data analysis. The proposed test contributes to the existing literature of count data analysis by providing a practical way for the determination of functional forms of independent variables.

Example

Patients with chronic diseases, such as congestive heart failure (CHF), must take medications regularly to prevent disease exacerbation that requires costly health care services such as emergency department (ED) visits and hospitalization admissions. In a study on medication adherence in older adults with CHF, participants were monitored for their medication use during a 1-year study period. Eligible participants were English-speaking, 50 years of age or older, had a diagnosis of CHF, and were currently prescribed for at least one cardiovascular medication, including angiotensin-converting enzyme inhibitors, angiotensin II-receptor antagonists, β -adrenergic receptor antagonists, digoxin, loop and nonloop diuretics, and an aldosterone antagonist. Upon enrollment, participants were provided electronic medication container lids for their cardiovascular medications. The electronic

container lids automatically recorded the dates and times of the lid openings (Tu et al., 2005). Assuming that the patient took the prescribed amount of medication each time the lid was opened, patient's medication adherence to the prescribed drug was calculated as the percentage of dose taken during the observation period according to the prescribed regimen.

For example, if 30 openings were recorded during a 1-month period for a b.i.d. (twice a day) drug, the medication adherence was $r = 30/60 = 50\%$, meaning the patient took only half of the medicine that he was supposed to take. Although 100% is the target level for medication adherence, values that are significantly less or more than 100% would represent suboptimal medication-taking behavior on the part of the patient. Therefore, in pharmacy practice, researchers often calculate the patient's deviation in medication consumption from the target level ($|1-r|$) and report an adjusted adherence $x = 1 - |1-r|$ as a percentage between 0 and 100%. For a more detailed discussion (see Hope et al., (2004).

When a patient was on multiple cardiovascular drugs, his overall adjusted medication adherence was summarized as the average level of the adjusted medication adherence values for all of the study drugs. An important issue of this study is to understand the relationship between adjusted medication adherence and disease exacerbation. Herein, the number of ED visits during the 1-year follow-up period is used as the primary outcome of interest.

For the purpose of illustration, consider a subset of the study data: 93 subjects who belong to the New York Heart Association (NYHA) Class III. The NYHA classification is one of the most commonly used clinical classification systems for patients with heart failure. Typical NYHA Class III patients experience a marked limitation of physical activities, such as walking one to two blocks on the level or climbing more than one flight of stairs under normal conditions. Patients are comfortable at rest, but more than usual physical activity causes fatigue, palpitation, dyspnea, anginal pain, or a combination thereof.

Methodology

Semiparametric Poisson Model

Using the previously introduced notation, we write the response variables as $Y_i \sim \text{Poisson}(\mu(x_i))$ for $i = 1, \dots, n$. To model the effect of the independent variable x_i on the response variable, link the mean function $\mu(x_i)$ to x_i via $g(\mu(x_i)) = h(x_i)$, where $g(\cdot)$ is a monotone differentiable link function, and $h(\cdot)$ is the predictor function. To differentiate the proposed model from the traditional loglinear predictor, write $g(\mu(x_i)) = s(x_i)$, where $s(x_i)$ is a smooth function to be estimated from the data. Under the commonly used log-link function, there is a semiparametric Poisson regression model:

$$g(\mu(x)) = \log(\mu(x)) = s(x). \quad (3.1)$$

Equivalently, write $\mu(x) = \exp(s(x))$. Because the B-spline basis is numerically more stable for the representation of a spline function than the truncated-power basis is, to approximate the unknown function $s(\cdot)$, parameterize it with the cubic B-splines as

$$s(x) = \sum_{k=1}^K \theta_k B_k(x), \quad (3.2)$$

where B_k are the cubic B-spline basis functions for s ; θ_k are spline coefficients; and $K = q + 4$, where q is the number of knots; see de Boor (1978) for details of computation of B-splines of any degree from B-splines of a lower degree. These knots were chosen to be equally spaced with respect to the quantiles of the distinct values of x_i and set $q = \min[(\text{number of distinct values of } x/6), 30]$, where $[a]$ is the greatest integer less than or equal to a ; for reference on the selection of q , (see Ruppert, 2002). Let $\mathbf{B}_{x_i} = (B_1(x_i), \dots, B_K(x_i))^T$ and $\boldsymbol{\theta} = (\theta_1, \dots, \theta_K)^T$ and expressing s in vector notation

as $s(x_i) = \mathbf{B}_{x_i}^T \boldsymbol{\theta}$, rewrite the Poisson density in (1.1) as

$$f(y_i | x_i) = \frac{\exp[-\exp(\mathbf{B}_{x_i}^T \boldsymbol{\theta})] \exp(\mathbf{B}_{x_i}^T \boldsymbol{\theta})^{y_i}}{y_i!}, \quad (3.3)$$

Parameter Estimation

To estimate $\boldsymbol{\theta}$ and prevent overfitting, employ a penalized likelihood approach with a discrete approximation to the integrated squared second derivative of s , $\int s''(x)^2 dx$, which is used as a measure of its roughness. Therefore, the penalized log-likelihood

$\ell(\boldsymbol{\theta}) - (1/2) \int s''(x)^2 dx$ is approximated by

$$\ell_{pen}(\boldsymbol{\theta}) = \ell(\boldsymbol{\theta}) - \frac{1}{2} \lambda \boldsymbol{\theta}^T \mathbf{K} \boldsymbol{\theta}, \quad (3.4)$$

where the log-likelihood $\ell(\boldsymbol{\theta})$ is

$$\ell(\boldsymbol{\theta}) = \sum_{i=1}^n \{y_i \mathbf{B}_{x_i}^T \boldsymbol{\theta} - \exp(\mathbf{B}_{x_i}^T \boldsymbol{\theta}) - \log y_i!\}.$$

λ is a smoothing parameter to be chosen. It is used to govern the tradeoff between goodness-of-fit and smoothness;

$$\boldsymbol{\theta}^T \mathbf{K} \boldsymbol{\theta} = \sum_{k=1}^K (\Delta^2 \theta_k)^2 \quad \text{for } \Delta^2 \theta_k = \theta_k - 2\theta_{k-1} + \theta_{k-2}$$

and $\mathbf{K} = \mathbf{D}_2^T \mathbf{D}_2$ for $\mathbf{D}_2$ being the matrix representation of the difference operator Δ^2 . For details of similar operation, see Eilers & Marx (1996). To estimate $\boldsymbol{\theta}$, set the first-order partial derivatives of the penalized log-likelihood in (3.4) with respect to $\boldsymbol{\theta}$ equal to $\mathbf{0}$, $q(\boldsymbol{\theta}) = \partial \ell_{pen}(\boldsymbol{\theta}) / \partial \boldsymbol{\theta} = \mathbf{0}$. Then, solve iteratively the following weighted least-squares equations in matrix notation:

$$(\mathbf{BWB} + \lambda \mathbf{K}) \boldsymbol{\theta} = \mathbf{B}^T \mathbf{W} \mathbf{y}^*, \quad (3.5)$$

where

$$\mathbf{B} = (\mathbf{B}_{x_1}^T, \dots, \mathbf{B}_{x_n}^T)^T,$$

$$\mathbf{W} = \text{diag}(\exp(\mathbf{B}_{x_1}^T \boldsymbol{\theta}), \dots, \exp(\mathbf{B}_{x_n}^T \boldsymbol{\theta})),$$

and

$$\mathbf{y}^* = (y_1^*, \dots, y_n^*)^T$$

is the working response vector for

$$y_i^* = \frac{y_i - \exp(\mathbf{B}_{x_i}^T \boldsymbol{\theta})}{\exp(\mathbf{B}_{x_i}^T \boldsymbol{\theta})} + \mathbf{B}_{x_i}^T \boldsymbol{\theta}.$$

The concept of the effective number of degrees of freedom (Edf) is used to choose the value of the smoothing parameter λ , $\text{Edf} = \text{tr}(\mathbf{S}_\lambda) - 1$, where

$$\mathbf{S}_\lambda = \mathbf{B}(\mathbf{B}\mathbf{W}\mathbf{B} + \lambda\mathbf{K})^{-1} \mathbf{B}^T \mathbf{W}$$

is called the smoother matrix (see Hastie & Tibshirani, 1990).

The solution to (3.5), denoted by $\hat{\boldsymbol{\theta}}_{pen}$, is called a maximum penalized likelihood estimate of $\boldsymbol{\theta}$. The cubic B-spline fitted mean function is $\hat{\mu}_B = \exp(\hat{s}_B(x)) = \exp(\mathbf{B}_x^T \hat{\boldsymbol{\theta}}_{pen})$.

Inference

Let $\mathbf{Q}(\boldsymbol{\theta}) = \partial^2 \ell_{pen}(\boldsymbol{\theta}) / \partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T$ be the second-order partial derivatives of the penalized log-likelihood in (3.4) with respect to $\boldsymbol{\theta}$. Then, approximate the covariance matrix of $\hat{\boldsymbol{\theta}}_{pen}$ as $\text{cov}(\hat{\boldsymbol{\theta}}_{pen}) \approx \{-\mathbf{Q}(\boldsymbol{\theta})\}^{-1} \text{var}\{\mathbf{q}(\boldsymbol{\theta})\} \{-\mathbf{Q}(\boldsymbol{\theta})\}^{-1}$ and, hence, estimate it as follows:

$$\hat{\text{cov}}(\hat{\boldsymbol{\theta}}_{pen}) \approx \{-\mathbf{Q}(\hat{\boldsymbol{\theta}})\}^{-1}. \quad (3.6)$$

From (3.6), obtain a confidence interval for $s(x)$ by computing the estimated variance of $\hat{s}_B(x)$ as follows:

$$\hat{\text{var}}(\hat{s}_B(x)) = \mathbf{B}_x^T \hat{\text{cov}}\{\hat{\boldsymbol{\theta}}_{pen}\} \mathbf{B}_x,$$

where

$$\hat{s}_B(x) = \mathbf{B}_x^T \hat{\boldsymbol{\theta}}_{pen}.$$

Accordingly, a confidence interval for $\exp(s(x))$ can be obtained by using the delta method and the estimated variance of $\hat{s}_B(x)$.

The proposed estimation method is used with deviance, or log-likelihood ratio statistic, to assess the adequacy of a postulated parametric form of the model in (1.2), i.e., testing the following parametric null hypothesis:

$$H_0 : \log(\mu(\cdot)) = h(\cdot; \boldsymbol{\beta}). \quad (3.7)$$

Then, test for the lack of fit of the postulated parametric model in (3.7) by using the log-likelihood ratio test (LRT) statistic

$$\begin{aligned} & \sup \prod_{i=1}^n \exp\{-\exp[h(x_i; \boldsymbol{\beta})]\} \exp[y_i h(x_i; \boldsymbol{\beta})] \\ & - 2 \log \frac{\prod_{i=1}^n \exp\{-\exp[\mathbf{B}_{x_i}^T \hat{\boldsymbol{\beta}}_{pen}]\} \exp[y_i \mathbf{B}_{x_i}^T \hat{\boldsymbol{\beta}}_{pen}]}{\prod_{i=1}^n \exp\{-\exp[\mathbf{B}_{x_i}^T \hat{\boldsymbol{\beta}}_{pen}]\} \exp[y_i \mathbf{B}_{x_i}^T \hat{\boldsymbol{\beta}}_{pen}]} \end{aligned} \quad (3.8)$$

and comparing its value to its asymptotic limiting chi-square distribution with D degrees of freedom, where $D = \text{Edf}$ - the number of the postulated parametric model parameters + 1 (see Hastie & Tibshirani, 1990). This is called a smoothing log-likelihood ratio test (SLRT). By comparing the likelihood of the postulated parametric model $h(\cdot; \boldsymbol{\beta})$ with that of a B-spline model, the SLRT allows for inference on the adequacy of the postulated model. For example, the SLRT can be used to assess the appropriateness of the loglinear effect of x by testing

$$H_0 : \log(\mu(x)) = \beta_0 + \beta_1 x$$

versus

$$H_a : \log(\mu(x)) = s(x),$$

where $s(x)$ is a general nonlinear smooth function.

Simulation Study

A Monte Carlo simulation study is conducted to assess the performance of the SLRT. The values of the independent variable are equally spaced design points $x_i = (2i-1)/2n$, $i = 1, \dots, n = 100$; 1000 data sets were generated for each configuration of the experiments. The goal is to test the adequacy of the following loglinear model:

$$H_0 : \log(\mu(x; \beta)) = \beta_0 + \beta_1 x. \quad (4.1)$$

To assess the empirical power of the SLRT, data were generated from the model in (1.1) with the following logarithmic mean functions:

$$\log(\mu(x; \beta, \gamma)) = \beta_0 + \beta_1 x + \gamma \sin(3\pi x), \quad (4.2)$$

where

$$\beta = (\beta_0, \beta_1) = (1.159, -0.675),$$

and

$$\gamma = 0, 0.05, 0.1, \dots, 0.5.$$

Note that $\gamma = 0$ corresponds to the null hypothesis. In this simulation study, the β values were chosen to reflect the estimated coefficient values of the example data, and the value of the smoothing parameter λ was chosen by fixing $\text{Edf} = \text{tr}(\mathbf{S}_\lambda) - 1 = 4$ while estimating the cubic B-spline coefficients. The null model is rejected if the observed value of the SLRT statistic in (3.8) with $h(x; \beta) = \beta_0 + \beta_1 x$, exceeds the 0.95-quantile of the chi-square distribution with $D = 3$ degrees of freedom. This is called an asymptotic smoothing log-likelihood ratio test (ASLRT).

An obvious variant of the ASLRT is to approximate the 0.95-quantile of the distribution of the SLRT statistic via 200 Monte Carlo simulations for each sample and reject the null model if the observed value of the SLRT statistic exceeds the approximated 0.95-quantile. This test is called the Monte Carlo smoothing log-likelihood ratio test (MSLRT).

For the purpose of comparative evaluation, it is important to establish a benchmark for the power of the inference when the true model is known. To do so, consider the following parametric likelihood ratio test for $\gamma = 0$ under the assumption that the true model is known:

$$-2 \log \frac{\sup \prod_{i=1}^n \exp\{-\exp[\beta_0 + \beta_1 x_i]\} \exp[y_i(\beta_0 + \beta_1 x_i)]}{\prod_{i=1}^n \exp\{-\exp[\beta_0 + \beta_1 x_i + \gamma \sin(3\pi x_i)]\} \exp[y_i(\beta_0 + \beta_1 x_i + \gamma \sin(3\pi x_i))]} \quad (4.3)$$

$$-2 \log \frac{\sup \prod_{i=1}^n \exp\{-\exp[\beta_0 + \beta_1 x_i]\} \exp[y_i(\beta_0 + \beta_1 x_i)]}{\prod_{i=1}^n \exp\{-\exp[a_0 + a_1 x_i + a_2 x_i^2]\} \exp[y_i(a_0 + a_1 x_i + a_2 x_i^2)]} \quad (4.4)$$

Because this test directly compares the likelihood of the postulated model (4.1) with the true parametric model (4.2) which generates the data, the parametric test in (4.3) is referred to as an exactly specified parametric log-likelihood ratio test (ESPLRT). The null model is rejected if the observed value of the LRT statistic in (4.3) was greater than the 0.95-quantile of the chi-square distribution with one degree of freedom. When the null model is appropriate, the exactly specified test ESPLRT in (4.3) follows an asymptotic chi-square distribution with degree of freedom and should have the best power among all competitors. This asymptotically optimal test, however, provides only a benchmark for the power comparison and is of limited practical values, because its use requires specific knowledge of the form of the true model.

In practical data analysis, when there are clear indications that an independent variable effect is not linear, data analysts often attempt to alleviate the lack-of-fit by including a quadratic term. To assess the potential power loss associated with such practice when a wrong model is used, consider a misspecified quadratic parametric model, $\log(\mu(x)) = a_0 + a_1x + a_2x^2$, and use it to construct a parametric likelihood ratio test:

Because the misspecified parametric model $\log(\mu(x)) = a_0 + a_1x + a_2x^2$ is used to fit data generated under the true model $\log(\mu(x; \beta, \gamma)) = \beta_0 + \beta_1x + \gamma \sin(3\pi x)$, in (4.2), this parametric test is referred to as a misspecified parametric likelihood ratio test (MSPLRT). By comparing the empirical power of the MSPLRT with that of the benchmark test, ESPLRT, and other competitors, it is possible to assess the power loss when a misspecified quadratic model is used in data analysis.

The empirical powers of the four candidate tests, ESPLRT, MSPLRT, ASLRT, and MSLRT, are depicted in Figure 1. While the empirical significance level of the ASLRT tends to be slightly higher than the nominal level 0.05, its power is the closest to that of the exactly specified parametric likelihood ratio test (ESPLRT), the benchmark test, among all three other candidates. A close second is the Monte Carlo version of the smoothing likelihood ratio

test, MSLRT. On the other hand, the misspecified parametric likelihood ratio test MSPLRT suffers a severe loss of power, highlighting the consequences of making inference under misspecified parametric regression models.

Example Data Analysis

The practical use of the proposed semiparametric Poisson regression model and lack-of-fit tests is illustrated by examining the effect of the adjusted medication adherence on ED utilization in a study of 93 NYHA Class III patients. Consider the number of all-cause ED visits as the response variable. All-cause ED visits include ED admissions for any reason. The use of all-cause ED visits in this analysis is justified, because acute exacerbation in patients with heart failure does not always occur in the form of CHF, coronary artery disease, or cardiovascular diseases. Sometimes, it results in complications in other organs, which would be recorded as noncardiovascular-related conditions in the medical records. The adjusted medication adherence to all prescribed cardiovascular medications is the independent variable of interest. Therefore, do not restrict the effect of the overall adjusted medication adherence (x) to be loglinear. Instead, use the proposed inference procedure to test for the loglinear effect of the independent variable x on the number of ED visits. That is, test the following hypotheses:

$$H_0 : \log(\mu(x)) = \beta_0 + \beta_1x,$$

versus

$$H_a : \log(\mu(x)) = s(x).$$

In this example, $\text{Edf} = \text{tr}(\mathbf{S}_\lambda) - 1 = 4$ is fixed to choose the value of λ for the estimation of cubic B-spline coefficients. By using the smoothing log-likelihood ratio test (SLRT) statistic with an asymptotic chi-square distribution with 3 degrees of freedom, it is found that the independent variable has a significantly non-loglinear effect on the number of ED visits (ASLRT p-value = 0.029).

The distribution of the SLRT statistic is approximated through 200 Monte Carlo simulations. The p-value from the Monte Carlo based test MSLRT is 0.015, which is the

Figure 1: Empirical power curve comparison of the ESPLRT, ASLRT, MSLRT, and MSPLRT for the null model $H_0: \log(\mu(x; \beta)) = \beta_0 + \beta_1 x$ and alternative model $\log(\mu(x; \beta, \gamma)) = \beta_0 + \beta_1 x + \gamma \sin(3\pi x)$, where $\beta = (\beta_0, \beta_1)^T = (1.159, -0.675)^T$. Abbreviations: ASLRT, asymptotic smoothing log-likelihood ratio test; ESPLRT, the exactly specified parametric log-likelihood ratio test; MSLRT, Monte Carlo smoothing log-likelihood ratio test; MSPLRT, misspecified parametric log-likelihood ratio test.

proportion of simulated values of the test statistic exceeding the observed value of the SLRT statistic 9.0033. Therefore, the SLRT based on the Monte Carlo simulations again confirmed the lack of log linearity in the medication adherence effect. Figure 2 shows the cubic B-spline fitted mean function $\mu(x)$ and 95% point-wise confidence interval for the mean function and the parametrically fitted mean function $\hat{\mu}(x) = \exp(1.159 - 0.675x)$; Figure 3 further confirms that the cubic B-spline fitted function and 95% point-wise confidence interval for the functional form of the effect of x and the parametrically fitted function $1.159 - 0.675x$.

From the perspective of pharmacotherapy, the lack of log linearity in the effect of medication adherence is perhaps not entirely surprising: underconsumption of

cardiovascular drugs often leads to decompensation in patients with CHF, and overdosing can cause dangerous hypotension. Both are likely to result in increased ED use. Because the adherence data are in the adjusted form $(x = 100(1 - |1 - r|)\%)$ where overconsumption of the medication was converted to a percentage less than 100%, a deviation from the target level (100%) could be the results of overconsumption as well as underconsumption. Figures 2 and 3 showed an increase in ED admission when adjusted medication adherence around 0.8, possibly caused by the folding of the raw adherence measure. Therefore, the loglinear relationship forced by the parametric Poisson regression model would not be adequate and the proposed semiparametric model would provide a relief in such a data situation.

Figure 2: Cubic B-spline fitted mean function $\hat{\mu}_B(x)$ and 95% point-wise confidence interval for the mean function $\mu(x)$ of medication adherence (x) and parametrically fitted mean function $\hat{\mu}(x) = \exp(1.159 - 0.675x)$ for $\mu(x)$.

Figure 3: Cubic B-spline fitted function $\hat{s}_B(x)$ and 95% point-wise confidence interval for the functional form $s(x)$ of the effect of medication adherence (x) and parametrically fitted function $1.159 - 0.675x$ for the effect of x .

Conclusion

Cubic B-spline basis functions can be used in Poisson regression analysis in a flexible manner, without imposing any particular functional form on the effects of independent variables. An easily implementable estimation procedure was examined for the coefficients of cubic B-spline basis functions by using a penalized likelihood approach. Fitting B-splines is usually not more difficult than that of a polynomial regression.

Because the selection of the number and locations of the knots is an important issue, it is the topic of much research in nonparametric regression methods (Ruppert, 2002; Lindstrom, 1999). Knots were chosen to be equally spaced with respect to the quantiles of the distinct values of the independent variable and set the number of chosen knots to be

$$\min \left[\left(\frac{\text{number of distinct values of covariate}}{6} \right), 30 \right]$$

(Ruppert, 2002).

This study has shown that by smoothing the effect of an independent variable, the proposed method allows for a test of the lack of fit of a postulated parametric model by the use of likelihood ratio method. As shown in the simulation study, the proposed test has the ability to detect more general alternative models and is superior to parametric likelihood ratio tests unless the true model is known. This is of great practical importance, because in most real data applications, the true parametric forms of independent variable effects are usually unknown. Therefore, investigators must consider the consequences of statistical inferences under misspecified parametric regression models. Specifically, this simulation study showed that the common practice of adding a quadratic term to the linear predictor could severely undercut the power of inference.

The scope was restricted to count data following Poisson distribution. But, as many have observed, count data often exhibit greater variability than that is provided by the Poisson distribution. In the presence of extra-Poisson variation, one could use regression models based

on negative binomial distribution (Tu & Piegorsch, 2003). This research can be extended by linking the negative binomial mean $\mu(x)$ to smooth function $s(x)$. The testing procedure associated with the extended model is currently under investigation.

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Using the Fractional Imputation Methodology to Evaluate Variance due to Hot Deck Imputation in Survey Data

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This article examines empirically the effect on the variance estimate due to the use of hot deck imputation with a nearest neighbor donor in comparison with the pairwise fractional hot deck imputation methodology in the 1999 Survey of Doctorate Recipients.

Key words: Ignorability, missing at random, item nonresponse, serpentine sorting, nearest neighbor, successive difference replication

Introduction

Imputation is commonly used to deal with nonresponse and incomplete data in surveys. Usually, the use of imputed values as observed values produces appropriate estimates of smooth statistics (totals, means, proportions, etc) as well as non-smooth statistics (quantiles, etc), if the imputation does not cause severe systematic bias. However, the dangers are well known of not correcting the variance estimates to reflect the uncertainty due to missing data. This may lead to larger underestimation as the proportion of imputed values increases when treating the imputed values as observed. Over the years, a number of methods have been suggested in the statistical literature to overcome these issues (Kalton & Kasprzyk, 1986; Brick & Kalton, 1996; Groves et al., 2004).

Among other reasons, imputation techniques typically are not used with survey data because their users are unfamiliar with techniques of analyzing missing data. Due to operational convenience, most of the commonly

used statistical packages do not incorporate adjustments for missing data into their analysis. For simplicity, often an entire observation with one missing variable response is eliminated.

Following Shao and Steel's (1999) description, two general perspectives exist to obtain variance estimators for large complex sample surveys after imputation: design-based and model-assisted perspective (including multiple imputation). Paraphrasing their definitions: the variance estimate in a design-based perspective accounts for repeated sampling from a fixed finite population and uniform nonresponse within an imputation cell.

Using the model-assisted perspective, the variance estimate is with respect to the sample design and response as well as to the model used for the imputation method (Särndal, Swensson, & Wretman, 1992; Shao et al., 1999). Variance estimators under a multiple imputation perspective (Rubin, 1987), are reasonable using Bayesian inference but are not applicable for design-based or deterministic imputation methods (Shao, 2002). The model-assisted perspective variance estimation methods will not be discussed any further.

Several variance estimation methods exist under the design-based perspective after imputation. Two examples are linearization methods (i.e., Taylor series expansions (Chen & Shao, 1997; Chen & Shao, 2000; Kim, 2001))

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and replication methods (i.e., Jackknife (Rao & Shao, 1992), bootstrap (Shao & Sitter, 1996) and balanced half samples (Lee, Rancourt, & Särndal, 1995; Rao & Shao, 1996; Shao, Chen, & Chen, 1998; Shao & Chen, 1999; Kim, 2001; Kim & Fuller, 2004). Lee, Rancourt and Särndal (2002) discussed the differences between these approaches. All these methods provide adequate estimates. The choice depends on the users, the need for the estimation of variance components, the computational burden, the adaptability of the sampling fraction and the response mechanism (Lee et al., 2002).

This article is focused on the effect on the variance estimates in the 1999 Survey of Doctorate Recipients (SDR) (National Science Foundation, Directorate for Social, & Division of Science Resources Statistics, 2002). In the next section, the 1999 SDR survey methods will be discussed. Next, a description of the aspects of nearest neighbor hot deck imputation method, fractional imputation, successive difference replication method and the effect of multiple weighting stages will be provided. All these methods are used here to evaluate the variance estimates of this survey. This study extends the proposal of pairwise fraction imputation by Kim and Fuller (1999) on the use of variance estimation with pairwise fractional hot deck imputation and the successive difference replication method.

The 1999 Survey of Doctorate Recipients (SDR)

The 1999 SDR is a National Science Foundation (NSF) survey conducted by the U.S. Census Bureau (National Science Foundation et al., 2002). The population of interest for this survey includes individuals who earned a doctoral degree from a United States (U.S.) institution in Science and Engineering (S&E) fields, are less than 76 years old and planned to stay in the U.S. after their degree (US Bureau of the Census, Demographic Statistical Methods Division, & Health Surveys and Supplements

Branch, 2003a). The SDR provides information about demographic and employment characteristics of the nation's science and engineering doctorate holders. The sampling frame consists of the doctorates records file which contains all research doctorate recipients from U.S. universities since 1920 (National Science Foundation et al., 2002).

The 1999 SDR survey sample size was 40,000. The sample was systematically selected from three groups using the probability proportional to size selection methodology. The three groups were the new cohort (doctoral recipients between July 1996 and June 1998), the nearly new cohort (doctoral recipients between July 1992 and June 1996) and the old cohort (doctoral recipients prior to July 1992) (National Science Foundation et al., 2002).

The sampling strata consisted of 240 strata for the old and nearly new cohorts and were defined by demographic group, degree field and sex. The same 240 strata (six of which were empty) defined the sampling strata for the new cohort (US Bureau of the Census et al., 2003a).

Item non-response was observed in this survey in all variables except seven. All seven were critical variables and had to be filled in order for the response to be considered complete. Hence, two imputation methods were used: logical imputation and hot deck imputation. Logical imputation was used when the answer to a question could be determined by the answer to another question either within the same survey year or from a prior survey round (US Bureau of the Census, Demographic Statistical Methods Division, & Health Surveys and Supplements Branch, 2001a). Logical imputation will not be addressed further in this article.

Hot deck imputation was implemented using a nearest neighbor donor. The auxiliary variables selected to identify the pool of donors were determined by prediction models for each

variable in the survey with item nonresponse. A serpentine sorting on the auxiliary variables was implemented to determine the nearest neighbor donor response (US Bureau of the Census et al., 2001a). This survey allowed for the use of information from any one donor a maximum of four times. The missing mechanism and the tentative reasons for missing values in this survey is likely missing at random (Perez, 2003).

Base weights of the 1999 SDR data were computed by the U.S. Census Bureau (US Bureau of the Census, Demographic Statistical Methods Division, & Health Surveys and Supplements Branch, 2001b). To obtain the final weights, the base weights underwent several adjustments to correct for duplicates, frame ineligibles, never earned doctorate case and control totals. Included in these weighting adjustments were a non-interview adjustment and a ratio adjustment via a raking methodology (US Bureau of the Census et al., 2001b). Variance estimates were calculated using successive difference replication methods with 160 replicates (US Bureau of the Census, Demographic Statistical Methods Division, & Health Surveys and Supplements Branch, 2003b; Sukasih & Jang, 2003). Point and variance estimates are currently reported using imputation values as observed values (National Science Foundation et al., 2002).

Methodology

Nearest Neighbor Hot Deck Imputation

Hot deck imputation refers to the process where missing responses or items are replaced by values selected from respondents within the same survey. The respondent selected as a donor is chosen by using observable values from auxiliary variables. The 1999 SDR survey used the hot deck imputation method based on imputation cells (US Bureau of the Census et al., 2001a). This means that in using auxiliary variables known for respondents and nonrespondents, the sample was divided into cells. Sorting was performed within each imputation cell and a neighboring case was selected as a donor for each missing value. Then, the missing value was replaced by the selected value within that cell (Chen et al., 2000).

Fractional imputation

Fractional imputation identifies the method where each missing response or item is replaced by several imputed values drawn from the responding values in an imputation cell (Fay, 1996; Kim et al., 1999). Fractional imputation provides an adjustment method for variance estimation in design-based estimators in the presence of missing values (da Silva & Opsomer, 2002).

Fractional imputation estimators were designed to reduce the imputation variance (Kim et al., 2004) by using more than one donor for a recipient and increasing the weight of the donor for each missing item by a value equal to a fraction of the original weight of the missing observation. Respondents who are not donors retain their original weights. Pairwise fractional hot deck imputation is a special case of fractional imputation where two distinct donors are selected for each missing item. The assumption for this method is that there are at least two donors in each imputation cell (Kim et al., 1999).

The Successive Difference Replication Method

The current approach in calculating the 1999 SDR variance estimates is the successive difference replication method (SDRM). Wolter (1984) developed the basic theory of the successive difference method and later Fay and Train (Fay & Train, 1995) extended this theory with replicates generating the SDRM. The variance estimator is calculated based on the squared differences between neighboring sample cases. The SDRM produces variance estimates with a greater number of degrees of freedom than other replication methods. To create the replicates, the SDRM variance estimator uses an orthogonal Hadamard matrix. Because the 1999 SDR used 160 replicates, a 160x160 Hadamard matrix was formed.

Notation

Paraphrasing, Kim and Fuller's (2004) notation: let P be a finite population containing indices $1, \dots, N$. P is stratified into H strata with N_h units in the h -th stratum. $n_h \geq 2$ units are selected following some probability sampling plan called the sampling mechanism.

Let S denote the sample. According to the sampling plan, survey weights $w_i, i \in S$ are constructed. This expectation is in respect to S . Let Y be a variable of interest and $Y = (y_1, y_2, \dots, y_N)$ denotes the population vector. The response mechanism (I) identifies the probability mechanism of the responses obtained in the sample. $I_i = 1$ if y_i is a respondent and $I_i = 0$ otherwise. Let the population characteristic of interest be $\theta_N = \theta(y_1, \dots, y_N)$ and let $\hat{\theta}$ be a linear estimator of θ_N based on the full sample, $\hat{\theta} = \sum_{i \in S} w_i y_i$.

The SDRM variance estimator for $\hat{\theta}$ can be defined without loss of generality as (ignoring the finite population correction factor) in equation (1):

$$V_{SDRM}(\hat{\theta}) = \frac{4}{k} \sum_{r=1}^k (\hat{\theta}^{(r)} - \hat{\theta})^2 \quad (1)$$

where r is the replicate sample ($r=1, \dots, k$). k is the total number of replicate samples, $\hat{\theta}^{(r)}$ is the r -th replicate of $\hat{\theta}$ and can be written as: $\hat{\theta}^{(r)} = \sum_{i \in S} w_i^{(r)} y_i$, where $w_i^{(r)}$ denotes the replicate weight for the i -th unit of the r -th replicate.

In the imputation procedure, let a_{ij} be the number of times that y_i is used as a donor for the missing y_j . S_R is the set of indices of the sample respondents and S_M is the set of indices of the sample nonrespondents. Let us define $a = \{a_{ij}; i \in S_R, j \in S_M\}$, then the distribution of a is called the imputation mechanism. In addition, when y_i is used as a donor for element j , let $w_{ij}^\bullet$ be the fraction of the original weight for element j . $w_{ij}^\bullet$ is called the imputation fraction (Fuller & Kim, 2001; Kim et al., 2004). $w_{ii}^\bullet = 1$ for $i \in S_R$ and $w_{ii}^\bullet = 0$ for $i \in S_M$. The a_{ij} are nonnegative and the sum of the imputation fractions of the donors for a missing item is mandatory to be one:

$\sum_{i \in S_R} a_{ij} w_{ij}^\bullet = 1, \forall j \in S$. In the case of a pairwise

fractional hot deck imputation, the imputation fractions, $w_{ij}^\bullet$, are equal to 0.5. A linear estimator using fractional hot deck imputation can be written as in equation (2):

$$\hat{\theta}_I = \sum_{i \in S_R} \left(w_i + \sum_{j \in S_M} a_{ij} w_{ij}^\bullet w_j \right) y_i \quad (2)$$

The term in parenthesis equation (2) is called the imputation adjustment weight. Kim and Fuller(1999) demonstrated that the linear estimator $\hat{\theta}_I$ is unbiased and consistent under an ignorable response mechanism. These authors also estimated the variance of this fractional hot deck imputation in terms of the imputation cells.

Variance Estimation After Pairwise Fractional Hot Deck Imputation

Extending the idea of variance estimation after imputation (Kim, 2002; Kim et al., 1999), if the imputed values from the pairwise fractional hot deck imputation are treated as true values and apply the successive difference replication method then the variance estimator can be expressed as in equation (3):

$$V_{SDRM,I}(\hat{\theta}) = \frac{4}{k} \sum_{r=1}^k (\hat{\theta}_I^{(r)} - \hat{\theta}_I)^2 \quad (3)$$

where $\hat{\theta}_I^{(r)}$ is the r -th replicate of $\hat{\theta}_I$ and can be

written as $\hat{\theta}_I^{(r)} = \sum_{i \in S_R} \left(w_i^{(r)} + \sum_{j \in S_M} a_{ij} w_{ij}^\bullet w_j^{(r)} \right) y_i$,

where $w_i^{(r)}$ denotes the replicate weight for the i -th unit of the r -th replicate and $w_j^{(r)}$ denotes the replicate weight for the j -th unit of the r -th replicate. Because a_{ij} and $w_{ij}^\bullet$ are the imputation mechanism and imputation fraction, respectively, they will take on the same value across all replicates. This is to ensure the correct calculation of the imputation adjustment weight.

Effect of Multiple Weighting Stages On Variance Estimation After Imputation

Frequently, multiple stages of weighting adjustments are implemented in survey (Valliant, 2004). The main aim of the weighting plan is to produce final weights that reduce the nonresponse bias in the survey estimates, balance for noncoverage, and adjust sample estimates to control totals. Each stage introduces a different source of variability in an estimator that may perhaps be important to reflect when estimating variances. The advantage of variance estimation through replication is that it can explicitly account for all the stages in estimation by repeating each adjustment separately for each replicate. This concept will be evaluated in this study.

Methods Implemented On 1999 SDR Data

As mentioned previously, this research focuses on variance estimation after imputation of the 1999 SDR. The pairwise fractional hot deck imputation procedure was evaluated and compared to the variance estimates with the ones obtained when treating the imputed values as observed. Five variables were selected: Race, Hispanic, Gender, Citizenship, and Median Basic Annual Salary of the doctoral scientist and engineers. The Woodruff (1952) method was used for calculating the median and its corresponding standard error was estimating using the program described by Gossett et al (2002). Employment status is a variable without missing data that was used in forming estimates for this study. Separate replicates were computed for each variable of interest as the response mechanism differs for each one. Employment, in combination with the aforementioned variables, was used to calculate 19 survey estimates.

After identifying two donors per missing value for each of the variables selected, the imputation adjustment weight was calculated. However, this imputation adjustment weight can be calculated at three stages of the weighting adjustment process: using the base weights, using the weights after the noninterview adjustment or using the final weights (US Bureau of the Census et al., 2001b). It was decided that all three stages should be explored and the corresponding replicates needed for the

SDRM under all three weighting stages were calculated for evaluation purposes. The three weighting stages being evaluated are discussed in Methods B, C and D below. Method A is the nearest neighbor hot deck imputation used in the 1999 SDR, and did not include an imputation weighting adjustment.

- Method A: The original sampling weights based on the one donor hot deck imputation methodology were used and the imputed values were treated as observed values. The imputation weight adjustment was not used in this method.
- Method B: The base weights were used to obtain the imputation adjustment weights. The imputation adjusted weights were then adjusted to include the non-interview and raking adjustments.
- Method C: The base weights were used to obtain the non-interview adjusted weights. The non-interview adjusted weights were then used to determine the imputation adjustment weights. Finally, the raking adjustments were the final weighting step in the weighting process for this method.
- Method D: After applying the non-interview and raking adjustments to the base weights to create the final weights, the final weights were then used to obtain the imputation adjustment weight.

This empirical evaluation will allow for a determination of the stage of the weighting process at which the imputation weighting adjustment should be performed. In addition, it will allow for an evaluation of the impact of using a single hot deck imputation versus a pairwise fractional hot deck imputation.

After the replicates were computed, the point estimates and their corresponding standard errors were obtained. Statistics combining employment status with variables with missing values used the imputation adjustment weight

for the variable with missing values. As an example, when the employed male estimate was formed, the imputation adjustment weight reflected the adjustments due to the gender variable being imputed.

The standard errors (SE) which do not take the imputation adjustment into account (Method A) were compared with the standard errors which take into account the imputation adjustment (Methods B, C and D). To assess this comparison, the relative difference (RD) was used. For example, when comparing method B versus method A the RD is in equation (4):

$$RD = 100\% * \frac{SE_B(\hat{\theta}_I) - SE_A(\hat{\theta}_I)}{SE_A(\hat{\theta}_I)}$$

The RD measures the magnitude of over or under estimation of the alternative method B compared with the current baseline method A. It is important to highlight that all SE are estimates of standard errors instead of true standard errors and furthermore all are subject to sampling errors.

Results

The imputation rates in the 1999 SDR are relatively low and are provided in table 1. Table 1 presents the point estimates for the 19 estimates selected on the doctoral scientists and engineers for methods A through D. As expected due to the low imputation rates, the point estimates did not vary significantly with either method across all the statistics selected.

Table 2 presents the variance estimates with methods A through D; and includes the relative variances comparing each method B, C and D to method A. The results in table 2 suggest that (i) the variance estimator is lower when the pairwise fractional imputation methods is used and (ii) there is no preference on the weighting stage of the adjustments, except for the median of the basic annual salary where a 17% reduction on its variance is obtained using method D.

Conclusion

The purpose of this article was to perform the pairwise fractional hot deck imputation to evaluate the effect on the variance estimates due to the imputation procedure. The use of this method shows a lower variance in comparison to the single hot deck imputation method which treated the imputed values as observed values. This is achieved in most of the variables of interest. Exceptions are Naturalized U.S. citizen and employed Naturalized U.S. citizen. For these exceptions, the relative difference is slight at most (1.1%) when compared with the hot deck imputation method.

Nevertheless, the effort involved may argue that the need of having an imputation adjustment weight for each variable may not have been necessary in this particular survey with its low imputation rates. Interestingly, this empirical evaluation confirms the disadvantage pointed out by Kim (2002) that its computation can be cumbersome for a large dataset such as the 1999 SDR.

There are limitations to the empirical evaluation. i) The dataset does not have a serious missing data problem which does not allow us to determine clearly which method should be preferred under what conditions. ii) Separate replicates were computed for each variable of interest, assuming an independent univariate missingness pattern. Neither the nearest neighbor hot deck nor the pairwise fractional hot deck imputation methods allows incorporation of multivariate missingness variables to estimate their replicates. iii) The true variance of the SDR data is unknown; for that reason this empiric investigation does not quantify the true relative efficiency.

Further investigation is needed on how to obtain an imputation adjustment weight for the entire survey, as well as how to use/obtain imputation adjustment weights for statistics where more than one variable with missing data are required. Monte Carlo simulations identifying the true variance for a pseudo SDR population as well as incorporating several patterns and missing data mechanisms beyond missing completely at random need to be explored.

Table 1. Doctoral scientist and engineers in 1999: Point estimates using four methods. Method A: hot deck imputation using one donor and treating the imputed values as observed values. Method B: pairwise fractional hot deck imputation using the base weight to obtain the imputation adjustment weight. Method C: pairwise fractional hot deck imputation using the noninterview weight to obtain the imputation adjustment weight. Method D: pairwise fractional hot deck imputation using the final weight to obtain the imputation adjustment weight.

Statistic/Variable	Sample Size	IR(%)*	Point Estimates			
			A	B	C	D
Total						
1 All	31,318		626,698	626,699	626,699	626,698
2 Hispanic	1,623	1.89	15,007	14,787	14,787	15,045
Race		0.89				
3 White [!]	22,949		508,447	508,859	508,863	508,417
4 African American	1,567		14,179	14,081	14,082	14,182
5 Asian or Pacific Islander	4,847		87,034	86,823	86,818	87,075
6 American Indian/Alaskan Native	332		2,032	2,009	2,011	2,017
Gender		0.01				
7 Male	22,432		476,495	476,511	476,511	476,503
8 Female	8,886		150,204	150,188	150,188	150,196
9 Employed Male	19,835		419,869	419,884	419,884	419,876
10 Employed Female	7,910		133,494	133,480	133,480	133,486
Citizenship		0.93				
11 Native Born U.S. Citizen	24,837		491,928	491,940	491,927	491,930
12 Naturalized U.S. Citizen	3,676		70,921	70,843	70,851	70,943
13 Non-U.S. Citizen. Permanent Resident	2,124		48,938	48,984	48,981	48,919
14 Non-U.S. Citizen. Temporary Resident	681		14,911	14,921	14,930	14,907
15 Employed Native Born U.S. Citizen	21,794		429,085	429,459	429,454	429,507
16 Employed Naturalized U.S. Citizen	3,243		62,507	62,460	62,461	62,540
17 Employed Non-U.S. Citizen. Permanent Resident	2,045		47,264	47,321	47,318	47,258
18 Employed Non-U.S. Citizen. Temporary Resident	663		14,507	14,527	14,536	14,514
19 Median Basic Annual Salary of Full Time Employed	25,686	4.27	70,000	68,000	68,000	68,000

Note: *: IR: Imputation rate (percentage); ! 'Other' race included with 'White'

Table 2. Doctoral scientist and engineers in 1999: Standard error estimates and relative differences using four methods. Method A: hot deck imputation using one donor and treating the imputed values as observed values. Method B: pairwise fractional hot deck imputation using the base weight to obtain the imputation adjustment weight. Method C: pairwise fractional hot deck imputation using the noninterview weight to obtain the imputation adjustment weight. Method D: pairwise fractional hot deck imputation using the final weight to obtain the imputation adjustment weight.

Statistic/Variable	Standard Error				Relative Difference		
	A	B	C	D	$\frac{B-A}{A}$	$\frac{C-A}{A}$	$\frac{D-A}{A}$
Total							
1 All	732.2	732.1	732.1	732.2	0.00	0.00	0.00
2 Hispanic	427.0	416.4	416.3	421.3	-0.02	-0.03	-0.01
Race							
3 White ¹	1,001.0	992.9	993.8	994.1	-0.01	-0.01	-0.01
4 African American	360.7	350.5	350.4	352.7	-0.03	-0.03	-0.02
5 Asian or Pacific Islander	819.8	814.7	813.8	819.0	-0.01	-0.01	0.00
6 American Indian/Alaskan Native	161.1	160.1	160.0	159.5	-0.01	-0.01	-0.01
Gender							
7 Male	694.5	693.9	693.9	694.2	0.00	0.00	0.00
8 Female	374.8	374.1	374.1	374.4	0.00	0.00	0.00
9 Employed Male	1,164.1	1,162.0	1,162.0	1,163.0	0.00	0.00	0.00
10 Employed Female	689.0	689.1	689.1	689.0	0.00	0.00	0.00
Citizenship							
11 Native Born U.S. Citizen	686.9	682.8	683.0	686.5	-0.01	-0.01	0.00
12 Naturalized U.S. Citizen	856.3	865.6	864.7	857.3	0.01	0.01	0.00
13 Non-U.S. Citizen. Permanent Resident	787.0	784.9	783.6	783.9	0.00	0.00	0.00
14 Non-U.S. Citizen. Temporary Resident	471.3	471.0	471.0	468.3	0.00	0.00	-0.01
15 Employed Native Born U.S. Citizen	1,253.6	1,239.7	1,239.1	1,247.6	-0.01	-0.01	0.00
16 Employed Naturalized U.S. Citizen	873.4	875.9	875.2	872.2	0.00	0.00	0.00
17 Employed Non-U.S. Citizen. Permanent Resident	797.8	791.6	790.3	791.1	-0.01	-0.01	-0.01
18 Employed Non-U.S. Citizen. Temporary Resident	486.5	486.3	486.5	483.8	0.00	0.00	-0.01
19 Median Basic Annual Salary of Full Time Employed	1,519	1,326	1,324	1,266	-0.13	-0.13	-0.17

Note: ¹ 'Other' race included with 'White'

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Practical Unit-Root Analysis Using Information Criteria: Simulation Evidence

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The information-criterion-based model selection method for detecting a unit root is proposed. The simulation results suggest that the performances of the proposed method are usually comparable to and sometimes better than those of the conventional unit-root tests. The advantages of the proposed method in practical applications are also discussed.

Key words: Information criteria, model selection, Monte Carlo simulation, pre-testing problem, unit root

Introduction

Since the seminal work of Dickey and Fuller (1979), numerous alternative methods have been developed to improve the size and power properties of unit-root tests. However, little attention has been paid to two practical problems encountered in unit-root tests. Consider the following augmented DF (ADF) regression for an observed time series y_t ($t = 1, \dots, T$):

$$\Delta y_t = \mu + \beta t + \rho y_{t-1} + \sum_{i=1}^k \phi_i \Delta y_{t-i} + e_t, \quad (1)$$

where $e_t \sim \text{NID}(0, \sigma^2)$. Three model classes and the corresponding t -statistics (denoted by $\hat{\tau}$) for a unit root are obtained by considering parameter restrictions on (1).

Model 1 (Statistics, Null, and Alternative)

$$\hat{\tau} \quad \mu = \beta = \rho = 0 \quad \mu = \beta = 0 \text{ and } \rho < 0$$

Model 2 (Statistics, Null, and Alternative)

$$\hat{\tau}_\mu \quad \mu = \beta = \rho = 0 \quad \beta = 0 \text{ and } \rho < 0$$

Model 3 (Statistics, Null, and Alternative)

$$\hat{\tau}_\tau \quad \beta = \rho = 0 \quad \rho < 0$$

Although there is no discussion on a statistical method for selecting a suitable model class from among these three alternatives, different statistics can lead to different conclusions. For example, in the seminal work of Nelson and Plosser (1982), the result obtained applying Model 3 suggested that the annual time series of U.S. unemployment rate is generated from the trend-stationary process. Forecasting the unemployment rate with the trend-stationary model in the very long horizon would provide a value less than zero or more than 1. If Model 1 is applied in place of Model 3, the null hypothesis of a unit root cannot be rejected. Which conclusion should be embraced? As discussed by Phillips (2005), there is little guidance from economic theory about the source and nature of the trending behavior. Thus, model selection criteria are expected to be applied in selecting a suitable model from among three alternatives.

Furthermore, the pretesting problem also arises. In the conventional ADF regression, the lag length k is selected by applying the Ng and

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Perron (1995) (NP) general-to-specific procedure. In this procedure, given the maximum lag length $k_{\max}$, by working backward from $k = k_{\max}$, the first value of k is selected such that the t -statistic on $\hat{\phi}_k$ is significant. Thus, in total, hypothesis testing has to be implemented at two stages. Every test has a nonzero frequency of rejecting the null hypothesis, thus causing Type I errors to accumulate. As discussed by Krolzig and Hendry (2001), it is important to distinguish between the individual test sizes and the overall test size.

These two practical problems have remained even in the recent literature. For example, although Elliott et al. (1996) have proposed more powerful unit root tests, there is no criterion in selecting deterministic components and there is the pretesting problem in selecting the lag length. The ADF test still has the most popularity even now in empirical analyses, while it is the oldest unit-root test and has low power. Thus, the ADF test remains a benchmark method in the present study.

The purpose of this article is to propose an information criterion (IC)-based model selection method for detecting a unit root in order to provide a solution to the above two problems. In this method, the following three steps are taken. First, several alternative models are considered by changing the model class (Models 1, 2, and 3 with and without a unit root) and the lag length, and each model is estimated with the corresponding IC. Second, the best model is selected from among the alternative models by using the minimum IC procedure. Finally, on the basis of the selected model, it is determined whether the observed data contain a unit root. In this article, the Akaike information criterion (AIC) proposed by Akaike (1974) and the Bayesian information criterion (BIC) proposed by Schwartz (1978) are applied. The AIC and BIC for Model (1) are obtained as follows:

$$\begin{aligned} \text{AIC} &= (T - k - 1) \ln \hat{\sigma}^2 + 2p, \\ \text{BIC} &= (T - k - 1) \ln \hat{\sigma}^2 + p \ln(T - k - 1), \end{aligned}$$

where p denotes the number of parameters. In the full model (Model 3 without a unit root), $p = 3 + k$, and the other values of p are obtained in correspondence with the number of parameter restrictions.

Simulation Studies: The Case Where the Model Specification is Known

Unlike the ADF tests described earlier, the DF likelihood ratio (DFLR, Dickey & Fuller, 1981) tests are now considered. This is because the AIC and BIC are both penalized likelihoods. However, DF argued that the limiting distribution of the LR test statistics is too complex to provide an analytical solution. DF presented empirical distributions using Monte Carlo simulations. In their simulation study, the following three cases are considered:

Null Alternative

$$\text{Case 1: } y_t = y_{t-1} + e_t \quad y_t = \mu + \rho y_{t-1} + e_t$$

$$\text{Case 2: } y_t = y_{t-1} + e_t \quad y_t = \mu + \beta t + \rho y_{t-1} + e_t$$

$$\text{Case 3: } y_t = \alpha + y_{t-1} + e_t \quad y_t = \mu + \beta t + \rho y_{t-1} + e_t.$$

In the subsequent study presented in this section, it is assumed that the model specification is known in each case. In the Monte Carlo simulation, the assumed data generating process (DGP) is

$$y_t = \theta y_{t-1} + e_t \text{ and } e_t \sim \text{NID}(0,1).$$

Each experiment is performed as follows. First, artificial time series are generated from the assumed DGP. Second, in each case, the DFLR test and the IC-based model selection are performed. Finally, the presence or absence of a unit root is determined in each method. In the DFLR test, three significance levels—10%, 5%, and 1%—are applied. In each experiment, three values of θ (0.9, 0.95, 1) and two values of T (100, 250) are considered. The number of replications in each experiment is 5,000.

Table 1 shows the frequency count of selecting stationary models. In Case 1, the frequency count of incorrectly selecting stationary models, which corresponds to test size in the terminology of hypothesis testing, is high in the AIC-based method. In the case of $T = 100$, this count is 0.41 and it is 0.43 in the case of $T = 250$. On the other hand, the performances of the BIC-based method are comparable to those of the DFLR tests. Interestingly, in the case of $T = 100$, the performances of the BIC-based method are identical to those of the DFLR tests at the 5% significance level. This is because the penalty on the likelihood of the stationary model in the BIC-based method is accidentally identical to that in the DFLR test. In Case 2, similar results are obtained. However, in Case 3, the frequency count of incorrectly selecting stationary models is slightly high in the BIC-based method in the case of $T = 100$. Thus, it can be concluded that

the performances of the BIC-based method are roughly comparable to those of the DFLR tests.

The Case Where Only the Lag Length is Unknown

The IC-based method is compared with the ADF tests using the NP lag length selection. The DGP considered here is partially similar to that considered by NP. Artificial time series are generated using the following process:

$$y_t = \rho y_{t-1} + \sum_{i=1}^3 \phi_i \Delta y_{t-i} + e_t,$$

where $e_t \sim \text{NID}(0,1)$. Three values of ρ — $\rho = 0.85, 0.95, 1$ —are considered, and four vectors of (ϕ_1, ϕ_2, ϕ_3) — $(\phi_1, \phi_2, \phi_3) = (0.6, 0, 0), (-0.6, 0, 0), (0.4, 0.2, 0), (0.2, 0.2, 0.2)$ —are considered. The maximum lag length $k_{\max}$ is assumed to be $k_{\max} = 8$. Given the observed

Table 1. Frequency count of selecting stationary models

θ	T	Methods				
		10%	5%	1%	AIC	BIC
<i>Null: $y_t = y_{t-1} + e_t$, Alternative: $y_t = \mu + \rho y_{t-1} + e_t$.</i>						
0.9	100	0.39	0.24	0.06	0.86	0.24
0.9	250	0.99	0.93	0.64	1.00	0.80
0.95	100	0.15	0.08	0.01	0.56	0.08
0.95	250	0.54	0.36	0.11	0.95	0.20
1	100	0.10	0.05	0.01	0.41	0.05
1	250	0.10	0.05	0.01	0.43	0.02
<i>Null: $y_t = y_{t-1} + e_t$, Alternative: $y_t = \mu + \beta t + \rho y_{t-1} + e_t$.</i>						
0.9	100	0.18	0.09	0.02	0.78	0.10
0.9	250	0.82	0.64	0.28	1.00	0.41
0.95	100	0.09	0.04	0.01	0.57	0.04
0.95	250	0.25	0.13	0.03	0.88	0.05
1	100	0.10	0.05	0.01	0.58	0.05
1	250	0.10	0.05	0.01	0.58	0.02
<i>Null: $y_t = \alpha + y_{t-1} + e_t$, Alternative: $y_t = \mu + \beta t + \rho y_{t-1} + e_t$.</i>						
0.9	100	0.28	0.15	0.04	0.96	0.39
0.9	250	0.90	0.77	0.41	1.00	0.88
0.95	100	0.13	0.07	0.01	0.83	0.21
0.95	250	0.36	0.22	0.06	0.98	0.33
1	100	0.11	0.06	0.01	0.75	0.18
1	250	0.09	0.05	0.01	0.74	0.08

Note: DGP: $y_t = \theta y_{t-1} + e_t$.

time series, the lag length selection is performed as follows. In the ADF tests, by working backward from $k = k_{\max}$, the first value of k is selected such that the t -statistic on $\hat{\phi}_k$ is significant. Three significance levels—10%, 5%, and 1%—are applied in the case of the ADF unit-root tests and the t -tests for the lag length selection.

In the IC-based method, alternative models are considered by changing the lag length as $k = 0, 1, \dots, k_{\max}$, and the best model is selected from $(1 + k_{\max})$ alternative models. Two values of T (100, 250) are considered, and each experiment is replicated 5,000 times.

Table 2 shows the frequency count of selecting stationary models. First, the size distortion does not occur, while it is well known that the incorrect lag length can cause the size distortion. As shown by NP, the general-to-specific procedure in selecting the lag length can prevent the size distortion. Second, the pretesting problem is not shown, similar to the results obtained by NP. Finally, the performances of the BIC-based method are roughly comparable to those of the ADF 5% tests in the case of $T = 100$ and to those of the ADF 1% tests in the case of $T = 250$.

Table 2. Frequency count of selecting stationary models

Parameters				Methods				
ρ	ϕ_1	ϕ_2	ϕ_3	10%	5%	1%	AIC	BIC
T = 100								
0.85	0.6	0	0	0.99	0.98	0.97	1.00	0.97
0.85	-0.6	0	0	0.78	0.63	0.26	0.89	0.49
0.85	0.4	0.2	0	0.98	0.97	0.90	0.99	0.95
0.85	0.2	0.2	0.2	0.98	0.94	0.64	0.99	0.78
0.95	0.6	0	0	0.86	0.76	0.43	0.94	0.66
0.95	-0.6	0	0	0.35	0.19	0.05	0.44	0.11
0.95	0.4	0.2	0	0.84	0.68	0.27	0.92	0.51
0.95	0.2	0.2	0.2	0.80	0.63	0.22	0.87	0.37
1	0.6	0	0	0.12	0.05	0.01	0.20	0.03
1	-0.6	0	0	0.11	0.05	0.01	0.19	0.04
1	0.4	0.2	0	0.11	0.06	0.01	0.19	0.04
1	0.2	0.2	0.2	0.11	0.05	0.01	0.20	0.06
T = 250								
0.85	0.6	0	0	1.00	1.00	1.00	1.00	1.00
0.85	-0.6	0	0	1.00	0.99	0.95	1.00	0.95
0.85	0.4	0.2	0	1.00	1.00	1.00	1.00	1.00
0.85	0.2	0.2	0.2	1.00	1.00	1.00	1.00	0.99
0.95	0.6	0	0	1.00	1.00	0.98	1.00	0.96
0.95	-0.6	0	0	0.76	0.55	0.20	0.87	0.28
0.95	0.4	0.2	0	1.00	1.00	0.96	1.00	0.96
0.95	0.2	0.2	0.2	1.00	0.99	0.92	1.00	0.93
1	0.6	0	0	0.11	0.05	0.01	0.20	0.02
1	-0.6	0	0	0.10	0.05	0.01	0.19	0.02
1	0.4	0.2	0	0.11	0.05	0.01	0.19	0.02
1	0.2	0.2	0.2	0.11	0.05	0.01	0.19	0.02

Note: DGP: $y_t = \rho y_t + \sum_{i=1}^3 \phi_i \Delta y_{t-i} + e_t$.

The Case Where the Model Class as Well as the Lag Length is Unknown

In this phase, the model class (Models 1, 2, and 3 in Section 1) as well as the lag length is unknown. Thus, the ADF tests should determine which model class is applied. No study has been devoted to this problem. Furthermore, there is little guidance from economic theory about the source and nature of the trending behavior. In the present study, therefore, the selection of the model class is performed based on statistical tests. Motivated by NP, general-to-specific modeling is performed in this subsection as follows. First, using Model 3, the ADF regression is performed with the NP lag length selection. If the t -statistic on $\hat{\beta}$ of the selected model is significant, Model 3 is obtained and the unit-root test is implemented. Otherwise, the ADF regression is performed using Model 2. If the t -statistic on $\hat{\mu}$ of the selected model is significant, Model 2 is obtained and the unit-root test is implemented. Otherwise, the ADF unit-root test is performed using Model 1. Three significance levels—10%, 5%, and 1%—are applied in the case of the ADF unit-root tests, the t -tests for the lag length selection, and the t -tests for $\hat{\beta}$ and $\hat{\mu}$. If each test is independent at three stages and is evaluated at the 10% significance level, the overall rejection probability under the null is $1 - (1 - 0.1)^3 = 0.271$, which is substantial.

In this simulation, artificial time series are generated using the following process:

$$y_t = \mu + \beta t + \rho y_{t-1} + \sum_{i=1}^3 \phi_i \Delta y_{t-i} + e_t,$$

where $e_t \sim \text{NID}(0,1)$. In order to obtain the stationary Models 1–3, the parameter vectors considered are $(\mu = 0, \beta = 0)$, $(\mu = 1, \beta = 0)$, and $(\mu = 0, \beta = 0.1)$, respectively. With regard to the nonstationary models, the parameter vectors considered are $(\mu = 0, \beta = 0)$ and $(\mu = 0.1, \beta = 0)$. The other parameter setting is implemented as follows. Two values of ρ — $\rho = 0.95, 1$ —are considered, and four vectors of (ϕ_1, ϕ_2, ϕ_3) —

$(\phi_1, \phi_2, \phi_3) = (0.6, 0, 0), (-0.6, 0, 0), (0.4, 0.2, 0), (0.2, 0.2, 0.2)$ —are considered. The maximum lag length $k_{\max}$ is assumed to be $k_{\max} = 8$. Two values of T (100, 250) are considered, and each experiment is replicated 5,000 times.

Table 3 shows the frequency count of selecting stationary models. Unlike in the preceding subsection, in this case, the pretesting problem is clearly shown. Consider the results of applying the 10% significance level for eight unit-root processes with $T = 100$. The frequency count of incorrectly selecting stationary models is from 26% to 31%. In the preceding subsection, it was shown that the lag length selection has little effect on the results of the unit-root tests under the assumption of the known model class. The size distortion is caused by the assumed method for selecting the model class. The selection of the model class with statistically significant deterministic components such as μ and β has a bias toward selecting a stationary model. The same results are obtained in the case of $T = 250$; however, in this case, the extent of size distortion is smaller. The frequency count of incorrectly selecting stationary models by the BIC-based method is from 12% to 19% in the case of $T = 100$ and from 5% to 9% in the case of $T = 250$. The performances of the BIC-based method are roughly comparable to those of the ADF 5% tests in the case of $T = 100$ and to those of the ADF 2.5% tests (not shown here) in the case of $T = 250$.

In particular, in the case of the trending process, it can be concluded that the BIC-based method outperforms the hypothesis-testing method. For example, compare the two cases of $(\rho, \mu, \beta, \phi_1, \phi_2, \phi_3) = (1, 0.1, 0, 0.6, 0, 0)$ and $(0.95, 0, 0.1, 0.6, 0, 0)$ with $T = 100$. In the case of the 10% significance level, the frequency counts of incorrectly and correctly selecting stationary models are 0.27 and 0.45, respectively. On the other hand, in the case of the BIC-based method, the frequency counts of incorrectly and correctly selecting stationary models are 0.15 and 0.49, respectively. In the terminology of hypothesis testing, the BIC-based method shows lower size and higher

Table 3. Frequency count of selecting stationary models

Parameters						Methods				
ρ	μ	β	ϕ_1	ϕ_2	ϕ_3	10%	5%	1%	AIC	BIC
T = 100										
0.95	0	0	0.6	0	0	0.84	0.78	0.46	0.98	0.72
0.95	0	0	-0.6	0	0	0.45	0.29	0.07	0.76	0.18
0.95	0	0	0.4	0.2	0	0.83	0.71	0.29	0.96	0.55
0.95	0	0	0.2	0.2	0.2	0.80	0.66	0.25	0.94	0.40
0.95	1	0	0.6	0	0	0.64	0.48	0.18	0.91	0.34
0.95	1	0	-0.6	0	0	0.29	0.17	0.04	0.65	0.08
0.95	1	0	0.4	0.2	0	0.58	0.40	0.11	0.88	0.22
0.95	1	0	0.2	0.2	0.2	0.55	0.36	0.10	0.84	0.15
0.95	0	0.1	0.6	0	0	0.45	0.32	0.10	0.96	0.49
0.95	0	0.1	-0.6	0	0	0.36	0.24	0.09	1.00	1.00
0.95	0	0.1	0.4	0.2	0	0.41	0.26	0.07	0.93	0.35
0.95	0	0.1	0.2	0.2	0.2	0.39	0.24	0.06	0.91	0.27
1	0	0	0.6	0	0	0.31	0.19	0.04	0.75	0.13
1	0	0	-0.6	0	0	0.30	0.17	0.04	0.72	0.12
1	0	0	0.4	0.2	0	0.30	0.17	0.03	0.74	0.13
1	0	0	0.2	0.2	0.2	0.28	0.16	0.04	0.76	0.16
1	0.1	0	0.6	0	0	0.27	0.16	0.04	0.77	0.15
1	0.1	0	-0.6	0	0	0.26	0.15	0.03	0.74	0.14
1	0.1	0	0.4	0.2	0	0.27	0.15	0.04	0.76	0.15
1	0.1	0	0.2	0.2	0.2	0.26	0.14	0.04	0.78	0.19
T = 250										
0.95	0	0	0.6	0	0	1.00	1.00	0.99	1.00	1.00
0.95	0	0	-0.6	0	0	0.73	0.57	0.21	0.94	0.31
0.95	0	0	0.4	0.2	0	1.00	1.00	0.96	1.00	0.99
0.95	0	0	0.2	0.2	0.2	0.99	0.99	0.92	1.00	0.95
0.95	1	0	0.6	0	0	0.97	0.96	0.85	1.00	0.89
0.95	1	0	-0.6	0	0	0.41	0.25	0.07	0.81	0.07
0.95	1	0	0.4	0.2	0	0.97	0.94	0.73	1.00	0.77
0.95	1	0	0.2	0.2	0.2	0.97	0.92	0.67	1.00	0.70
0.95	0	0.1	0.6	0	0	0.92	0.88	0.66	1.00	0.94
0.95	0	0.1	-0.6	0	0	1.00	1.00	0.99	1.00	1.00
0.95	0	0.1	0.4	0.2	0	0.90	0.83	0.55	1.00	0.84
0.95	0	0.1	0.2	0.2	0.2	0.89	0.80	0.50	1.00	0.79
1	0	0	0.6	0	0	0.24	0.14	0.03	0.71	0.06
1	0	0	-0.6	0	0	0.24	0.14	0.03	0.70	0.05
1	0	0	0.4	0.2	0	0.25	0.13	0.03	0.71	0.05
1	0	0	0.2	0.2	0.2	0.25	0.15	0.03	0.73	0.06
1	0.1	0	0.6	0	0	0.19	0.10	0.02	0.76	0.08
1	0.1	0	-0.6	0	0	0.18	0.10	0.02	0.74	0.07
1	0.1	0	0.4	0.2	0	0.20	0.11	0.02	0.77	0.08
1	0.1	0	0.2	0.2	0.2	0.19	0.11	0.02	0.76	0.09

Note: DGP: $y_t = \mu + \beta t + \rho y_t + \sum_{i=1}^3 \phi_i \Delta y_{t-i} + e_t$.

power than the hypothesis-testing method. Similar results are obtained in other trending process of $(\rho = 1, \mu = 0.1)$ and $(\rho = 0.95, \beta = 0.1)$.

Conclusion

This article focused on the two problems encountered in the conventional unit-root tests: the absence of a criterion for selecting a suitable model class and the presence of the pretesting problem. In order to provide a solution to these problems, the IC-based model selection method was proposed. In this method, alternative models with and without a unit root are considered by changing the model class and the lag length. All the possible models are estimated and the corresponding IC values are stored. Finally, the best model is selected from among the alternatives. Thus, on the basis of the selected model, it is determined whether the observed time series contain a unit root. The simulation results suggested that the performances of the BIC-based method are usually comparable to and sometimes better than those of the DFLR and ADF unit-root tests.

In comparison with the conventional hypothesis testing methods, this BIC-based model selection method has two advantages. First, by the introduction of the minimum BIC procedure, the subjective judgment required in the hypothesis testing procedure for determining the levels of significance is completely eliminated, thus enabling a semiautomatic execution. The well-known criticism of the IC-based method is that it cannot control the test size. However, as shown in Table 3, the conventional hypothesis testing method causes the pretesting problem and cannot control the overall test size.

Second, the selection of the model class can be performed automatically and consistently using the IC-based method. Furthermore, flexible time-series modeling, such as the introduction of measurement error (Fukuda, 2005a) and/or regime switching (Fukuda, 2005b), is applicable in the proposed method, and the efficacy of a model change can be

consistently evaluated via the minimum BIC procedure. In the case of hypothesis testing, different models require different statistics; this makes time-series analyses very complex.

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A Fano-Huffman Based Statistical Coding Method

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Statistical coding techniques have been used for lossless statistical data compression, applying methods such as Ordinary, Shannon, Fano, Enhanced Fano, Huffman and Shannon-Fano-Elias coding methods. A new and improved coding method is presented, the Fano-Huffman Based Statistical Coding Method. It holds the advantages of both the Fano and Huffman coding methods. It is more easily applicable than the Huffman coding methods and it is more optimal than Fano coding method. The optimality with respect to the other methods is realized on the basis of English, German, Turkish, French, Russian and Spanish.

Key words: Fano-Huffman based statistical coding method, probability distribution of language, entropy, information, optimal code.

Introduction

Problem Statement

Huffman's algorithm is a well-known encoding method that generates an optimal prefix encoding scheme, in the sense that the average code word length is minimum. As opposed to this, Fano's method has not been used so much because it generates prefix encoding schemes that can be sub-optimal (Rueda & Oommen, 2004).

In this article, an improved coding method is presented, which has been named the Fano-Huffman Based Statistical Coding method and applications of this method. This method holds the both advantages of Fano and Huffman coding method. So, it is more easily applicable than the Huffman coding method and is more optimal than Fano coding method. The optimality of the mentioned coding method with

respect to the other coding methods is realized on the basis of English, German, Turkish, French, Russian and Spanish.

The classical coding methods and the concept of optimality are described in the section titled Classical Coding Methods and Optimality.

An improved coding method, Fano-Huffman Based Coding Method by which encoding schemes, which are arbitrarily close to the optimum, can be easily constructed, is introduced in the section called Fano-Huffman Based Statistical Coding Method.

In the following section, the tables of constructed binary codes are given and comparisons of considered methods in sense of optimality are made.

In the conclusion, the interpretation of optimality of these results is made subject to classical coding methods and suggestions are given.

Overview

Assume that a source alphabet, $S = \{s_1, s_2, \dots, s_n\}$, whose probabilities of occurrence are $P = \{p_1, p_2, \dots, p_n\}$, and a code alphabet, $A = \{a_1, a_2, \dots, a_r\}$ is given. The propose of this study is the generation of an encoding scheme, $\{s_i \rightarrow w_i\}$, in such a way

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that $\bar{l} = \sum_{i=1}^n p_i l_i$ is minimized, where l_i is the length of w_i .

Information theory has important applications in probability theory, statistics and communication systems. Lossless encoding methods used to solve this problem include Huffman's algorithm (Huffman, 1952), Shannon's method (Shannon & Weaver, 1949), arithmetic coding (Sayood, 2000), Fano's method (Hankerson, Harris, & Johnson, 1998), enhanced Fano-based coding algorithm (Rueda & Oomen, 2004) etc. Adaptive versions of these methods have been proposed, and can be found in (Faller, 1973; Gallager, 1978; Hankerson et al., 1998; Knuth, 1985; Rueda, 2002; Sayood, 2000). The survey is necessarily brief as this is a well-reputed field.

Also, assume that the source is memoryless or zeroth-order, which means that the occurrence of the next symbol is independent of any other symbol that has occurred previously. Higher-order models include Markov models (Hankerson et al., 1998), dictionary techniques (Ziv & Lempel, 1977; Ziv & Lempel, 1978), prediction with partial matching (Witten, Moffat, & Bell, 1999), grammar based compression (Kieffer & Yang, 2000), etc., and the techniques introduced here are also readily applicable for such structure models.

Classical Coding Methods and Optimality

In this section, the fundamental steps of classical coding methods are described and the concept of optimality of codes is expounded.

Classical coding methods

Suppose that source alphabet (alphabet of language) $S = \{s_1, s_2, \dots, s_n\}$ and its probability distribution $P = \{p_1, p_2, \dots, p_n\}$ are given.

Ordinary Coding Method

This method requires the following steps:

(a) Determine number ℓ satisfying the inequality $\ell \geq \log_2 N$, where ℓ is the

length of codeword and N is the the number of symbols in source alphabet;

(b) Enumerate letter ignoring the frequency;

(c) Convert numbers determined by (b) from base 10 to base 2 such that ℓ is the length of converted number (Roman, 1997).

Shannon Coding Method

Construction of Shannon Codes is provided by steps:

(a) Put $P = \{p_1, p_2, \dots, p_n\}$ in ascending order $p_1 \geq p_2 \geq \dots \geq p_n$;

(b) Calculate $\ell_i = \lceil \log_2 p_i^{-1} \rceil$ the length of codeword, $i = 1, 2, \dots, n$;

(c) Let define dyadic fraction as $F_1 = 0$ and $F_k = \sum_{i=1}^{k-1} p_i$, $2 \leq k \leq n$. Then calculate F_i , $i = 1, 2, \dots, n$;

(d) Convert dyadic fraction F_i to binary form by using Koblitz's trick, then select first ℓ_i bits as a code corresponding to s_i (Hankerson et. al., 2003).

Fano Coding Method

This method involves the steps:

(a) Perform the probabilities of symbols in source alphabet in ascending order $p_1 \geq p_2 \geq \dots \geq p_n$;

(b) Divide the set of symbols into two subsets such that the sum of the probabilities of occurrences of symbols in each subset are equal or almost equal. Then, assign a 0 to first subset and a 1 to second;

(c) Repeat step (a) until all subsets have a single element (Венцель, 1969).

Enhanced Fano Coding Method

This method proposed the following steps:

- (a) Consider the source alphabet $S = \{s_1, s_2, \dots, s_n\}$ whose probability distribution of occurrences is $P = \{p_1, p_2, \dots, p_n\}$, where $p_1 \geq p_2 \geq \dots \geq p_n$;
- (b) Obtain $\phi: s_1 \rightarrow w_1, \dots, s_n \rightarrow w_n$ the encoding scheme by Fano's method;
- (c) Rearrange $w_1, w_2, \dots, w_n$ into $w'_1, w'_2, \dots, w'_n$ such that $\ell'_i \leq \ell'_j$ for all $i < j$, and simultaneously maintain $s_1, s_2, \dots, s_n$ in the same order, to yield the encoding scheme: $\phi': s_1 \rightarrow w'_1, \dots, s_n \rightarrow w'_n$ (Rueda & Oommen, 2004).

Huffman Coding Method

This method is bottom-up while the others are top-down. It can be explained more clearly as follows:

- (a) Sort symbols of source alphabet in decreasing order of their probabilities;
- (b) Merge the two least-probable letter into a single output whose probability is the sum of the corresponding probabilities;
- (c) Go to step (a) if the number of remaining outputs is more than 2;
- (d) Assign a 0 and a 1 arbitrarily as code words for the two remaining outputs;
- (e) Append the current codeword with a 0 and a 1 to obtain the codeword the preceding outputs and repeat step (e) if an output is the result of the merger of two outputs in a preceding step. Stop if no output is preceded by another output in a preceding step (Aazhang, 2004).

Shannon-Fano-Elias Coding Method

This method can be explained by steps:

- (a) Perform the source alphabet $S = \{s_1, s_2, \dots, s_n\}$ whose probability distribution of occurrences is $P = \{p_1, p_2, \dots, p_n\}$ and the order of probabilities isn't important;
- (b) Obtain the cumulative distribution by the function $F(s) = \sum_{a \leq s} p(a)$;
- (c) Consider modified cumulative distribution function $\bar{F}(s) = \sum_{a < s} p(a) + \frac{1}{2} p(s)$, where $\bar{F}(s)$ denotes the sum of probabilities of all symbols less than s plus half the probability of the symbols;
- (d) Obtain the length of codeword by the formula $\ell_i(s) = \left\lceil \log \frac{1}{p(s)} \right\rceil + 1$, where $\lceil \cdot \rceil$ denotes rounding up;
- (e) Convert dyadic fraction $\bar{F}(s)$ to binary form by using Koblitz's trick such that the codeword has $\ell_i(s)$ bits (Cover & Thomas, 1991).

The concept of optimality of codes

There exists a uniquely decodable code whose codeword lengths are given by the sequence $\{\ell_i\}_{i=1}^n$ if Kraft inequality $\sum_{i=1}^n 2^{-\ell_i} \leq 1$ holds. Due to Kraft inequality (Cover, 1991), the conditions for optimal codes are as follows:

- (a) The average codeword length $\bar{\ell} = \sum_{i=1}^n p_i \ell_i$ of an optimal code for a source S is greater than or equal to its entropy $H(S) = - \sum_{i=1}^n p_i \log_2 p_i$;

(b) The average codeword length $\bar{\ell}$ of an optimal code for a source S is strictly less than $H(S)+1$.

For source alphabet $S = \{s_1, s_2, \dots, s_n\}$ whose probability distribution of occurrences is $P = \{p_1, p_2, \dots, p_n\}$, the average codeword length is given by $\bar{\ell}$, and entropy of the source alphabet is given by $H(S)$.

Under these conditions, it is required to transmit as well as possible information by using codes consists of fewer bits. So, this problem can be considered as optimization problem

which is consist of minimizing $\bar{\ell} = \sum_{i=1}^n p_i \ell_i$

subject to constraint $\sum_{i=1}^n D^{-l_i} \leq 1$, where D is

dimension of codebook, i.e. if the codebook is $\{0,1\}$ then $D=2$ etc.

This problem is solved by using Langrange Multipliers, and the following result is obtained:

$$l_i^* = -\log_D p_i; \quad (2.1)$$

$$\bar{\ell} = \sum_{i=1}^n p_i l_i^* = -\sum_{i=1}^n p_i \log_D p_i = H_D(S); \quad (2.2)$$

$$\bar{\ell} = H_D(S). \quad (2.3)$$

But it isn't possible to find an interger number for codeword length that satisfies (2.1). For this reason, it is necessary to obtain the entropy lower bound (Cover & Thomas, 1991; Roman, 1997) satisfying the following inequality:

$$\bar{\ell} = \sum_{i=1}^n p_i l_i^* \geq H_D(S). \quad (2.4)$$

Moreover, if S is a stationary stochastic process,

$$\bar{\ell} \rightarrow H(S), \quad (2.5)$$

where $H(S)$ is the entropy rate of the process.

Under the mentioned knowledge, the information per symbol (letter) is given by

$$I_{\text{inf/letter}} = \frac{H(S)}{\bar{\ell}} \text{ and the optimality criteria}$$

for codes is considered as $I_{\text{inf/letter}} \rightarrow 1$ (Венцель, 1969). Moreover, the optimality means that if the text is coded by an optimal coding method, the number of 1s and the number of 0s are nearly equal in sence of maximum entropy. Hence, the optimal codes means that they transmit nearly maximum information since 1s and 0s aren't always equal probable.

Fano-Huffman Based Statistical Coding Method

In this section, a new and improved coding method is proposed, which can be considered as a hybrid method that holds the both advantages of Fano and Huffman coding methods.

It is well known that Fano coding method is a suboptimal procedure for constructing a source code (Rueda & Oommen, 2004). In this method, the source symbols and their probabilities are sorted in a non-increasing order of the probabilities and then the set of symbols is divided into two subsets such that the sum of the probabilities of occurrences of symbols in each subset are equal or almost equal. The main advantage of this method is the division of the set of symbols. Because, it requires pure computations. Hence, the first goal of the improved coding method is to hold this advantage.

Huffman coding method is a optimal procedure (Cover & Thomas, 1991). In this method, the source symbols and their probabilities are also sorted in decreasing order and then the two least-probable symbols are merged into a single output whose probability is the sum of the corresponding probabilities. Thus, by this recursive procedure, the optimal Huffman codes are constructed. The advantage of this coding method is that the procedure is from bottom to top. In this way, the short code

words are attain to the symbols that occur frequently and long code words are attain to the symbols that occur rarely. This advantage of Huffman coding method constitutes the second goal of the improved coding method.

Considering the advantages of these two coding procedure a hybrid coding method is presented. So, the coding method is more easily applicable than the Huffman coding methods and is more optimal than Fano coding method. The codes performed by that coding method are prefix codes and satisfy the sibling property.

The Fano-Huffman based statistical coding method is now proposed in the following form:

- (a) Perform the probabilities of symbols in source alphabet in ascending order $p_1 \geq p_2 \geq \dots \geq p_n$;
- (b) Choose k such that $\left| \sum_{i=1}^k p_i - \sum_{i=k+1}^m p_i \right|$ is minimized. This number k divides the source symbols into two sets of almost equal probability.
- (c) Merge the two least-probable letter in each set into a single output whose probability is the sum of the corresponding probabilities;
- (d) Go to step (c) if the number of remaining outputs is more than 2;
- (e) Assign a 0 and a 1 arbitrarily as codewords for the two remaining outputs;

- (f) Append the current codeword with a 0 and a 1 to obtain the codeword the preceding outputs and repeat step (e) If no output is preceded by another output in a preceding step merge the two least-probable subset into a single output whose probability is the sum of the corresponding probabilities;

- (g) Stop if no output is preceded by another output in a preceding step.

Note that, according to step (b) due to size of source alphabet, the set of symbols can be divided into more subsets (2^n , $n=1,2,\dots$) of equal or almost equal probabilities.

The advantages of the proposed method arise from the comparisons of this method with the other aforesaid coding methods. The applications of this method and comparisons are given in the following section.

Tables, Computational Details and Comparisons

In this section, in order to indicate the advantages of our proposed method, Fano-Huffman Based statistical coding method, we compare it with the traditional coding methods. Various binary codes for English, German, Turkish, French, Russian and Spanish symbols are constructed in sense of optimality.

French, German, Spanish and English symbols (letters) are the Latin characters consisting of 26 letters which are given in Table 1a.

The probabilities of French, German and Spanish symbols (letters) were established in 1939 by Fletcher Pratt (Stephens, 2002; Pratt, 1939), the probabilities of English symbols (letters) were established by Nam Phamdo (2001) and they are given in Table 1b.

Table 1a. French, German, Spanish and English Symbols

A	B	C	D	E	F	G	H	I	J	K	L	M
a	B	c	d	e	F	g	h	i	j	k	l	m
N	O	P	Q	R	S	T	U	V	W	X	Y	Z
n	O	p	q	r	s	t	u	v	w	x	y	z

Table 1b. Probabilities of French, German, Spanish and English Symbols

Symbols	English	French	German	Spanish
A	0.065174	0.08147	0.06506	0.12529
B	0.012425	0.00876	0.02566	0.01420
C	0.021734	0.03063	0.02837	0.04679
D	0.034984	0.04125	0.05414	0.05856
E	0.104144	0.17564	0.16693	0.13676
F	0.019788	0.00959	0.02044	0.00694
G	0.015861	0.01051	0.03647	0.01006
H	0.049289	0.00721	0.04064	0.00704
I	0.055809	0.07559	0.07812	0.06249
J	0.000903	0.00598	0.00191	0.00443
K	0.005053	0.00041	0.01879	0.00004
L	0.033149	0.05783	0.02825	0.04971
M	0.020212	0.02990	0.03005	0.03150
N	0.056451	0.07322	0.09905	0.06712
O	0.059630	0.05289	0.02285	0.08684
P	0.013765	0.02980	0.00944	0.02505
Q	0.000861	0.01361	0.00055	0.00875
R	0.049756	0.06291	0.06539	0.06873
S	0.051576	0.08013	0.06765	0.07980
T	0.072936	0.07353	0.06742	0.04629
U	0.022513	0.05991	0.03703	0.03934
V	0.008290	0.01557	0.01069	0.00895
W	0.017127	0.00020	0.01396	0.00023
X	0.001369	0.00350	0.00022	0.00221
Y	0.014598	0.00116	0.00032	0.00895
Z	0.000784	0.00072	0.01002	0.00523
#	0.191818	-	-	-

Turkish Source Alphabet consists of 29 symbols (letters). The capital and small letters of the Turkish Alphabet are given in Table 2a.

Probabilities of occurrence of Turkish symbols (letters) are given in Table 2b (Shamilov & Yolacan, 2005; Dalkilic & Dalkilic, 2002). Considered probabilities have been constituted from a corpus consist of words from many variety of fields, i. e. scientific

articles, newspapers, poetics etc., 12.5 million characters in total.

Russian uses Cyrillic alphabet consisting of 32 symbols (letters) which are given in Table 3a. Probabilities of Russian symbols are given in Table 3b., where # denotes the space symbol (Венцель, 1969; Yaglom & Yaglom, 1966).

Table 2a. Turkish Source Alphabet

A	B	C	Ç	D	E	F	G	Ğ	H	İ	ı	J	K	
a	b	c	ç	d	e	f	g	ğ	h	ı	i	j	k	
L	M	N	O	Ö	P	R	S	Ş	T	U	Ü	V	Y	Z
l	m	n	o	ö	p	r	s	ş	t	u	ü	v	y	z

Table 2b. Probabilities of Turkish Symbols

Letter	Frequency	Letter	Frequency	Letter	Frequency
A	0.1026	I	0.0444	R	0.0604
B	0.0237	İ	0.0723	S	0.0264
C	0.0084	J	0.0003	Ş	0.0157
Ç	0.0102	K	0.0407	T	0.0287
D	0.0400	L	0.0530	U	0.0284
E	0.0782	M	0.0320	Ü	0.0171
F	0.0038	N	0.0633	V	0.0087
G	0.0114	O	0.0214	Y	0.0295
Ğ	0.0092	Ö	0.0074	Z	0.0130
H	0.0096	P	0.0073	#	0.1329

Table 3a. Russian Symbols (Cyrillic alphabet)

А	Б	В	Г	Д	Е	Ж	З	И	Й	К	Л	М	Н	О	
а	б	в	г	д	е	ж	з	и	й	к	л	м	н	о	
П	Р	С	Т	У	Ф	Х	Ц	Ч	Ш	Щ	Ъ(Ь)	Ы	Э	Ю	Я
п	р	с	т	у	ф	х	ц	ч	ш	щ	ъ(ь)	ы	э	ю	я

Table 3b. Probabilities of Russian Symbols

Symbols	Probabilities	Symbols	Probabilities
А	0.064	Р	0.041
Б	0.015	С	0.047
В	0.039	Т	0.056
Г	0.014	У	0.021
Д	0.026	Ф	0.002
Е	0.074	Х	0.009
Ж	0.008	Ц	0.004
З	0.015	Ч	0.013
И	0.064	Ш	0.006
Й	0.010	Щ	0.003
К	0.029	Ъ(Ь)	0.015
Л	0.036	Ы	0.016
М	0.026	Э	0.003
Н	0.056	Ю	0.007
О	0.095	Я	0.019
П	0.024	#	0.145

In order to construct binary codes for English, German, Turkish, French, Russian and Spanish, the classical coding methods are applied to considered source alphabets. Consequently, the constructed binary codes are

given respectively in Tables 4-9. Moreover, Fano-Huffman Based statistical coding method is also applied to considered languages. Binary Codes constructed by Fano-Huffman based statistical coding are given in Table 10.

Table 4 Binary Codes for Probability Distribution of English Symbols

English Alphabet	No	Ordinary Codes	S-F-E Codes	Ordered Alphabet	Shannon Codes	Fano Codes	Enhanced Fano Codes	Huffman Codes
A	0	00000	00001	#	000	000	000	001
B	1	00001	00010010	E	0011	001	001	100
C	2	00010	0001011	T	0100	010	010	0101
D	3	00011	000111	A	0101	0110	0110	0011
E	4	00100	00101	O	01101	0111	0111	0111
F	5	00101	0011111	N	01111	1000	1000	0000
G	6	00110	0100010	I	10001	1001	1001	1000
H	7	00111	010011	S	10011	1010	1010	0010
I	8	01000	010110	R	10100	10110	10110	1010
J	9	01001	011000010011	H	10110	10111	10111	0110
K	10	01010	011000011	D	11000	11000	11000	01101
L	11	01011	011001	L	11001	11001	11001	01011
M	12	01100	0110110	U	110100	11010	11010	01110
N	13	01101	011101	C	110110	110111	11100	11110
O	14	01110	100001	M	110111	110110	110110	011101
P	15	01111	10001111	F	111000	11100	110111	111101
Q	16	10000	100100011001	W	111001	111010	111010	011011
R	17	10001	100110	G	111011	111011	111011	001111
S	18	10010	101001	Y	1111000	111100	111100	101111
T	19	10011	10110	P	1111010	111101	111101	011111
U	20	10100	1100000	B	1111011	111110	111110	111111
V	21	10101	11000101	V	1111101	1111110	1111110	0111011
W	22	10110	1100100	K	11111100	11111110	11111110	01111011
X	23	10111	110001010110	X	1111111000	111111110	111111110	011111011
Y	24	11000	11001100	J	11111110100	1111111110	1111111110	101111011
Z	25	11001	110011101100	Q	11111110110	11111111110	11111111110	0111111011
#	26	11010	1110	Z	11111110111	11111111111	11111111111	1111111011

Table 5. Binary Codes for Probability Distribution of German Symbols

German Alphabet	No	Ordinary Codes	S-F-E Codes	Ordered Alphabet	Shannon Codes	Fano Codes	Enhanced Fano Codes	Huffman Codes
A	0	00000	00001	E	000	000	000	000
B	1	00001	0001001	N	0010	001	001	001
C	2	00010	0001101	I	0100	010	010	0100
D	3	00011	001001	S	0101	0110	0110	0010
E	4	00100	0100	T	0110	0111	0111	1010
F	5	00101	0101100	R	0111	1000	1000	0110
G	6	00110	011000	A	1000	1001	1001	0011
H	7	00111	011010	D	10011	1010	1010	0111
I	8	01000	01111	H	10101	10110	10110	0101
J	9	01001	10000100010	U	10110	10111	10111	01100
K	10	01010	1000011	G	10111	11000	11000	01110
L	11	01011	1000110	M	110001	11001	11001	11110
M	12	01100	1001010	C	110011	11010	11010	01011
N	13	01101	10100	L	110101	11011	11011	11011
O	14	01110	1011010	B	110111	11100	11100	01111
P	15	01111	10111000	O	111000	111010	111010	01101
Q	16	10000	101110011111	F	111010	111011	111011	011100
R	17	10001	11000	K	111011	111100	111100	111100
S	18	10010	11010	W	1111001	111101	111101	011111
T	19	10011	11100	V	1111011	1111100	1111100	011101
U	20	10100	111100	Z	1111101	1111101	1111101	111101
V	21	10101	11111000	P	1111110	1111110	1111110	0111111
W	22	10110	11111011	J	111111100	11111110	11111110	01111111
X	23	10111	11111101001011	Q	1111111100	111111110	111111110	011111111
Y	24	11000	1111110100111	Y	11111111011	1111111110	1111111110	0111111111
Z	25	11001	11111110	X	111111111001	1111111111	1111111111	1111111111

Table 6. Binary Codes for Probability Distribution of Turkish Symbols

Turkish Alphabet	No	Ordinary Codes	S-F-E Codes	Ordered Alphabet	Shannon Codes	Fano Codes	Enhanced Fano Codes	Huffman Codes
A	0	00000	00001	#	000	000	000	001
B	1	00001	0001110	A	0010	001	001	000
C	2	00010	00100001	E	0011	0100	0100	0011
Ç	3	00011	00100011	İ	0101	0101	0101	0111
D	4	00100	001010	N	0110	0110	0110	0101
E	5	00101	00111	R	01110	0111	0111	0010
F	6	00110	0100001111	L	10000	1000	1000	0110
G	7	00111	01000101	I	10010	1001	1001	0100
Ğ	8	01000	01001000	K	10011	10100	10100	01011
H	9	01001	01001010	D	10100	10101	10101	01111
I	10	01010	010100	M	10110	10110	10110	01101
İ	11	01011	01100	Y	101110	10111	10111	01010
J	12	01100	0110100111111	T	101111	11000	11000	11010
K	13	01101	011011	U	110001	11001	11001	01110
L	14	01110	011110	S	110011	11010	11010	01100
M	15	01111	100001	B	110101	110110	110110	11100
N	16	10000	10010	O	110110	110111	110111	011011
O	17	10001	1001110	Ü	111000	111000	111000	011101
Ö	18	10010	101000001	Ş	111001	111001	111001	011110
P	19	10011	101000101	Z	1110100	111010	111010	111110
R	20	10100	101010	G	1110110	111011	111011	0111011
S	21	10101	1011011	Ç	1110111	1111000	1111000	0011111
Ş	22	10110	1011101	H	1111000	1111001	1111001	1011111
T	23	10111	1100000	Ğ	1111010	1111010	1111010	0111111
U	24	11000	1100100	V	1111011	1111011	1111011	1111111
Ü	25	11001	1100111	C	1111100	1111100	1111100	0111101
V	26	11010	11010001	Ö	11111011	1111101	1111101	1111101
Y	27	11011	1101011	P	11111101	1111110	1111110	01111011
Z	28	11100	11011100	F	111111101	11111110	11111110	011111011
#	29	11101	1110	J	111111111110	11111111	11111111	111111011

Table 7. Binary Codes for Probability Distribution of French Symbols

French Alphabet	No	Ordinary Codes	S-F-E Codes	Ordered Alphabet	Shannon Codes	Fano Codes	Enhanced Fano Codes	Huffman Codes
A	0	00000	00001	E	000	000	000	00
B	1	00001	00010101	A	0010	001	001	0101
C	2	00010	0001101	S	0100	010	010	0001
D	3	00011	001001	I	0101	0110	0110	1001
E	4	00100	0011	T	0110	0111	0111	0011
F	5	00101	01010111	N	0111	1000	1000	1011
G	6	00110	01011010	R	1000	1001	1001	0111
H	7	00111	010111001	U	10011	1010	1010	0110
I	8	01000	01100	L	10101	1011	1011	0010
J	9	01001	011100011	O	10111	1100	1100	1010
K	10	01010	0111001001100	D	11001	11010	11010	01101
L	11	01011	011110	C	110101	11011	11011	01111
M	12	01100	1000010	M	110111	11100	11100	01110
N	13	01101	10010	P	111001	111010	111010	11110
O	14	01110	101000	V	1110110	111011	111011	011111
P	15	01111	1010110	Q	1111000	111100	111100	0111101
Q	16	10000	10110010	G	1111010	1111010	1111010	0011101
R	17	10001	10111	F	1111011	1111011	1111011	1011101
S	18	10010	11001	B	1111100	1111100	1111100	0111111
T	19	10011	11100	H	11111011	1111101	1111101	1111111
U	20	10100	111100	J	11111101	1111110	1111110	01111101
V	21	10101	11111101	X	111111101	11111110	11111110	011111101
W	22	10110	11111111000101	Y	1111111111	111111110	111111110	0111111101
X	23	10111	1111111110	Z	00000000001	1111111110	1111111110	01111111101
Y	24	11000	00000000001	K	000000000101	11111111110	11111111110	011111111101
Z	25	11001	000000000110	W	0000000001110	11111111111	11111111111	111111111101

Table 8. Binary Codes for Probability Distribution of Russian Symbols

Russian Alphabet	No	Ordinary Codes	S-F-E Codes	Ordered Alphabet	Shannon Codes	Fano Codes	Enhanced Fano Codes	Huffman Codes
A	0	00000	00010	#	000	000	000	000
Б	1	00001	00010010	О	0010	001	001	001
В	2	00010	000110	Е	0011	0100	0100	011
Г	3	00011	00100000	А	0101	0101	0101	0010
Д	4	00100	0010001	И	0110	0110	0110	1010
Е	5	00101	00110	Т	01110	0111	0111	0111
Ж	6	00110	00111100	Н	01111	1000	1000	0011
З	7	00111	00111111	С	10001	1001	1001	0101
И	8	01000	01001	Р	10011	10100	10100	00100
Й	9	01001	01010010	В	10100	10101	10101	01100
К	10	01010	0101011	Л	10101	10110	10110	01110
Л	11	01011	011000	К	101101	10111	10111	01011
М	12	01100	0110100	М	101111	11000	11000	01101
Н	13	01101	011100	Д	110001	110010	11010	11101
О	14	01110	10000	П	110011	110011	110010	010100
П	15	01111	1001010	У	110100	11010	110011	110100
Р	16	10000	100111	Я	110101	110110	110110	011100
С	17	10001	101010	Ы	110111	110111	110111	011110
Т	18	10010	101101	З	1110000	111000	111000	001111
У	19	10011	1011111	Ь(ь)	1110010	111001	111001	101111
Ф	20	10100	1100001011	Б	1110100	111010	111010	011111
Х	21	10101	11000100	Г	1110110	111011	111011	011011
Ц	22	10110	110001011	Ч	1110111	111100	111100	111011
Ч	23	10111	11001000	Й	1111001	1111010	1111010	0111100
Ш	24	11000	110010100	Х	1111010	1111011	1111011	0111110
Щ	25	11001	1100101110	Ж	1111100	1111100	1111100	1111110
Ъ(ъ)	26	11010	11001101	Ю	11111010	1111101	1111101	0111111
Ы	27	11011	1101000	Ш	11111011	11111100	11111100	01111100
Э	28	11100	1101010001	Ц	11111101	11111101	11111101	11111100
Ю	29	11101	110101011	Щ	111111100	11111110	11111110	01111111
Я	30	11110	1101100	Э	111111110	111111110	111111110	011111111
#	31	11111	1110	Ф	111111111	111111111	111111111	111111111

Table 9. Binary Codes for Probability Distrubution of Spanish Symbols

Spanish Symbols	No	Ordinary Codes	S-F-E Codes	Ordered Alphabet	Shannon Codes	Fano Codes	Enhanced Fano Codes	Huffman Codes
A	0	00000	0001	E	000	000	000	000
B	1	00001	00100001	A	001	001	001	001
C	2	00010	001010	O	0100	010	010	0010
D	3	00011	001101	S	0101	0110	0110	1010
E	4	00100	0101	R	0110	0111	0111	0110
F	5	00101	011000101	N	0111	1000	1000	0100
G	6	00110	01100100	I	10010	1001	1001	1100
H	7	00111	011001101	D	10100	1010	1010	0101
I	8	01000	011011	L	10101	1011	1011	0011
J	9	01001	011110000	C	10111	11000	11000	1011
K	10	01010	0111100011111011	T	11001	11001	11001	0111
L	11	01011	011111	U	11010	11010	11010	01110
M	12	01100	100010	M	11011	11011	11011	01101
N	13	01101	10010	P	111001	11100	11100	01111
O	14	01110	10101	B	1110110	111010	111010	011110
P	15	01111	1011100	G	1111000	111011	111011	011111
Q	16	10000	10111100	Y	1111001	111100	111100	111111
R	17	10001	11000	V	1111010	1111010	1111010	0111110
S	18	10010	11011	Q	1111011	1111011	1111011	1111110
T	19	10011	111010	H	11111001	1111100	1111100	0011101
U	20	10100	111101	F	11111011	1111101	1111101	1011101
V	21	10101	11111010	Z	11111101	1111110	1111110	0111101
W	22	10110	11111100000110	J	11111110	11111110	11111110	01111101
X	23	10111	1111110001	X	111111111	111111110	111111110	011111101
Y	24	11000	111111101	W	0000000001000	1111111110	1111111110	0111111101
Z	25	11001	111111111	K	000000000101001	1111111111	1111111111	1111111101

Table 10. Binary Codes Constructed by Fano-Huffman Based Statistical Coding Method

Turkish Alphabet	Fano-Huffman based Codes for Turkish symbols	Russian Alphabet	Fano-Huffman based Codes for Russian symbols	English, French, German, Spanish Alphabet	Fano-Huffman based Codes for English symbols	Fano-Huffman based Codes for French symbols	Fano-Huffman based Codes for German symbols	Fano-Huffman based Codes for Spanish symbols
A	110	A	1101	A	0101	0001	0010	011
B	10111	Б	011100	B	111100	0001100	11110	111000
C	0100101	B	11000	C	110000	11100	01010	1110
Ç	0011001	Г	011010	D	11000	10000	0110	0010
D	01001	Д	10110	E	0001	11	001	101
E	0000	Е	0101	F	101000	1100000	001000	1011010
F	010000001	Ж	1010100	G	001100	0100000	00100	0110000
G	1000001	З	001100	H	00000	1001100	10000	0011010
Ğ	0111001	И	0011	I	1010	0101	111	1100
H	1011001	Й	1100000	J	1010000100	11000000	01101110	00111010
I	1111	К	01010	K	00000100	010101000000	101000	1110111010
İ	1000	Л	00100	L	10100	0110	11010	0110
J	110000001	М	00110	M	001000	01010	10100	01010
K	10001	Н	0010	N	0010	1000	011	0100
L	1011	О	111	O	1101	1110	000000	111
M	10101	П	000000	P	011100	11010	0101110	010000
N	0010	Р	10000	Q	0110000100	0000000	011101110	1011000
O	100001	С	1110	R	1110	0100	1100	1001
Ö	1100101	Т	1011	S	0110	1001	0101	0001
P	00000001	У	001000	T	1001	1101	1101	00000
R	1010	Ф	110100000	U	010000	0010	11000	01000
S	00111	Х	0010100	V	1000100	101100	0100000	0011000
Ş	011101	Ц	01111100	W	100100	110101000000	001110	0110111010
T	00011	Ч	111010	X	0010000100	001000000	1111101110	010111010
Ü	10011	Ш	00100000	Y	101100	1101000000	0111101110	1110000
Û	000101	Щ	11111100	Z	1110000100	00101000000	1100000	1111010
V	1111001	Ъ(Ь)	101100	#	11			
Y	01101	Ы	110100					
Z	111101	Э	010100000					
#	100	Ю	0111100					
		Я	101000					
		#	001					

In order to determine the information per letter for considered alphabets due to the mentioned coding methods, the following stages are presented:

1) The entropy of each mentioned languages $H(S)$ is calculated.

2) The codeword length of each codes shown in Tables 4-10 is obtained by counting the bits of the code words and thus average codeword length $\bar{\ell}$ is computed for each coding methods.

3) The information per letter $I_{\text{inf/letter}} = \frac{H(S)}{\bar{\ell}}$ is get for interpretation of optimality of codes.

The results of these stages are given in Table 11. As previously presented, the optimality criteria for codes is $I_{i/s} \rightarrow 1$. Obviously, it is seen from Table 11 that, binary codes constructed for each symbols of different alphabet by Fano-Huffman based statistical coding method is more optimal than Fano coding method and is as optimal as constructed by Huffman coding method but it is more easily applicable than Huffman coding method. Also, the improved coding method is more optimal than the others. Moreover, if a file is coded by Fano-Huffman based codes then the dimension of the file will be less than the files coded by the other considered coding methods. Hence, this means faster communication.

Table 11 Information per letter sent by constructed binary codes

Source Alphabet	Ordinary Codes (bits)	Shannon Codes (bits)	Fano Codes (bits)	Improved Fano Codes (bits)	Shannon Fano Elias Codes (bits)	Huffman Codes (bits)	Fano-Huffman based Codes (bits)
English	0.8145	0.8801	0.9834	0.9839	1.0792	0.9905	0.9888
Turkish	0.8732	0.9075	0.9937	0.9937	1.0955	0.9939	0.9939
French	0.7971	0.8885	0.9854	0.9854	1.0911	0.9899	0.9899
German	0.8190	0.9100	0.9901	0.9901	1.1083	0.9915	0.9901
Spanish	0.8032	0.9150	0.9909	0.9909	1.1161	0.9924	0.9916
Russian	0.8839	0.9085	0.9925	0.9936	1.2142	0.9936	0.9936

Conclusion

It is seen that, binary codes constructed by Fano-Huffman based statistical coding method carry information per letter as much as codes constructed by Huffman coding method. However, by this coding method the less subset you divide the more optimal codes you obtain. Thus, this result make Fano-Huffman based statistical coding method preferred coding methods as Huffman coding method for each of the considered languages. Fano-Huffman based statistical coding method takes less time than Huffman coding method to construct binary codes. However, it require more pure computation than Huffman coding method by means of dividing the source alphabet to subsets and this means faster coding.

As it is commonly known, operating system of computers based on American Standard Code for Information Interchange (ASCII) which is ordinary binary codes. Therefore, another main result from this study is the advantage of Fano-Huffman based codes rather than ASCII. Obviously, it can be concluded from this study that ordinary codes are not optimal because they have the highest average codeword length and the least information per letter. Hence, since ASCII codes are ordinary codes, the text coded by them will be larger in size contrary to Fano-Huffman based codes. So, ASCII codes are not preferred codes.

Consequently, Fano-Huffman based codes can be used in computer systems for data compression rather than ASCII for faster communication. Because, if a file is coded by Fano-Huffman based codes then the dimension of the file will be less than file coded by ASCII but it will transmit the same information by using codes consist of less bits.

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A Comparison of One-High-Threshold and Two-High-Threshold Multinomial Models of Source Monitoring

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A data simulation study comparing the one-high-threshold (1HT) and two-high-threshold (2HT) multinomial models suggested that 2HT models are more likely to misestimate the underlying parameter values, due to inflation of some parameters (b and d), and deflation of others (D).

Key words: Multinomial modeling, source monitoring, data simulation

Introduction

Source monitoring and reality monitoring studies have proven to be extremely useful in understanding a variety of memory processes in the normal and clinical populations (Brebion, Gorman, Amador, Malaspina, & Sharif, 2002; Hoffman, 1997; Johnson, Hashtroudi, & Lindsay, 1993; Keefe, Arnold, Bayen, McEvoy, & Wilson, 2002; Lindsay, Johnson, & Kwon, 1991). Consider a simple source monitoring experiment with two sources: A and B. Single words are presented in a random fashion from the two sources, and the final recognition test consists of a mix of old A and B items along with new distracters N. The analysis of data from such a study typically examines item detection (the number of previously presented items that are correctly identified as being old), source recognition (the number of times the source of the item was correctly attributed), and

the false positive error rates (the number of new items that are incorrectly identified as being old).

However, traditional methods of analysis are unable to separate guessing biases and meta-cognitive response strategies from true item and source recognition. For example, when subjects notice that they are recognizing too few items from the (less memorable) external source, they tend to compensate by increasing the number of external-source guesses (Batchelder & Riefer, 1990). Therefore, in order to accurately measure externalizations, increases in strategic external guesses must be excluded. Similarly, to accurately estimate source recognition, it must be separable from both biases and strategic guessing. Multinomial modeling allows these distinct cognitive mechanisms can be disentangled. Multinomial modeling is a statistically sophisticated, yet simple method of separating item recognition, source recognition and response biases in discrimination tasks such as source monitoring, allowing estimation of guessing strategies and biases separately from source-discrimination processes.

Multinomial models attempt to explain discrete responses in a particular psychological paradigm by postulating latent cognitive processes that combine in different ways to determine the response category. The basic idea is that any given response category may occur as a consequence of one or more processing sequences, where each processing sequence is characterized by a series of successful or unsuccessful processing events. The processing

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sequences are represented in a tree structure (see Figure 1). The root (or initial node) represents the beginning of the processing sequence, the intermediate nodes represent stages involving a choice between two or more processing events, and the terminal nodes correspond to the observable response categories. The application of multinomial models to source monitoring has been reviewed in detail elsewhere (Batchelder & Riefer, 1999; Bayen, Murname, & Erdfelder, 1996).

One theoretical divide with implications for future research and interpretability of prior research findings lies in the selection of the basic model used for the analyses. Bayen et al. (1996) described three classes of models: the one-low-threshold (1LT), one-high-threshold (1HT) and two-high-threshold (2HT) models. The 1LT model has been used in some studies (Macmillan & Creelman, 1991), but the lack of a recognition bias parameter greatly weakens the LT model as a general purpose model of source monitoring (Bayen et al., 1996). The major theoretical debate therefore remains between the use of the 1HT and 2HT classes of models.

In 1HT models there is a single high threshold that divides the decision space into two discrete areas that correspond to detect as old and undetected. In 1HT models, it is assumed that only old items can cross the high threshold. If the threshold is crossed on presentation of a test item, the item is detected as old. If the threshold is not crossed, the item is said to be in an undetected state. All the new items and the old items that do not cross the threshold are categorized as old or new only on the basis of guessing. The probability with which an undetected item is guessed as being old is labeled b (see Figure 1).

In a 2HT model, there are two high thresholds that divide decision space into three discrete areas that correspond to detect as old, detect as new and undetected. It is assumed that only old items can cross the detect as old threshold, and only new items can cross the detect as new threshold. If either threshold is crossed on presentation of a test item, the item is detected as either old or new, depending on which threshold was crossed. If neither threshold is crossed, the item goes undetected, and is guessed to be new or old. As can be seen from

Figure 1, the 2HT source monitoring model can be constructed from the 1HT model by adding a parameter (labeled D_N) indicating the probability that a new item will be detected as new. Conversely, the 1HT model described earlier can be derived from the 2HT model by imposing the restriction $D_N = 0$. A 1HT model may thus always be regarded as a special case of a 2HT model, where the probability of crossing the second threshold is zero for all classes of items.

The nature of this debate centers around three issues. The primary theoretical issue is one of how an item is recognized as being old or new. In 2HT model space, the detection of an item as new requires it to cross a discrete threshold, which would determine it to be previously unseen. The 1HT model instead argues that the failure to cross the detection threshold for the item being old would imply that it remains unrecognized, and in the absence of a false positive recognition, the person would conclude that the item is new.

The second issue is an empirical one, stated as follows: for a given set of data, does including a D_N parameter affect the values of the other parameters (even though it is thought to represent a distinct, independent cognitive process), and if so, what is the nature of these changes?

A third issue lies in the interpretability of the parameters in the two classes of models. Specifically, in the 1HT and 2HT models (but not the 1LT model), the b parameter represents the probability of guessing that a word is a target item, when it has not actually crossed one of the thresholds. This parameter is reflected in two separate scenarios: (1) for previously seen words, it is an indicator of the tendency to guess that the word is old even when it has not been detected as being old, and (2) for new words, it is an indicator of the tendency to make false positive errors. It is assumed that these two scenarios are underpinned by the same cognitive process, and hence are assigned a common parameter. But how representative are the b parameters generated by the 1HT and 2HT model of this cognitive process?

The empirical question of how estimating a D_N parameter affects the values of the other parameters by way of a data simulation of a three-source source monitoring

Figure 1 One- and two-high-threshold models of source monitoring.

Notes. A = Source A item; B = Source B item; C = Source C item; N = distracter item; Item recognition parameters: D_1 = probability of detecting an item from source A; D_2 = probability of detecting an item from source B; D_3 = probability of detecting an item from source C; D_N = probability of detecting that a distracter item is new; Source recognition parameters: d_1 = probability of correctly discriminating the source of an item from source A; d_2 = probability of correctly discriminating the source of an item from source B; d_3 = probability of correctly discriminating the source of an item from source C; Guessing biases: a = probability of guessing that a detected item is from source A; a_1 = probability of guessing that a detected item is from source B; b = probability of guessing that an undetected item is old; g = probability of guessing that an undetected item is from source A; g_1 = probability of guessing that an undetected item is from source B.

study was addressed. The three source model was used as it allows for greater flexibility with model specification, which is not limited by the available degrees of freedom (Keefe et al., 2002; Riefer, Hu, & Batchelder, 1994; Woodward et al., 2006). The data simulation results are also pertinent to the theoretical and interpretational issues mentioned above, and these issues are addressed in the Discussion section.

The simulation of the to-be-analyzed data involved generating frequency tables from tree models for which all parameter values were set, with the exception of D_N , which was varied between 0 and .90. Varying the D_N parameter in this fashion allowed us to simulate a situation where, as is assumed by the 1HT model, there is no cognitive process that is captured by D_N , as well as three other situations whereby detection of new items is the true state of affairs, to varying degrees.

Then, these frequency tables were analyzed using 1HT and various 2HT models. Performance was assessed by examining the inflation and deflation of estimated parameter values that occur when the 1HT and 2HT underlying assumptions did or did not match the true state of affairs (the true state of affairs being the state where the estimated D_N parameter value matched the generating D_N parameter value). In this fashion, the underlying assumptions (i.e., 1HT or 2HT generating parameter values) and the methods of analysis (i.e., 1HT or 2HT estimated parameter values) were completely crossed. Both the 1HT and 2HT models were expected to perform well when the method of analysis matched the underlying assumptions determined by the generating parameters, but inflations and deflations in parameter estimates were expected when a mismatch occurred between the method of analysis and the underlying assumptions. The conclusions are based on the net inflation or deflation of parameter values for the 1HT and 2HT models under these mismatch conditions.

Methodology

A series of simulated frequency tables of responses from a three-source source monitoring task were created, similar to one used by Keefe and colleagues (Keefe et al., 2002) and one used

by Woodward, Menon, and Whitman (in press). The frequency tables were created under the constraint of 100 old items from each of the three sources (labeled A, B and C), and 300 new items. A set of underlying parameter values (i.e., the generating parameters) were specified, and these were used to create sets of response frequencies, under the restrictions of 300 old and 300 new items, as mentioned above. The final probabilities for each source/response combination were computed by multiplying the generating parameters down the processing tree, and summing together the events that lead to each specific source/response combination. For example, for the 1HT and 2HT models shown in Figure 1, the probability of participants responding "A" given stimulus A can be arrived at by multiplying the following parameters:

$$P("A" | A) = D_1 * d_1 + D_1 * (1-d_1) * a + (1-D_1) * b * g \quad (1)$$

The simulated response frequencies were created by multiplying the final probabilities associated with each source/response combination (as specified in Figure 1, and exemplified in Equation 1) by the number of responses for that source. For example, multiplying the summed probability shown in Equation (1) by 100 generates the number of times participants responded "A" for stimuli from source A.

The generating parameter values were fixed across simulated sets of frequencies, with the exception of the D_N parameter (the item recognition parameter for new items), which was varied (0, .30, .60 and .90). This method of creating sets of frequencies is similar to the method used by Reifer and Batchelder (1991) in their Monte Carlo simulation. The sets of frequencies created when $D_N = 0$ represent patterns of frequencies that would be generated under the assumptions underlying 1HT model, whereas the sets of frequencies created when $D_N > 0$ represent patterns of frequencies that would be generated under the assumptions underlying various 2HT models. The frequency tables generated for the analyses are presented in Appendix A. Note that the only variation in the sets of frequencies generated using the various

values of D_N occurred in the number of false positive responses generated by the new words.

Then, the data were analyzed using an Excel spreadsheet specialized for multinomial modeling (Dodson, Prinzmetal, & Shimamura, 1998). In the analysis, the value of the D_N parameter was first fixed at the different values (0, .30, .60 and .90) to test the impact of varying degrees of mismatch between the underlying model assumptions (as determined by the generating parameter values) and the methods of analysis. Following this, the 2HT analysis was carried out allowing all parameters (including D_N) to vary freely. In the Excel spreadsheet, the optimum parameter values are found by allowing them to vary in an iterative fashion using the solver function. Starting values for probability estimates were .50, and the log likelihood ratio statistic G^2 was used to assess overall fit. G^2 asymptotically has a chi-square distribution, and the optimized solution is the one that minimizes the G^2 value (Riefer & Batchelder, 1988).

Results

The estimated parameter values are presented as a function of varying generating and estimating D_N parameter values in Table 1, and in Figures 2-6. From these results it is apparent that, within each set of response frequencies, varying the value of the D_N parameter (which in theory should only affect the recognition of new items) affected the value of the other parameters in a variety of important ways. As was expected, all models were very accurate when the method of analysis matched the underlying assumption (i.e., when the estimating D_N was equal to the generating D_N). However, in the case of mismatches, occasionally severe inflation and deflation of the underlying parameters occurred. Specifically, underestimation of D_N parameter resulted in overestimation of the other D parameters and underestimation of b and d parameters, whereas overestimation of D_N resulted in underestimation of D and overestimation of b and d parameters.

With respect to the comparative performance of 1HT and 2HT models, the most important pattern that can be derived from Table

1 and Figures 2-6 is that the consequences of overestimating D_N are far more severe than the consequences of underestimating D_N . As Figures 2-6 show, the changes in the generating parameter values had the least effect when estimated using the 1HT model (i.e., $D_N = 0$), while the variability of the estimated parameters increased greatly when a 2HT model is used, particularly with high D_N parameter values.

For example, consider the results based on a generating D_N parameter of .60 (see Table 1). An instructive comparison can be made between when D_N was underestimated by .30 and when D_N was overestimated by .30 for this condition. When the D_N parameter was underestimated by .30 (i.e., estimated $D_N = .30$), D_1 and D_2 increased to .70 (from .67), D_3 increased to .78 (from .75), and the d_1 and d_2 parameters decreased to .57 (from .60), a net change of .03 on all these parameters. This also resulted in a reduction in the value of the b parameter to .11 (from .20). However, in the comparison condition when D_N was overestimated by .30 (i.e., estimated $D_N = .90$), D_1 decreased to .40 (from .67), the d_{1-2} parameters increased to 1.0 (from .60, indicating perfect source recognition), a net change of .27 and .40, respectively. In addition, the b parameter increased to .59 (from .20).

Following the analysis where the estimating D_N parameter was fixed at various values, we also examined the results using an unconstrained 2HT model (i.e., all parameters, including the D_N parameter, were free to vary). The results are shown in Table 1 (bottom row). The unconstrained 2HT model did not retrieve the generating parameters in any of the lower D_N conditions (i.e., generating $D_N = 0$, .30 or .60), despite a perfect fit (i.e., very low G^2 values). Instead the model tended to estimate D_N values that were higher than the generating D_N values, resulting in a corresponding elevation of the b and d parameter values, and a reduction in the D parameter values.

Both 1HT and 2HT models estimated the guessing parameters a , a_1 , g and g_1 accurately, and their values did not change with changes in the value of the estimating D_N parameter; therefore, they are not presented here.

Table 1. Estimated Parameter Values Presented as a Function of Varying Generating and Estimating D_N

Parameter Values													
Generating D_N Parameter													
$D_N = 0$ (1 HT) FP = .20							$D_N = .30$ FP = .14						
Est D_N	D_{1-2}	D_3	d_{1-2}	d_3	b	Fit	Est D_N	D_{1-2}	D_3	d_{1-2}	d_3	b	Fit
$D_N = 0$	.67	.75	.60	.59	.20	0 (.99)	$D_N = 0$	.69	.77	.58	.58	.14	0 (.99)
$D_N = .30$	.63	.72	.64	.61	.29	0 (.99)	$D_N = .30$	.67	.75	.60	.59	.20	0 (.99)
$D_N = .60$	.47	.60	.85	.74	.50	0 (.98)	$D_N = .60$	.59	.69	.68	.64	.36	0 (.99)
$D_N = .90$	.37	.44	1.0	1.0	.68	62.8 (.0)	$D_N = .90$	.38	.45	1.0	1.0	.65	26.3 (.0)
$D_N = .53$	.54	.66	.74	.68	.43	0 (.99)	$D_N = .61$	.58	.69	.69	.65	.37	0 (.99)

Generating D_N Parameter													
$D_N = .60$ FP = .08							$D_N = .90$ FP = .02						
Est D_N	D_{1-2}	D_3	d_{1-2}	d_3	b	Fit	Est D_N	D_{1-2}	D_3	d_{1-2}	d_3	b	Fit
$D_N = 0$	.71	.78	.57	.56	.08	0 (.99)	$D_N = 0$	.73	.80	.55	.55	.02	0 (.99)
$D_N = .30$	.70	.78	.57	.57	.11	0 (.99)	$D_N = .30$	.73	.80	.55	.56	.03	0 (.99)
$D_N = .60$	.67	.75	.60	.59	.20	0 (.99)	$D_N = .60$	.72	.79	.56	.56	.05	0 (.99)
$D_N = .90$	.40	.52	1.0	.74	.59	2.6 (.10)	$D_N = .90$	.67	.75	.60	.58	.20	0 (.99)
$D_N = .73$	.63	.72	.65	.62	.30	0 (.99)	$D_N = .91$	.67	.75	.61	.59	.21	0 (.99)

Note. The generating probabilities used were: $D_1/D_2 = .67$, $D_3 = .75$, $d_1/d_2 = .60$, $d_3 = .60$, $a = .60$, $b = .20$, $g = .60$, $a_1 = .50$, $g_1 = .50$. FP refers to false positives, and Fit refers to Chi-square values of the final model (p values are bracketed, such that $p < .05$ indicates poor fit). When estimating, all parameters were free to vary with the exception of D_N , which was fixed (Est D_N). The bottom row displays the results when the D_N parameter was also allowed to vary. The models generated guessing parameters (a , a_1 , g , g_1) that were identical to the generating probabilities and did not vary across the different simulations, and are therefore not listed in the above table.

Figure 2 Estimated D_1/D_2 parameter values plotted as a function of generating and estimated D_N parameters (True $D_1/D_2 = .67$).

Figure 3. Estimated D_3 parameter values plotted as a function of generating and estimated D_N parameters (True $D_3 = .75$).

Figure 4 Estimated d_1/d_2 parameter values plotted as a function of generating and estimated D_N parameters (True $d_1/d_2 = .60$).

Figure 5. Estimated d_3 parameter values plotted as a function of generating and estimated D_N parameters (True $d_3 = .60$)

Figure 6. Estimated b parameter values plotted as a function of generating and estimated D_N parameters (True $b = .20$).

Conclusion

This simulation was designed to compare the 1HT and 2HT approaches to multinomial modeling on their ability to accurately estimate underlying parameter values under a number of experimental conditions. The results suggest that the 1HT model is a more conservative choice for the analysis of data from source monitoring tasks, because the 2HT models are more likely to misestimate the underlying parameters. Specifically, the simulation showed that use of the 2HT models lead to an artificial inflation of the b parameter (probability of guessing that an item not detected as old was actually seen before), which in turn caused inflation of d (source recognition), and deflation of D (item recognition) parameter values. The 1HT model showed less variability and gave parameter estimates that were closer to the underlying parameter values, even when the underlying assumptions were those held by the 2HT perspective. As the simulation shows, the unconstrained 2HT solution (where the D_N parameter value was not fixed - Table 1 bottom row) typically produced a D_N parameter value

that was in excess of the true generating D_N value, which in turn affected many of the other parameters as outlined above. With respect to a behavioral interpretation, the 2HT models produce parameter values that suggest artificially reduced item recognition for old items, increased guessing of undetected old items, and increased source recognition compared to the 1HT model. For instance, with the high estimated D_N parameter values, the 2HT models suggest a state with perfect source recognition even though item recognition is occurring much less frequently, which is counterintuitive, given that item recognition is generally regarded as a less demanding process than source recognition.

With respect to the theoretical issue mentioned in the Introduction, whether or not the recognition of new items occurs via the new items crossing a definite threshold (as suggested by the 2HT model) or simply by not being recognized as being old (as suggested by the 1HT model) remains open to debate. What the simulation results show is that, given that these theoretical issues cannot currently be resolved, the 1HT model is a more conservative choice for

the analysis of data from source monitoring tasks, because the 2HT models are more sensitive to possible mis-estimation of the underlying parameters.

With respect to interpretability of the b parameter (the probability of guessing that an undetected item is actually a target item), as can be seen in Table 1, the results show that only the 1HT model (i.e., $D_N = 0$) produced a b parameter value equal to the false positive error rate. In the 2HT model, increasing values of D_N resulted in b parameter values that were far higher than the proportion of false positives. As mentioned earlier, the parameter is an indicator of two separate scenarios. For previously seen words, it is an indicator of the tendency to guess that the word is old even when it has not been detected as being old, and for new words, it is the tendency to make false positive errors (i.e., detect them as being old). However, the crucial difference between these two processes is that the tendency to make false positive errors can be estimated (by observing raw frequencies of the number of false positive recognition errors), while the same cognitive process for old words (making fortuitous false positive recognitions, which in turn elevates the hit rate), remains a hidden process.

If both these patterns of false recognition are driven by the same cognitive processes, then the b parameter should reflect both in equal measure. The use of the 1HT model, which generates the value of the b parameter corresponding to the proportion of false positive error rates, has an intuitive appeal from this perspective. The 2HT model is likely to produce a b parameter that is inflated, possibly leading to the false conclusion that much of the recognition reflected by the raw frequencies occurs through fortuitous guessing. Moreover, an increase in b causes corresponding decreases and increases in the D and d parameters, respectively, leading to the false conclusion that recognition has decreased and source discrimination has increased, respectively.

In an important study that suggested the superiority of the 2HT model over the 1HT model in source monitoring, Bayen et al. (1996) studied the impact of increased distracter similarity on the ability to carry out item

detection and source recognition. On the assumption that increased distracter similarity (but not increased source similarity) would decrease item detection, they analyzed their results using 1HT and 2HT models. They found that D parameter values decreased with increasing distracter similarity only when the 2HT model was used, and argued on these grounds that the 2HT is more sensitive to changes in item detection, making it a superior model of source monitoring. However, as Bayen et al. (1996) pointed out, increasing distracter similarity only serves to increase the number of false alarms and not the hit rate (p 205, Appendix C pg 215), casting doubt on their assumption that increasing distracter similarity should decrease item detection. Moreover, the simulation results demonstrate that use of the 2HT model is likely to lead to artificial decreases in the recognition parameter D , suggesting that Bayen et al.'s (1996) recommendations may have been based on an artifact of the 2HT model, as opposed to the purported superiority of the 2HT model in detecting an experimental-manipulation-induced true decrease in recognition.

There are two reasons to suggest that the recognition parameters may have been affected by the model selected rather than the experimental manipulation. First, the Bayen et al. (1996) models used one D parameter for both old and new items (i.e. $D_N = D_1 = D_2$), and as a result, the increase in false positives, which should cause a decrease in D_N but not in D_1 or D_2 , affected all three of these parameters. Secondly, due to the reciprocal relationship between b and D in the 2HT model (as can be seen from Figures 2, 3 and 6), an increase in the b parameter (which is often well in excess of the true proportion of false alarms in the experimental data) caused a reduction in the D parameter. That is to say, use of the 2HT model can lead to apparent decreases in item detection as an artifact of increases in false positives, even in the absence of an experimental manipulation affecting item detection.

In the aforementioned Bayen et al. (1996) study, the 1HT model, on the other hand, showed a slight decrease in the D parameter due to an increase in false alarms, and a significant decrease in the D parameter only when the hit

rate decreased. This pattern of results would be expected from a model that was appropriately reflecting factors affecting false alarms independently from those affecting item detection.

Bayen et al. (1996) computed decreases in the signal detection measure d' for item detection. They showed decreases in d' with increasing source similarity, and, based on this measure, concluded that their experimental manipulations had affected the true recognition rate. Batchelder, Riefer and Hu (1994) and Thomas and Olzak (1992) explicitly pointed out that d' can be used as a means to compare item recognition only when false alarm rates are comparable across conditions. For a paradigm such as that used by Bayen et al. (1996), where the manipulation specifically affected the false alarm rates, d' is expected to underestimate item detection as the false alarm rate increases. It therefore seems likely that the fundamental assumption of their experimental manipulation (i.e., that increasing distracter similarity causes decreases in item detection) is debatable, and that the decreases in recognition parameters that they observed when employing the 2HT model may have instead reflected an artifact of the 2HT model.

The data simulation indicates that the 1HT model generally provides more accurate estimates of the underlying parameter values than the 2HT model, and is more robust to variation in the generating D_N parameters. In addition, with respect to interpretation, the 1HT model produces a b parameter value that accurately reflects the true proportion of false positives and the 2HT model inflates the b parameter value, which in turn spuriously reduces the item detection parameters and inflates the source recognition parameters. In the light of these considerations, use of the 1HT model over the 2HT model is recommended in the analysis of data from source monitoring studies.

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Appendix A

Table of frequencies generated with varying 2HT assumptions

Source	Response			
	Experimenter	Computer	Self	New
$D_N = 0$				
Experimenter	50 (.50)	10 (.10)	13 (.13)	26 (.26)
Computer	10 (.10)	50 (.50)	13 (.13)	26 (.26)
Self	11 (.11)	11 (.11)	58 (.58)	20 (.20)
New	18 (.06)	18 (.06)	24 (.08)	240 (.80)
$D_N = .30$				
Experimenter	50 (.50)	10 (.10)	13 (.13)	26 (.26)
Computer	10 (.10)	50 (.50)	13 (.13)	26 (.26)
Self	11 (.11)	11 (.11)	58 (.58)	20 (.20)
New	13 (.04)	13 (.04)	17 (.06)	258 (.86)
$D_N = .60$				
Experimenter	50 (.50)	10 (.10)	13 (.13)	26 (.26)
Computer	10 (.10)	50 (.50)	13 (.13)	26 (.26)
Self	11 (.11)	11 (.11)	58 (.58)	20 (.20)
New	7 (.02)	7 (.02)	10 (.03)	276 (.92)
$D_N = .90$				
Experimenter	50 (.50)	10 (.10)	13 (.13)	26 (.26)
Computer	10 (.10)	50 (.50)	13 (.13)	26 (.26)
Self	11 (.11)	11 (.11)	58 (.58)	20 (.20)
New	2 (.007)	2 (.007)	2 (.007)	294 (.98)

Note. Row percentages are presented in brackets. Correct responses are in bold.

Examining Cronbach Alpha, Theta, Omega Reliability Coefficients According to the Sample Size

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Differentiations according to the sample size of different reliability coefficients are examined. It is concluded that the estimates obtained by Cronbach alpha and teta coefficients are not related with the sample size, even the estimates obtained from the small samples can represent the population parameter. However, the Omega coefficient requires large sample sizes.

Key words: Cronbach alpha, theta, omega, reliability, scale, sample size.

Introduction

A scale is needed to measure and that scale must be reliable and valid. The scale's reliability does not matter in the case of measuring the concrete characteristics. But, it is an important problem in the case of measuring the abstract characteristics. So, it is necessary to analyze the reliability of the scales using some statistical

methods. In making a reliability analysis, the reliability coefficients that are suitable in obtaining the reliability of the scale and the structure of the empirical study must be examined. Sample size is also important to determine the reliability level of the scale. Thus, one of the dimensions that must be examined is the changes in Cronbach alpha, theta, and omega coefficients according to the sample size.

Reliability

The scale, used to get some information on a defined subject, must have some properties. Reliability, a property that a scale must have, is an indicator of consistency of measurement values obtained from the measurements repeated under the same circumstances (Gay, 1985; Carmines & Zeller, 1982; Arkin & Colton, 1970; O'Connor, 1993; Carey, 1988).

The reliability of the scale can be examined by different ways. The reliability of the scale can be examined by applying the scale once, applying the scale twice or applying the equivalent scales once. In case of applying the scale once, the reliability of internal consistency is examined. The reliability coefficient ranges between 0 and 1.

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Methods of Internal Consistency

If the reliability can be estimated by applying the scale once, the error in reliability estimation will be less than the other reliability estimation methods. In this kind of reliability estimation, wrong management, scoring, temporary changes in personal performance affect the internal consistency, the leading affect will be the content sampling (O'Connor, 1993).

Another method, split-half, denotes the homogeneity indices of the items in the scales. It pertains to the relationship level between the responses of the items and the total scale score (Oncu, 1994). An increase in homogeneity in the set of items increases this reliability estimate (O'Connor, 1993). The idea that the internal consistency methods depend upon is that every measurement tool is constructed to realize an objective and those have known equal weights (Karasar, 2000). The internal consistency methods are preferred because they are economical and easy to apply (Oncu, 1994).

Cronbach Alpha

The Alpha coefficient method (Cronbach, 1951), is a suitable method that can be used for likert scale items (e.g., 1-3, 1-4, 1-5). Thus, it is not limited to the true-false or correct-incorrect format (Oncu, 1994).

Cronbach alpha coefficient is weighted standard variations mean, obtained by dividing the total of the k items in the scale, to the general variance (Thorndike et al., 1991).

$$\alpha = \frac{n}{(n-1)} \left[1 - \frac{\sum_{i=1}^n \sigma_{Y_i}^2}{\sigma_x^2} \right]$$

n : Number of the items

σ_{Y_i} : ith item's standard deviation

σ_x : General standard deviation

(2.1)

If the items are standardized, coefficient is calculated by using the items' correlation mean or variance-covariances' mean (Carmines & Zeller, 1982; Ozdamar, 1999a; SPSS, 1991; SPSS, 1999).

Calculation of alpha coefficient due to the correlation mean,

$$\alpha = \frac{n \bar{\rho}}{1 + (n-1) \bar{\rho}} \quad (2.2)$$

Calculation of alpha coefficient due to the variance-covariance mean,

$$\alpha = \frac{n \overline{\sigma_{XX}} / \overline{\sigma_X}}{1 + (n-1) \overline{\sigma_{XX}} / \overline{\sigma_X}} \quad (2.3)$$

When the formula for calculating Cronbach alpha using the correlation means between items is examined, it can be seen that it is proportionally related with the number of the items and the mean of the correlation between items (Carmines & Zeller, 1982). If the correlation between the items is negative, alpha coefficient will also be negative. Because this situation will spoil the scale's additive property, it also causes a spoil in the reliability model and the scale is no more additive (Ozdamar, 1999a). The coefficient is equal to the mean of all probable coefficients using split-half method (Carmines & Zeller, 1982; Gursakal, 2001).

Theta Coefficient

The Theta coefficient depends on the principal components analysis. In principal components analysis, the components are in descending order due to the variances of each of the constructions (Carmines & Zeller, 1982). The first component is the linear component with the maximum variance. The second component is the linear component with the second maximum variance. Components can be explained by the component variances defined by the percentage values to explain the variance of the original data set in order (Ozdamar, 1999b). Theta coefficient depends on that property. The Theta coefficient, takes into account the eigenvalue that maximum explains the event, is calculated as follows:

$$\theta = (N / N - 1)(1 - 1 / \lambda_i)$$

N : Number of items

λ_i : The largest eigenvalue (the first eigenvalue)

(2.4)

Omega Coefficient

Another coefficient for linear dependencies is the Omega coefficient proposed by Heise and Bohrnstedt (1970). It depends on the factor analysis model. Omega coefficient is modeled on factor analysis. In this type of modeling, in calculating the coefficient, before factoring "1" values on diagonal in the correlation matrix are replaced with the communality values. The Omega coefficient can be calculated with two ways, using variance-covariance matrix and correlation matrix (Carmines & Zeller, 1982).

When studied with variance-covariance matrix,

$$\Omega = 1 - \left(\sum \sigma_i^2 - \sum \sigma_i^2 h_i^2 \right) / \left(\sum \sum \sigma_{x_i x_j} \right)$$

h_i^2 : Communality of the i^{th} item

(2.5)

When studied with correlation matrix,

$$\Omega = 1 - \left(a - \sum h_i^2 \right) / (a + 2b)$$

a: Number of items

b: Sum of the correlations among items

(2.6)

There are some differences between the Theta and Omega coefficients. They depend on different factor-analytic models. The Theta coefficient depends on principal components model, whereas the Omega coefficient depends on factor analysis model. Therefore, in calculating the eigenvalues for Theta coefficients, the diagonal 1.0 values are used, but in calculating the Omega coefficients,

communality values that are not related with 1.0 values are used (Carmines & Zeller, 1982).

There is a relationship between Alpha, Theta, and Omega coefficients. If the items take parallel values, three coefficients are equal each other and will be 1.0. Otherwise, the relationship of magnitude for the coefficients will be $\alpha < \theta < \Omega$. Among these internal consistency coefficients, α gives the lower bound of the reliability coefficient and Ω gives the upper bound of the reliability coefficient (Carmines & Zeller, 1982).

Methodology

To compare the Alpha, Theta and Omega coefficients, a data set has been used from an instrument developed by Ercan et al. (2004) to measure patient satisfaction in the secondary health-care units. To obtain the effects of different number of items and different sample sizes, 3 different scales are constructed with 39, 34, and 30 items by subtracting some items from the scale with 43 items. Because all the subjects did not answer all the items, the subject numbers in the scales are also different. There are 170 subjects answered all of the 43 items, 240 subjects answered all of the 39 items, 230 subjects answered all of the 34 items, and 320 subjects answered all of the 30 items.

After giving a number to each of the subjects, samples are constructed by producing random numbers using MINITAB 13.2 beginning from 10 and increasing 10 units each of those random numbers. The same procedure was repeated 10 times and for each of the samples Cronbach alpha, Theta and Omega reliability coefficients are calculated.

SPSS 13.0 was used for these analyses. Statistical comparisons are performed in order to determine if alpha, theta and omega coefficients change or not according to the sample size and in order to determine the sample size that the reliability coefficients begin to get stable. Before the between group comparisons, the homogeneity of variances is tested using the Levene statistic. If the variances are found to be homogeneous, then analysis of variance

Table-4.1: The homogeneity test results for the scale with 30 items

	Levene Statistic	Degree of Freedom 1	Degree of Freedom 2	Significance level (p)
α	5.631	31	288	<0.001
θ	5.578	31	288	<0.001
Ω	1.531	31	288	0.040

Table-4.2: Significance level in comparison of α , θ and Ω reliability coefficients according to different sample sizes using Kruskal-Wallis test for the scale with 30 items

	α	θ	Ω
χ^2	23.706	46.720	259.636
Degree of freedom	31	31	31
Significance level (p)	0.822	0.035	<0.001

Bonferroni correction: $\alpha^* = 1 - (1 - \alpha)^{1/k}$

$$\alpha^* = 1 - (1 - 0.05)^{1/32} = 0.0016$$

and Tukey HSD post-hoc comparison test are applied. If the variances are heterogeneous, Kruskal-Wallis and Mann-Whitney U tests are applied to make reliability comparisons according to sample size. The level of significance in multiple comparisons is determined after Bonferroni correction ($\alpha^* = 1 - (1 - \alpha)^{1/k}$ k: number of groups).

Results

The results of comparisons α , θ and Ω coefficients according to different sample sizes are given in Table 4.1, 4.2, 4.3, 4.4 for the scale with 30 items.

n	10	20	30	40	50	60	70	80	90	100	110	120	130	140	150	160	170	180	190	200	210	220	230	240	250	260	270	280	290	300	310	320
10	631	315	315	315	280	353	393	393	353	353	393	393	353	315	353	315	353	353	315	315	315	353	353	353	393	315	315	315	436	436	436	
20		912	684	796	529	579	100	529	631	529	529	529	631	353	315	190	165	089	123	190	123	123	123	105	089	165	052	075	075	123	075	063
30			315	393	218	315	529	247	218	218	190	190	190	165	143	105	105	089	105	123	075	089	089	105	123	063	075	075	075	123	105	089
40				853	684	912	796	579	853	481	529	353	280	218	143	123	123	123	123	123	089	143	123	123	123	089	063	075	123	123	123	
50					529	971	853	436	684	353	529	190	165	247	143	052	034	052	075	105	105	105	035	052	075	075	052	035	023	023	023	
60						796	353	971	912	912	100	912	912	796	739	529	436	247	315	481	436	436	218	218	393	190	190	247	353	165	123	
70							739	739	912	631	796	393	436	529	247	165	143	089	190	143	165	105	105	165	218	143	105	063	075	075	089	
80								315	529	247	280	105	089	123	052	011	004	009	011	023	019	019	004	005	009	009	005	005	002	002	002	
90									971	796	971	739	796	579	353	280	247	218	353	280	165	165	123	190	315	089	089	105	105	143	218	
100										739	796	481	481	315	315	218	190	165	190	218	143	165	218	143	247	123	143	105	218	190	143	
110											971	796	853	529	481	315	315	247	247	280	165	190	247	165	280	105	143	143	165	165	143	
120												579	684	739	315	190	105	105	315	190	315	075	063	143	247	089	089	035	035	052	075	
130													631	971	971	631	529	123	190	436	353	280	105	105	481	105	123	247	165	075	023	
140														853	739	481	315	143	143	247	353	247	052	075	123	123	105	075	023	043	023	
150															579	280	190	218	353	280	436	190	165	247	393	218	190	075	075	075	089	
160																529	280	190	393	436	529	631	143	315	529	315	280	105	075	123	123	
170																	631	315	796	912	971	100	436	739	912	739						

[illegible]

The results of comparisons α , θ and Ω coefficients according to different sample sizes

are given in Table 4.5, 4.6, 4.7 for the scale with 34 items.

Table-4.5: The homogeneity test results for the scale with 34 items

	Levene Statistic	Degree of freedom 1	Degree of freedom 2	Significance level (p)
α	11.003	22	207	<0.001
θ	10.477	22	207	<0.001
Ω	3.238	22	207	<0.001

Table-4.6: Significance level in comparison of α , θ and Ω reliability coefficients according to different sample sizes using Kruskal-Wallis test for the scale with 34 items

	α	θ	Ω
χ^2	6.329	8.960	176.741
Degree of freedom	22	22	22
Significance level (p)	1.000	0.994	<0.001

Bonferroni correction: $\alpha^* = 1 - (1 - \alpha)^{1/k}$

$$\alpha^* = 1 - (1 - 0.05)^{1/23} = 0.0022$$

[illegible]

The results of comparisons α , θ and Ω coefficients according to different sample sizes

are given in Table 4.8, 4.9, 4.10, 4.11 for the scale with 39 items.

Table-4.8 : The homogeneity test results for the scale with 39 items

	Levene Statistic	Degree of freedom 1	Degree of freedom 2	Significance level (p)
α	10.692	23	216	<0.001
θ	12.048	23	216	<0.001
Ω	1.418	23	216	0.104

Table-4.9: Significance level in comparison of α and θ reliability coefficients according to different sample sizes using Kruskal-Wallis test for the scale with 39 items

	α	θ
χ^2	7.206	8.702
Degree of freedom	23	23
Significance level (p)	0.999	0.997

Table-4.10: Significance level in comparison of Ω reliability coefficients according to different sample sizes by analysis of variance for the scale with 39 items

	Sum of Squares	Degrees of freedom	Sum of Squares	F	Significance level (p)
Between groups	0.00536	23	0.0002329	142.881	<0.001
Within groups	0.000352	216	0.00000163		
Total	0.00571	239			

Bonferroni correction: $\alpha^* = 1 - (1 - \alpha)^{1/k}$

$$\alpha^* = 1 - (1 - 0.05)^{1/24} = 0.0021$$

for the scale with 39 items ($\alpha^*=0.0021$).

[illegible]

The results of comparisons α , θ and Ω coefficients according to different sample sizes

are given in Table 4.12, 4.13, 4.14 for the scale with 43 items.

Table-4.12: The homogeneity test results for the scale with 43 items

	Levene Statistic	Degree of freedom 1	Degree of freedom 2	Significance level (p)
α	6.313	16	153	<0.001
θ	7.654	16	153	<0.001
Ω	2.463	16	153	0.002

Table-4.13: Significance level in comparison of α , θ and Ω reliability coefficients according to different sample sizes using Kruskal-Wallis test for the scale with 43 items

	α	θ	Ω
χ^2	11.248	7.026	141.750
Degree of freedom	16	16	16
Significance level (p)	0.794	0.973	<0.001

Bonferroni correction: $\alpha^* = 1 - (1 - \alpha)^{1/k}$

$$\alpha^* = 1 - (1 - 0.05)^{1/17} = 0.003$$

Table-4.14: Significance level (p values $\times 10^{-3}$) in comparison of Ω reliability coefficients according to different sample sizes using Mann-Whitney U test for the scale with 39 items ($\alpha^*=0.003$)

n	10	20	30	40	50	60	70	80	90	100	110	120	130	140	150	160	170
10		000	000	000	000	000	000	000	000	000	000	000	000	000	000	000	000
20			000	000	000	000	000	000	000	000	000	000	000	000	000	000	000
30				143	000	000	000	000	000	000	000	000	000	000	000	000	000
40					001	000	000	000	000	000	000	000	000	000	000	000	000
50						353	015	002	000	000	000	000	000	000	000	000	000
60							123	011	003	000	000	000	000	000	000	000	000
70								218	089	009	003	000	000	000	000	000	000
80									353	105	105	005	001	000	000	000	000
90										393	315	035	015	009	002	001	002
100											912	280	190	089	035	029	023
110												280	165	105	035	029	009
120													631	481	190	075	023
130														912	579	123	043
140															436	218	063
150																481	165
160																	481
170																	

Conclusion

The answer to the question of sample size in this context is important. The accuracy of reliability coefficients changes according to the sample size. There is high positive correlation between number of items and reliability coefficient as mentioned in Carmines and Zeller (1982). Also, the difference in number of items must be taken into account.

Significant differences are not observed due to the sample size in the commonly used Cronbach Alpha, and with the Theta coefficient which is based on principal components. However, with the Omega coefficient, based on factor analysis, large differences were observed due to the sample size. With an increase in item numbers, however, the Omega coefficient is stabilized even for smaller sample sizes.

Ozdamar (1999a) mentioned that the sample size should be more than 50 in reliability

analysis applications. According to the results of this study, that sample size is not important for the Cronbach alpha or theta coefficients, and is stable even for a small number of items (although of course an increase in the number of items will increase the magnitude.) However, in order to estimate the population parameter with Omega coefficient, the item number is important. With an increase in item number, either the consistency of estimation or the reliability level increases.

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Modeling Longitudinal Ordinal Response Variables for Educational Data

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This article presents applications for the analysis of multilevel ordinal response data through the proportional odds model. Data are drawn from the public-use *Early Childhood Longitudinal Study*. Results showed that gender, number of family risk characteristics, and age at kindergarten entry were associated with initial reading proficiency (0 to 5 scale). The number of family risks and age were associated with time-slopes. Three issues are highlighted: building multilevel ordinal models, interpretation of multilevel effects; and determination of predicted probabilities based on results of the multilevel proportional odds models.

Key words: Proportional odds models, multilevel models, ordinal data.

Introduction

Prior to the fitting of statistical models to investigate relational characteristics of data, researchers must first consider the much more fundamental process of measurement. Stevens

(1946) referred to the measurement process as the development of a model that “represent[s] aspects of the empirical world” (p. 677) that are consistent with the nature of the objects under study. In education as well as the social and behavioral sciences, many outcomes are measured on an ordinal rather than an interval or ratio scale, reflecting of course the underlying nature of the phenomenon under study. As an example of an ordinal scale, consider the Concerns-Based Adoption Model (CBAM), developed to characterize the progression of teacher and administrator concerns regarding implementation of innovations within their classrooms or schools (Hall, George & Rutherford, 1986; van den Berg, Slegers & Pelkmans, 2002, etc.).

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Responses on the CBAM correspond to eight ordinal categories, representing progressive stages ranging from self-concern, task-concern to other-concern. This stage-based model is currently being adapted to characterize agency capacity for implementation of evidence-based HIV prevention interventions (O'Connell, Cornman & Heybruck, 2003). Examples of ordinal scales can be found in many different contexts. Proficiency on statewide educational assessments has been characterized as ordinal, with students identified as below basic, basic, proficient, goal, and advanced in mathematics and reading (Beaudin, 2003). The goals set by No Child Left Behind (<http://www.nclb.org/>)

require 100% of students within schools to attain proficiency in order to demonstrate effectiveness, making an understanding of ordinal measures and their statistical treatment important for schools, teachers, administrators, districts and state personnel.

In fact, most variables that are used to detect educational or behavior change are ordinal in nature. For example, change in proficiency during the kindergarten year in early reading or mathematics can be characterized as ordinal (i.e., achieved or did not achieve a particular level within a hierarchy of proficiency goals, pre- and post-school year); so can frequency of condom use before and after an intervention (never, sometimes, almost always, always). Many health intervention studies have relied on the transtheoretical model to characterize individual change before and after participation (Bowen & Trotter, 1995; Hedeker & Mermelstein, 1998; Lauby et al., 1998; Prochaska & DiClemente, 1983, 1986; Prochaska, DiClemente, & Norcross, 1992; Prochaska, Redding, Harlow, Rossi, & Velicer, 1994; Stark et. al, 1996). Other examples include change in severity of illness or physical condition with scale categories such as mild, moderate, and severe (Knapp, 1999), and the common approach of using endorsement of responses to a particular statement (strongly disagree, disagree, neutral, agree, strongly agree) to assess attitudes before and after an event or period of time.

As these examples suggest, the use of ordinal-level variables in education and the social sciences are abundant. This should not be surprising, as Cliff (2003, 1996, and 1993) has consistently pointed out in much of his work on ordinal measurement that the questions we ask of our data are primarily ordinal in nature as well (Did students perform better after a school-based intervention?). However, there is inconsistency in the fidelity between ordinal measurement of a behavioral or cognitive outcome and how these quantities are analyzed in statistical models (Cliff, 2003, 1996, 1993; O'Connell, 2000; Clogg & Shihadeh, 1994; Long, 1997; Agresti, 1996). The accurate

interpretation of relationships among variables is dependent on the application of appropriate statistical techniques, yet the treatment of ordinal responses present challenges for many applied researchers in the educational and behavioral sciences. Similar to the field of biomedical and epidemiological research, the underutilization of ordinal regression models in the educational and behavioral sciences may be partially explained by researcher unfamiliarity with software programs capable of fitting these models, confusion about model assumptions and how to investigate these assumptions, and problems in interpretation of model results (Bender & Benner, 2000). These challenges are multiplied when the study purports to consider change in an ordinal outcome over time. In this paper, the hierarchical generalized linear model (HGLM; Goldstein, 2003; McCullagh & Nelder, 1989; Raudenbush & Bryk, 2002) for ordinal responses is demonstrated and explained, using a small number of potential explanatory variables for illustration purposes.

Data applications that characterize an approach to analyzing change over time in ordinal response variables are presented. The data used is drawn from the Early Childhood Longitudinal Study (ECLS), a national database developed and managed through the National Center for Education Statistics (NCES). The ECLS-K (Kindergarten cohort) follows nearly 20,000 students from kindergarten through the first grade, with additional follow-ups in 3rd and 5th grade. The outcome of interest in the models constructed is student proficiency for early reading and literacy assessed across kindergarten and 1st grade, which was measured using six ordinal categories (Table 1). Particular attention is paid to interpretation of the model estimates and assumptions, and the effects of independent variables on proficiency over time. HLM version 6.03 is used for these analyses (Raudenbush, Bryk, Cheong & Congdon, 2004). The goal is to make a contribution to the applied literature on use and interpretation of hierarchical ordinal models, as well as to highlight the methodological challenges of modeling longitudinal ordinal outcomes.

Table 1. Percent of Sample Reaching Reading Proficiency Levels Across Four Waves of ECLS-K.

Proficiency Level	Baseline			
	0 months <i>n</i> = 3242	8 months <i>n</i> = 3346	12 months <i>n</i> = 3380	20 months <i>n</i> = 3425
0. Did not pass level 1	28.0	4.5	2.0	0.2
1. Identifying upper/lower case letters	34.6	14.8	8.3	1.1
2. Associating letters with sounds at the beginning of words	17.2	23.3	17.6	3.0
3. Associating letters with sounds at the end of words	17.0	40.9	44.0	11.8
4. Recognizing words by sight	2.1	11.3	17.5	37.9
5. Recognizing words in context	1.2	5.2	10.6	46.0

Methodology

Context: Proficiency in Early Literacy

In the ECLS-K, proficiency in early literacy is represented as a series of stepping-stones, which reflect the skills that form the foundation for further learning in reading (West, Denton, & Germino-Hausken, 2000). The categorization of early literacy proficiencies represented in the ECLS-K assessment instrument is consistent with the skills that have been identified as the building blocks of reading mastery: phonemic awareness (the understanding that letters represent spoken sounds), phonics (understanding the sounds of letters in combination), fluency, vocabulary and text-comprehension (CIERA, 2001). Six categories of hierarchical skill levels are used to establish the proficiency scale (Table 1). Mastery is defined as passing 3 out of 4 items in a cluster representing each successive proficiency level.

Research has indicated that children who experience difficulty learning to read in the early primary grades tend to begin school with limited proficiency for early-literacy skills (Burns, Snow & Griffen, 1998). These early skills in reading carry-over to performance at later grades in reading as well as in other

subjects, and children who experience difficulties early in school tend to experience continuation of these difficulties as they progress through school (Bayder, Brooks-Gunn, & Furstenberg, 1993; Butler, Marsh, Sheppard & Sheppard, 1985; Juel, 1988; McCoach, O'Connell, Reis, & Levitt, 2006). Even prior to formal schooling, much is happening in the way of literacy skill development via the interaction between life experience and language development. The notion of emergent literacy suggests that children do indeed enter kindergarten with diverse literacy skills that may have an important predictive relationship with later reading abilities (Lonigan, Burgess, & Anthony, 2000).

Initial data summaries from the Early Childhood Longitudinal Study-Kindergarten (ECLS-K) cohort indicate that some children do enter kindergarten with greater preparedness and readiness to learn relative to other children, perhaps putting them a step ahead of their peers for the important early grades at school (West, Denton, Germino-Hausken, 2000). ECLS-K studies have shown that children entering kindergarten from families with particular characteristics (living in a single parent household, living in a family that receives welfare payments or food stamps, having a

mother with less than a high school education, or having parents whose primary language is not English) tended to be at risk for low reading skills (Zill & West, 2001). Pre-kindergarten experiences related to family life, pre-school or daycare and personal characteristics (e.g., gender, persistence) may relate to children's initial proficiency in reading as well as their potential growth in skills and abilities across the kindergarten year and beyond. For example, girls typically enter kindergarten with slightly greater early literacy ability than boys. Child-focused predictors of success and failure in early reading are helpful for understanding how individual children may be at risk for reading difficulties. From a policy and practice perspective it is clearly desirable that teachers, school administrators, parents, and other stakeholders be aware of these individual factors related to entry-level proficiency as well as to growth in proficiency in order to develop curriculum and instructional practices that can promote achievement for all students relative to their kindergarten entry skills.

School and instructional characteristics have also been shown to be associated with student ability in early literacy, but it is not entirely clear how the differing educational experiences of children across schools (teacher and school effects) might affect growth in proficiency. The National Research Council (1998) reviewed predictors of success and failure in early reading at the neighborhood, school, and community level. In the continuing work using the ECLS-K, the effects of specific school-level variables on proficiency have been modeled separately across the four years of available data. These models included frequency of use of ability-grouping in kindergarten, principals' ratings on the success of various teacher instructional practice, attendance at public versus private schools, school socioeconomic status, and neighborhood climate including the presence of racial tensions, litter, drug/alcohol use in the neighborhood, and extent of crime (Levitt & O'Connell, 2002; McCoach, O'Connell, Levitt & Reis, 2006; O'Connell & Levitt, 2002).

Although instructional, organizational and neighborhood effects on children's entry-level reading ability and growth in reading are

critical to understanding how to create and implement effective school-supported teaching strategies, these effects have not been modeled here. Instead, as the purpose of this article is on the methodology for developing and interpreting multilevel models for ordinal responses, the focus herein is on the development and interpretation of two-level models investigating the effect of child-level characteristics on reading growth across four time points (fall and spring of kindergarten, and fall and spring of first grade); extensions to the three-level case are relatively straightforward.

Hierarchical Ordinal Regression Models

Explanatory models for ordinal outcome data collected during a single time frame have been previously reviewed by O'Connell (2000; 2006) and others (e.g., Agresti, 1989, 1990, 1996; Bender & Benner, 2000; Clogg & Shihadeh, 1994; Long, 1997; McCullagh, 1980). This work can be adapted to fit the needs of a hierarchical context. Wong and Mason (1985) and Hedeker and Mermelstein (1998) provided examples of extensions of models for dichotomous and ordinal outcomes for hierarchical data. In addition, the latest version of the HLM program (HLMv6.03; Raudenbush, Bryk, Cheong, and Congdon, 2004) includes options for modeling the cumulative odds for ordinal hierarchical data. An article by Plewis (2002) in the *Multilevel Modeling Newsletter* describes the fitting of multilevel ordinal data using MLwiN.

The most common ordinal outcome model is the regression-type proportional or cumulative odds (PO) model (Agresti, 1996; Armstrong & Sloan, 1989; Long, 1997; McCullagh, 1980). In this approach, the (log of the) odds of a response at or below each of the ordinal categories form the quantities of interest. For example, with a six-category ordinal outcome ($K=6$), the K-1 formulas shown in Table 2 would be used to compute the cumulative probabilities and consequently the cumulative odds (note: consistent with the ECLS-K categories, the possible outcomes are 0 through 5). The cumulative probabilities are the probabilities that the response for the i^{th} student nested within the j^{th} school (or, for longitudinal data, the i^{th} student at the t^{th} time point) is at or

Table 2. Cumulative Odds Model for $K=6$ ($K=0, 1, \dots, 5$), Where R_{ti} Represents the Proficiency Outcome (Response) for the i^{th} Student at the T^{th} Wave.

Category	Cumulative Probability	Cumulative Odds [Y'_{kti}]	Probability Comparison
$k=0$ (Proficiency 0)	$P(R_{ti} \leq 0)$	$\frac{P(R_{ti} = 0)}{P(R_{ti} > 0)}$	Proficiency 0 versus all levels above
$k=1$ (Proficiency 1)	$P(R_{ti} \leq 1)$	$\frac{P(R_{ti} \leq 1)}{P(R_{ti} > 1)}$	Proficiency 0 and 1 combined versus all levels above
$k=2$ (Proficiency 2)	$P(R_{ti} \leq 2)$	$\frac{P(R_{ti} \leq 2)}{P(R_{ti} > 2)}$	Proficiency 0,1,2 combined versus 3, 4, 5 combined
$k=3$ (Proficiency 3)	$P(R_{ti} \leq 3)$	$\frac{P(R_{ti} \leq 3)}{P(R_{ti} > 3)}$	Proficiency 0,1,2,3 combined versus 4,5 combined
$k=4$ (Proficiency 4)	$P(R_{ti} \leq 4)$	$\frac{P(R_{ti} \leq 4)}{P(R_{ti} > 4)}$	Proficiency 0,1,2,3,4 versus proficiency 5

below a given proficiency level. The odds is a ratio of the probability of an event occurring to the probability of an event not occurring. Accordingly, the cumulative odds [Y'_{kti}] represent the odds that any given response would be in at most category k (rather than beyond category k), for the i^{th} child at the t^{th} wave of data collection. From Table 2, it may be seen that the cumulative odds, in order, correspond to the probability of being in proficiency level 0 relative to all categories above it; the probability of being in proficiency level 0 or 1 relative to all above it; and so on until arriving at the probability of being in categories 0, 1, ...4 relative to being in category 5. The K^{th} or final cumulative probability would always be 1.0 (being at or below the last possible level), and its probability and associated odds are therefore not included in the table. It is common to refer to the value marking each of these binary comparisons as cutpoints or cumulative splits. For example, the cutpoint for the first comparison is 0 (proficiency level 0 versus above 0); the cutpoint for the second

comparison is 1 (proficiency 0 and 1 versus above 1), etc.

To better understand how the PO model works, imagine if the separate comparisons indicated in the last column of Table 2 were investigated using corresponding binary (hierarchical) logistic regressions at each of the associated cumulative splits. The simultaneous fitting of each of these separate $K-1$ (in this example, $K-1=5$) logistic models represents the overall PO approach. For this approach to be valid, a critical assumption must be made of the data. This assumption of proportionality states that the effects of the explanatory variables cannot be statistically different across these cutpoint comparisons. This is also called the cumulative odds assumption or the equal slopes assumption and can be restrictive but is the most common choice for ordinal regression models (Hedeker & Gibbons, 2006; O'Connell, 2006). For non-hierarchical data, the assumption of equal slopes can easily be tested within SAS or SPSS, for example. However, in a multi-level context direct tests of this assumption are not currently available. Interaction terms can be

used to test for non-proportionality of some or all of the predictors, or an ad hoc approach can be applied that investigates the consistency of slope estimates across the cumulative splits described in Table 2. Space does not allow for a demonstration of this assessment here; interested readers can find further discussion and examples in O'Connell, Goldstein, Rogers & Peng (in press), as well as in Hedeker, et al., 2006).

General Model: Students Nested Within Schools.

A brief description of the ordinal HGLM is presented for analyses focused at one point in time; in the next section it is expanded this to cover repeated ordinal measures. For the i^{th} student in the j^{th} school, the hierarchical proportional odds model is fit according to the following equations (Raudenbush & Bryk, 2002):

Student level:

$$\begin{aligned} \ln(Y'_{kij}) &= \ln\left(\frac{P(R_{ij} \leq k)}{P(R_{ij} > k)}\right) \\ &= \beta_{0j} + \sum_{q=1}^Q \beta_{qj} X_{qij} + \sum_{k=2}^{K-1} D_{kij} \delta_k \end{aligned} \quad (1)$$

School or Context level:

$$\beta_{qj} = \gamma_{q0} + \sum_{s=1}^{S_q} \gamma_{qs} W_{sj} + u_{qj} \quad (2)$$

where $[Y'_{kij}]$ represents the cumulative odds for each category k , with $k=1 \dots K-1$ levels of the ordinal response and $q = 1 \dots Q$ independent variables at the student level. For these models, the term on the left side of equation (1) is the log of the cumulative odds for each category k , and is referred to as the logit for the cumulative distribution. The terms on the right can be interpreted similar to any logistic regression model, with the β_{qj} representing the expected change in the logit for each one unit change in the q^{th} explanatory variable, X_{qj} . Its exponentiation will provide the estimate of the cumulative odds for that variable. However, an

important difference between an ordinal model and a binary logistic regression model is that with $K-1$ ways to characterize the cumulative odds, the slope parameters for each of the independent variables are restricted to be constant across all the separate possible cumulative splits derived according to the second column of Table 2. That is, the model assumes that the effect of any independent variable can be represented by a common cumulative odds ratio, $\exp(\beta)$; this is the assumption of proportional odds. If this assumption does not hold, then the PO model is not a plausible one for the data and less restrictive models should be investigated.

The collection of estimates at the far right of equation (1) are referred to as thresholds or delta coefficients, and they operate as deviations from the baseline intercept for each of the $K-1$ separate binary comparisons beyond the first, with β_{0j} as the baseline intercept (i.e., for the first cumulative comparison). D_{kij} is the indicator variable for each category beyond the first. In other words, each cumulative comparison has its own intercept, while the effects of the explanatory variables are assumed to be constant across each comparison.

Changes Over Time in an Ordinal Response.

When data are gathered over time, methodologies for the treatment of ordinal outcomes need to be combined with methods that address the multilevel nature of longitudinal data. As with other studies of growth, change was modeled in the logit as a linear effect. With only four time points, this approach is reasonable (Murray, 1998). At level one, the repeated measures are modeled over time, and at level two student characteristics are used to look at changes in intercepts or growth trajectories across children. For demonstration purposes, the focus is on the two-level model in this article rather than include a third level for modeling school effects. To investigate child-level variability in baseline (entry) proficiency and in the trajectory of change, we considered the following child-level variables: age at kindergarten entry, gender (boys = 1), attending half-day rather than full-day kindergarten (half-day = 1), previously attending any center-based

care (yes = 1), frequency with which parents read books to their child, socio-economic status, count of family risks, and a model-based approach was used to adjust for oversampling of Asian and Pacific Islanders (API) by including API (yes = 1) in all preliminary analyses. The general level one and level two models are provided below.

Time level:

$$\ln(Y'_{kti}) = \ln\left(\frac{P(R_{ti} \leq k)}{P(R_{ti} > k)}\right) = \pi_{0i} + \pi_{1i}T_{ti} + \sum_{k=2}^{K-1} D_{kti}\delta_k \quad (3)$$

Student level:

$$\pi_{qi} = \beta_{q0} + \sum_{s=1}^{S_q} \beta_{qs} X_{si} + u_{qi} \quad (4)$$

The last term in equation 3 is used to estimate the increasing intercepts for each of the underlying cumulative models, and is described in depth in the next section. Not unsurprisingly, these multilevel ordinal models were difficult to converge. Therefore, each independent variable was considered separately, consistent with Raudenbush and Bryk's (2002) suggestions regarding strategies for building complex multilevel models. Based on these preliminary analyses, two were selected that were found to be associated with proficiency in the simpler (univariate) models, and known to be associated with early literacy: gender and family-risk characteristics. The sum of the number of family-risk characteristics was used as a contextual variable in models predicting baseline proficiency (intercept) as well as change in proficiency (slope) over time. Once the contextual model was derived, age at kindergarten entry was included to control for age-effects. These few variables were selected to illustrate how contextual models may be developed and interpreted for longitudinal ordinal outcomes, and below an application of the PO model is presented in the prediction of change in reading proficiency across four years of data using the ECLS-K.

The following section describes the process by which the repeated measures and hierarchical ordinal models were developed.

Procedures

A sample of $n=3440$ children were selected from the ECLS-K. Since the primary purpose of this presentation is to illustrate the application of a multilevel approach to ordinal data, the sample was limited to children who did not change schools from kindergarten to first-grade, had four waves of data (a 30% subsample of the original data were included in a fall first-grade wave of data collection), were first-time kindergarteners only (no repeaters were included), and had no missing observations on the child-level (level-2) characteristics investigated for this study (gender, family-risk, and age at kindergarten entry). These criteria were applied to minimize complexity of the statistical design regarding number of data points available per child, convergence issues, and concerns regarding the impact of cross-classification of children changing schools during the study period. The resulting data set represents a sample of first-time kindergarteners assessed twice in kindergarten and twice in first grade.

HGLM, the non-linear counterpart to hierarchical linear modeling (HLM), was used to model the ordinal outcomes (Raudenbush and Bryk, 2002). The most general case of an HGLM for ordinal data assumes proportional odds across successive cumulative categories. Proportionality implies that the effect of an independent variable remains constant across the cumulative categories of the outcome variable.

In the PO model, the likelihood (or odds) of an observation falling into category k or below is assessed over time. Similar to the familiar logistic regression model, the PO analysis predicts a transformation of the odds, i.e., the logit, which is the log of the odds. A logit of zero corresponds to an odds of 1.0, which implies that there is no difference between the probability of being in a certain category (or below) and being above that category ($.5/.5 = 1.0$, $\ln(1.0) = 0$). A positive logit implies that the likelihood of being in lower categories is greater (e.g., $.7/.3 = 2.33$, $\log(2.33) = .847$); and a negative logit implies

that the likelihood of being *in higher* categories is greater (e.g., $.3/.7 = .429$, $\log(.429) = -.847$).

Using the HLM program, the desired data structure is similar to that in other multilevel analyses of longitudinal data. The level-one data file represents the repeated measures outcomes, and contains the proficiency score as an ordinal-level response variable for each child at each of the four time points. With 3440 children, there would be at most 4×3440 or 13,760 observations at level one. Some children were missing proficiency scores at some point during the four waves of data collection; thus there were 13,393 observations overall at level one for the analytic sample. The level-two data contains the child-level characteristics, including gender, the number of family risk characteristics, and age at kindergarten entry. Although three level ordinal models are now available in HLMv6.03 (Raudenbush et al., 2004), the models presented in this article illustrate the assessment of child-level effects (level two) on changes in proficiency over time (level one), and work is continuing on how these models might be extended to incorporate school effects as a third level.

Although many different models were investigated, only three are reported here. The final models include a random coefficients model (Table 4), with time in months as the sole predictor of proficiency (more precisely, as the predictor of the logits for the cumulative odds for proficiency). Next, a contextual model was developed using gender and the number of risk factors as the explanatory child-level variables at level 2 (Table 4). This contextual model was designed to illustrate how the effects of gender and the number of family risk factors may moderate the change in cumulative odds over time. These effects were included as predictors of the intercepts or baseline values and as predictors of the slope for time. This model was then adjusted to include age at kindergarten entry (grand mean centered) as a control variable for predicting both the intercept and the slope from level one, as well as deleted non-statistically significant predictors. Results of this final model are provided in Table 5.

The random coefficients analysis looks at the thresholds between (cumulative) adjacent proficiency levels and estimates the odds of a

person being in proficiency level k or below over time. If changes in proficiency can be reliably detected over time, the effect of time on the logit should be negative, so that the likelihood of being in higher categories increases over time. With a six-category outcome ($k = 0, 1, 2, 3, 4, 5$) and time measured in months from baseline ($t = 0, 8, 12, 20$), five models are fit simultaneously, as shown below.

Level one:

$$\begin{aligned}\ln(Y'_{0ti}) &= \pi_{0i} + \pi_{1i}(\text{time})_{ti} \\ \ln(Y'_{1ti}) &= \pi_{0i} + \pi_{1i}(\text{time})_{ti} + \delta_2 \\ \ln(Y'_{2ti}) &= \pi_{0i} + \pi_{1i}(\text{time})_{ti} + \delta_3 \\ \ln(Y'_{3ti}) &= \pi_{0i} + \pi_{1i}(\text{time})_{ti} + \delta_4 \\ \ln(Y'_{4ti}) &= \pi_{0i} + \pi_{1i}(\text{time})_{ti} + \delta_5\end{aligned}\quad (5)$$

Level two:

$$\begin{aligned}\pi_{0i} &= \beta_{00} + u_{0i} \\ \pi_{1i} &= \beta_{10} + u_{1i}\end{aligned}\quad (6)$$

In the collection of equations for level one, the terms on the left, $\ln(Y'_{3ti})$ for example, represents the log of the odds for being in category 3 or below (rather than beyond category 3), consistent with the approach described in Table 2.

The critical assumption of proportional odds implies that the effect of time is constant across the cumulative splits identified through the level one model. The level one effects, π_{0i} and π_{1i} , represent, respectively, the baseline estimates (at the first wave of data collection (entry into kindergarten)) for the log of the odds of being in category k or below, and the effect of time (slope) on these logits. These intercepts and slopes are free to vary from person to person. This variability is captured by the level two random effects, u_{0i} and u_{1i} , with variance components, respectively, of τ_{00} and τ_{11} ($\text{var}(u_{0i}) = \tau_{00}$ and $\text{var}(u_{1i}) = \tau_{11}$). The thresholds, δ_2 to δ_5 , represent the differences in the logit for each successive cumulative category relative to the

first logit; for example, in this sample the estimate at baseline for the log(odds) of being in category 3 or below would be $\beta_{00} + \delta_3$.

The first contextual model analysis considers the effects of gender (1=male) and the number of risk characteristics (0 through 4) on the baseline logits and the slopes. The level one model remains the same as (5), but now the level-two models used to describe the effects of gender and number of family risks on the intercept and slope are:

$$\begin{aligned}\pi_{0i} &= \beta_{00} + \beta_{01}(\text{gender})_i + \beta_{02}(\text{risknum})_i + u_{0i} \\ \pi_{1i} &= \beta_{10} + \beta_{11}(\text{gender})_i + \beta_{12}(\text{risknum})_i + u_{1i}\end{aligned}\quad (7)$$

Finally, in the second contextual model analysis age at kindergarten entry was included (grand mean centered) in the level two models for both the intercepts and the slopes. The gender effect was deleted from the model for time-slopes due to lack of statistically significant results for gender in a preliminary run.

Results

Table 1 contains the proportion of children classified into each literacy proficiency level from kindergarten through first grade. Table 3 shows the proportion of children making specific transitions in literacy proficiency across the four waves. Most children made a positive change across the kindergarten year; most did not change during the summer between kindergarten and first grade, but then children tended to increase again by one or two proficiency levels across the first grade year.

Results of the random coefficients model are provided in Table 4. These results show that overall across children, the expected log odds of being in proficiency level 0 at baseline is negative ($\beta_{00} = -1.73$, $p < .01$), which implies that at baseline it is more likely for a child to be at least in level 1 or higher. There is a statistically significant linear trend in the cumulative logits for time ($\beta_{10} = -.41$, $p < .01$), indicating that as a child progresses in school, the likelihood of being at or below category 0 decreases (stated differently, the negative slope

for time implies that the probability of being beyond category 0 is increasing with time). This is consistent with what we see in Tables 1 and 3. At baseline, children are more likely to be beyond category 0, and this likelihood increases over time. The model estimates are predicted logits. To transform to odds and then to probabilities, odds = $\exp(\beta)$, and probability = odds/(1 + odds) are used. For this example, the odds at baseline of a child being in proficiency level 0 or below is $\exp(-1.73) = .1773$; this corresponds to a probability of $.1773/(1+.1773) = .15$. For this random coefficients model containing no child-level predictor variables, 15% of children would be predicted to be at or below category 0 at baseline. For the predicted logit of being at or below category 0 at time 2 (8 months), the model estimates the logit as: $-1.73 + (-.41)(8) = -5.01$. Thus, at the end of kindergarten, the model predicts that the odds of being in category 0 or below is decreased ($\exp(-5.01) = .0067$), and the associated probability of being at or below proficiency category 0 at the end of kindergarten is .007, or .7%.

To examine the model predictions at other splits in the cumulative hierarchy, for example, model predictions for being at or below category three at baseline, δ_4 is used in addition to the baseline intercept and the slope (see equation 5). For this data, the new intercept, or threshold, becomes $\beta_{00} + \delta_4 = -1.73 + 7.86 = 6.13$. Accordingly, the probability of a child being at or below proficiency level 3 at baseline is .998 or 99.8%. At time 2 (8 months), the predicted logit is $\beta_{00} + \beta_{10}*(8 \text{ months}) + \delta_4 = -1.73 + (-.41)*(8) + 7.86 = 2.85$, where $\exp(2.85) = 17.29$, and the predicted probability of being at or below proficiency category three at the end of kindergarten is .945, or 94.5%. These predictions, based on a model with no explanatory variables, are reasonably consistent with the data in Table 1.

Finally, reviewing the variance components for the model, it may be seen that considerable variation remains in the intercepts, $\tau_{00} = 8.35$, $p < .01$, as well as in the slopes, $\tau_{11} = .003$, $p < .01$.

The first contextual model (Table 4) describes the effect of gender and the number of family risk factors on the baseline logits and the

Table 3. Change in Proficiency Across the Kindergarten (K1 & K2) and First Grade (FG1 & FG2) Years.

<i>Raw Change in Proficiency</i>	K2-K1	FG1-K2	FG2-FG1
-3	0.0	0.1	0.0
-2	0.3	0.8	0.1
-1	1.7	7.7	0.7
0	21.3	46.5	18.5
1	33.6	32.6	40.9
2	27.5	8.3	29.9
3	9.0	1.0	7.1
4	0.5	0.0	0.8
5	0.01	0.0	0.0

Table 4. Multilevel Ordinal Models for Prediction of Proficiency Using Four Waves Of ECLS-K; Ivs are Gender and Number of Family Risks.

Effect	Coeff. (s.e.)	t (df)	Coeff. (s.e.)	t (df)
Intercept (π_{0i})				
β_{00}	-1.73 (.068)	-25.41 ** (3439)	-2.56 (.097)	-26.48 ** (3437)
β_{01} (gender (M=1))			0.62 (.114)	5.48 ** (3437)
β_{02} (number of risks)			1.07 (.078)	13.75 ** (3437)
Time Slope (π_{1i})				
β_{10}	-.41 (.004)	-98.46 ** (3439)	-.41 (.005)	-77.45 ** (3437)
β_{11} (gender (M=1))			-.001 (.005)	-0.21 (3437)
β_{12} (number of risks)			-.01 (.003)	-2.18 * (3437)
For Thresholds:				
δ_2	2.75 (.053)	51.71 ** (13387)	2.78 (.054)	51.58 ** (13383)
δ_3	4.69 (.060)	77.28 ** (13387)	4.71 (.061)	77.03 ** (13383)
δ_4	7.86 (.077)	101.46 ** (13387)	7.88 (.079)	101.17 ** (13383)
δ_5	10.32 (.091)	112.88 ** (13387)	10.35 (.092)	112.61 ** (13383)

Note: * $p < .05$; ** $p < .01$

	Random Coefficients Model			Contextual Model		
<i>Random Effects</i>	<i>Variance</i>	<i>df</i>	<i>Chi-square</i>	<i>Variance</i>	<i>df</i>	<i>Chi-square</i>
Variance in Base- K1 (τ_{00})	8.346	3391	10350.03 **	7.75	3389	10025.82 **
Variance in Time slope (τ_{11})	.003	3392	3615.27 **	.003	3392	3626.38 **

Note: * $p < .05$; ** $p < .01$

slopes for time. Gender has a statistically significant effect on the baseline logits ($\beta_{01} = .62$, $p < .01$). Being a boy tends to increase the logit, making the likelihood of being in higher proficiency categories lower for boys relative to girls. The number of risk factors also has a statistically significant effect on the baseline logit ($\beta_{02} = 1.07$, $p < .01$). Because the logit is positive, it may be seen that as the number of family-risk characteristics increases, the likelihood that a child would be in lower proficiency categories (i.e., at or below any category k) increases, relative to a child with fewer risks.

Attention is now turned to interpretation of the effects of gender and the number of risk characteristics on the slope for time. $\beta_{10} = -.41$ may be interpreted as the estimated slope for girls with out any family risks. Controlling for the number of risk factors, gender has no effect on the slopes ($\beta_{11} = -.001$, $p > .05$); thus gender does not affect the rate of change in proficiency. The number of risk factors does impact rate of change ($\beta_{12} = -.01$, $p < .05$). On the surface this would suggest that the likelihood is greater that a child with more risk characteristics improves over time even beyond that of a child with fewer risks. However, on closer inspection of the model predictions – particularly in terms of predicted probabilities across the four time points of being at or below any category k – it is seen that children with increased family risks tend not to improve as readily over time as their non-risk peers.

This complexity of ordinal model interpretation can be overcome by estimating outcomes for discrete cases of children. For example, substituting into the prediction model, a female child (gender = 0) from a family with 0 risk characteristics would be expected to have a predicted logit for the first cumulative comparison (proficiency level 0 or below) at baseline (time=0) of -2.56, which corresponds to a cumulative odds of $\exp(-2.56) = .08$ and cumulative probability of being at or below proficiency category 0 of .072, or 7.2%. For a girl at baseline from a family with 1 risk characteristic, the predicted logit is -1.49, corresponding to a cumulative odds of .23, and a probability of .187 or 18.7%. This is a large

proportion of girls estimated to be at or below proficiency level 0 (rather than beyond category 0), given the addition of just one risk factor. In fact, the odds ratio for the variable number of risks is $\exp(1.07) = 2.92$. The model suggests that, at baseline, the odds of being at or below any category increases by a factor of 2.92 for every one unit increase in a child's number of family risks. Baseline is the simplest case for making predictions; moving to time 2 at 8 months, the model estimates now need to include gender and family risk effects on the effect of time, but the process of estimating outcomes is similar to the process demonstrated above. Based on the parameter estimates from the model, probability predictions for being at or below proficiency category 0 at time 2 (8 months) are .29%, 1.56%, and 13.24% for girls with 0, 1, and 4 family risk factors, respectively.

The variance estimates for this contextual model indicates that variability in the baseline logits and in the time slopes continues to be statistically different from zero, which suggests that additional variables may be useful in understanding proficiency growth (initial status and rate of change). Table 5 provides the model estimates for an adjusted contextual model. In this modified model, age at kindergarten entry (grand-mean centered) is included in the models, and gender is removed from the level 2 models for the slope due to its lack of contribution to that model. The predictions for baseline or initial proficiency remain fairly similar to the contextual model estimates in Table 4. All three predictors contribute to the prediction of the baseline logits, with age at kindergarten entry having a negative effect ($\beta_{03} = -.13$, $p < .01$). This implies that for older children at kindergarten entry, the probability of being in higher categories of proficiency increases. After adjusting for age at kindergarten entry, the number of family risks is still a statistically significant predictor of the trajectory (slope) in the proficiency logits from baseline through the end of first grade ($\beta_{11} = -.01$, $p < .05$), with little change in magnitude from the previous model. In addition, age at kindergarten entry is positively related to the time slopes ($\beta_{12} = .002$, $p < .01$); based on model predictions, older children tend to improve over time more readily than their younger peers.

Table 5. Multilevel Ordinal Model for Prediction of Proficiency Controlling for Kindergarten Entry Age; Ivs are Gender, Number of Family Risks, and Age at Kindergarten Entry.

Contextual Model 2			
Effect	Coeff (s.e.)	t(df)	p
Intercept (π_{0i})			
β_{00}	-2.58 (.089)	-28.91 ** (3436)	.000
β_{01} (gender (M=1))	.67 (.089)	7.514 ** (3436)	.000
β_{02} (number of risks)	1.05 (.077)	13.65 ** (3436)	.000
β_{03} (age at K entry)	-.13 (.014)	-9.09 ** (3436)	.000
Time Slope (π_{1i})			
β_{10}	-.41 (.005)	-90.98 ** (3437)	.000
β_{11} (number of risks)	-.01 (.004)	-2.08 * (3437)	.037
β_{12} (age at K entry)	.002 (.001)	3.72 ** (3437)	.000
For Thresholds:			
δ_2	2.76 (.054)	51.54 ** (13382)	.000
δ_3	4.71 (.061)	76.99 ** (13382)	.000
δ_4	7.88 (.078)	101.10 ** (13382)	.000
δ_5	10.35 (.092)	112.53 ** (13382)	.000

Note: * $p < .05$; ** $p < .01$

Random Components			
Random Effects	Variance	df	Chi-square (p)
Variance in Base- K1 (τ_{00})	7.47	3388	9818.72 (p=.000) **
Variance in Time slope (τ_{11})	.003	3392	3611.19 (p=.005) **

Note: * $p < .05$; ** $p < .01$

Despite the addition of entry age to both the intercept and slope models, however, significant variability remains in the initial status and the growth trajectories across children ($\tau_{00} = 7.47$, $p < .01$; $\tau_{11} = .003$, $p < .01$).

Table 6 provides predictions based on the random coefficients model and the final contextual model for the probability of a child being at or below proficiency level 3 across all four waves, and contains the actual proportion of children for comparison. Probabilities decline over time, as expected, because it is hoped that children are moving beyond category three by the end of first grade. Among the notable comparisons possible based on this simple table is the predicted probability at the end of first grade for a hypothetical male child of average age with no family risk characteristics (prob =

.097) relative to the predicted probability for a male average-age child with four family risk characteristics (prob = .763). Recall that these probabilities are cumulative, and represent the probabilities of being at or below proficiency category 3. These differences are quite large. Further, at the end of first grade, the likelihood that boys do not achieve proficiency in the highest categories in comparison to girls' likelihood is large as well. These predicted probabilities help to make clear the utility of hierarchical ordinal models for understanding effects of child-demographic variables on growth in proficiency for early literacy skills in a way that the basic interpretation of parameter estimates from the models in Tables 5 and 6 cannot easily do.

Table 6. Probability Predictions (at or Below Category 3) for Each Time Point Based on Models in Tables 5 And 6 (Age is Grand Mean Centered).

	K-entry (0 months)	K-completion (8 months)	FG-entry (12 months)	FG-completion (20 months)
At or below Category 3: Actual Data	.967	.835	.719	.161
Random Coefficients Model	.998	.945	.770	.112
Contextual Model 2				
Female				
Average age	.995	.883	.594	.052
Family Risks = 0				
Female				
Average age	.999	.997	.984	.622
Family Risks = 4				
Male				
Average age	.997	.936	.741	.097
Family Risks = 0				
Male				
Average age	.999	.997	.992	.763
Family Risks = 4				

Conclusion

These examples illustrate the application and interpretation of ordinal regression models to longitudinal data. Given that ordinal responses are best analyzed using ordinal methods, it is important that educational statisticians add these techniques to their toolkit. The ECLS provides a rich data set for investigating many challenging statistical issues. However, some issues need more clarity before these models can be effectively applied.

In this article, the focus has been on the cumulative odds or proportional odds model; however, this assumption may not always hold. Other options are routinely available for researchers dealing with single-level ordinal response data such as the continuation ratio model or non-proportional odds models (Agresti, 1989, 1990; Armstrong & Sloan, 1989; Cox, 1972; Greenland, 1994; Goodman, 1983;

McCullagh, 1980; O'Connell, 2000, 2006). In addition, multilevel software programs are somewhat limited in terms of ordinal model methodology, and the default model may often be based on the (untested) assumption of proportional odds. Ultimately, the choice for what approach to take should be guided by theory or an a-priori expectation of which approach would be most appropriate for a given situation (Agresti, 1990; Armstrong & Sloan, 1989). It is hoped that this article has helped to familiarize applied researchers with some of these issues as well as with the interpretation of multilevel ordinal models. Yet, further work is necessary to clarify model fitting for multilevel ordinal data when the assumption of proportional odds is violated, and for when three-level models might offer the best structure for the research data being analyzed.

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Estimation of Risk for Developing Cardiac Problem in Patients of Type 2 Diabetes as Obtained by the Technique of Density Estimation

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High levels of cholesterol and triglyceride are known to be strongly associated with development of cardiac problem in patients of type 2 diabetes. In a hospital-based study, patients showing ECG positive were compared with those who were not. The observations on cholesterol and triglyceride were considered for estimation of risk for developing the cardiac problem. The technique of density estimation employing Epanechnikov kernel was used for estimating bivariate probability density functions with respect to observations on cholesterol and triglyceride of the two groups. Using the odds form of Bayes' rule, the estimates of posterior odds were computed.

Key words: Density estimation, kernel, logistic regression, probability density function.

Introduction

The technique of Density Estimation is a non-parametric approach and involves no assumptions as it deals directly with the experimental data. The method of density estimation describes the probability distribution of people with respect to the parameter under investigation. This technique has found favour with many applied statisticians in the past. Scott, Gotto, Cole, and Gorry (1978) used density

estimation for assessing plasma lipids as collateral risk factors in coronary artery disease. Bithell (1990) gave an application of this technique in Geographical Epidemiology. Mukherjee, Kumar, Mittal, and Saxena (2002) used density estimation for estimating risk of developing goiter in an endemic area. Silverman (1986) provided an excellent account of various approaches to Density Estimation in his book.

High levels of cholesterol and triglyceride are known to be strongly associated with development of cardiac problem in patients of type 2 diabetes. However, the extent of risk posed by elevated levels of these two risk factors in patients of type 2 diabetes has not been studied extensively. The present article describes an alternative methodology whereby risk of developing cardiac problem in patients of type 2 diabetes can be estimated using cholesterol and triglyceride as risk factors.

Methodology

In a hospital-based study conducted by Indian Council of Medical Research in 1989-92, 4637 patients of Non Insulin Dependent Diabetes Mellitus (NIDDM) also known as Type2 Diabetes were enrolled. Various bio-chemical investigations and electrocardiogram (ECG) were carried out at regular intervals. The 311

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patients showing ECG positive and thereby indicating coronary artery disease (CAD +), formed the first group. The remaining patients numbering 4326 formed the second group. The Epanechnikov kernel, which is known to have 100% efficiency in terms of mean integrated square error (Silverman, 1986), was employed in the technique of density estimation for estimating probability density functions of the patients falling in the two groups with respect to their cholesterol and triglyceride levels. Using the odds form of Bayes' rule, the estimate of odds ratio (OR) was obtained. A simulation study was undertaken and 100 estimates of OR were generated using the approach of density estimation giving a mean estimated odds ratio and an estimate of standard deviation.

Let the number of patients in the first group be denoted by N_{CAD+} and that in the second group by N_{NID} . Let x and y in general denote the observations on cholesterol and triglyceride of the patients with x_i and y_i being the observations on the i th patient. Then the bivariate kernel density estimator for the first group is given by

$$\begin{aligned} f_{CAD+} &\equiv f_{CAD+}(x, y) \\ &= \frac{1}{N_{CAD+} h_x h_y} \sum_{i=1}^{N_{CAD+}} K\left(\frac{x - x_i}{h_x}\right) K\left(\frac{y - y_i}{h_y}\right) \end{aligned}$$

the quantities h_x and h_y are called bandwidths of the function f_{CAD+} and are appropriately chosen.

The function $K(z)$ which is known as Epanechnikov kernel, is defined as follows:

$$K(z) = \begin{cases} \frac{3}{4} \left(1 - \frac{1}{5} z^2\right) / \sqrt{5}, & \text{if } |z| \leq \sqrt{5} \\ 0, & \text{otherwise} \end{cases}$$

Similarly, the Epanechnikov kernel density estimator for the other group namely, $f_{NID} \equiv f_{NID}(x, y)$ can also be worked out.

The Likelihood Ratio (LR) will then be given by

$$LR = \frac{f_{CAD+}}{f_{NID}}.$$

Further, the odds form of Bayes' rule states that

$$O'(D) = O(D) * LR,$$

where $O'(D)$ is the posterior odds and $O(D)$

is prior odds and is given as $O(D) = \frac{N_{CAD+}}{N_{NID}}$.

For the present set of data, $N_{CAD+} = 311$ and $N_{NID} = 4326$. For estimating f_{CAD+} , the optimum values of h_x and h_y were obtained by objectively starting the process of smoothing with $h_x = h_y = 5$ giving an increment of 5 until $h_x = h_y = 35$. Thereafter, the process of smoothing was continued by giving a unit increment. The estimates of density stabilized with values of h_x and h_y at 40, 41, 42, 43 to five decimal places. Hence, $h_x = h_y = 40$ was accepted as an optimum value of h_x and h_y .

Similarly, the values of h_x and h_y for estimating f_{NID} were also obtained to be 40 each. The estimate of probability density function for the first group i.e., f_{CAD+} is as depicted in Figure 1.

Computation of OR

Consider the following transformation

$$P = \frac{1}{1 + e^{-Y}}, \text{ where}$$

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_k X_k + \varepsilon.$$

It can be shown that

Fig.1. Bivariate Probability Density Function of patients with CAD+ at different values of Cholesterol and Triglyceride using Epanechnikov Kernel

Results

$$\log\left(\frac{P}{1-P}\right)=Y$$

or

$$\log\left(\frac{P}{1-P}\right)=\beta_0+\beta_1X_1+\beta_2X_2+\dots+\beta_kX_k+\varepsilon$$

Thus β_i gives average quantum of change in log(odds) per unit change in X_i , $i=1,2,\dots,k$ and e^{β_i} gives the odds ratio with respect to X_i keeping other predictors at constant levels.

Keeping cholesterol fixed at 250 and varying the value of triglyceride from 209 to 254, the posterior odds at three pairs of values of cholesterol and triglyceride viz., (250,209), (250,254) and (250, 260) were worked out to be respectively 0.0629, 0.08047 and 0.08549. Thus, keeping cholesterol fixed at 250 and increasing triglyceride by a margin of 45 and 51 units from 209, led to respectively 1.28 and 1.34 times increase in odds for developing a cardiac problem. Further, considering first two of the above three pairs of values of cholesterol and triglyceride, the following would be obtained:

$$\beta_Y = \frac{\log(0.08047) - \log(0.0629)}{45}$$

or

$$\beta_Y = 0.005474$$

Therefore OR is given by $e^{\beta_Y} = 1.005489$. Drawing a simple random sample of 100 consecutive pairs of values of cholesterol and triglyceride and using the above methodology, 100 estimates of OR were obtained with a mean value of OR as 1.0025 and S.D. of 0.0027 giving 95% C.I. as {1.0020, 1.0031}. The OR as estimated by Logistic Regression model was 1.0029 with a 95% C.I. of {0.9984, 1.0074}.

Conclusion

It is seen that with the technique of density estimation employing Epanechnikov kernel, it is possible to obtain an estimate of the probability density function of the patients of type 2 diabetes falling in the two groups with respect to their cholesterol and triglyceride levels. It has also been demonstrated in the present article, how the posterior odds vary with increasing levels of triglyceride keeping cholesterol at a constant high level, which ultimately led to an estimate of odds ratio (Table 1).

From table 1, it is clear that the estimate of odds ratio as obtained by the method of density estimation is in close proximity to the estimate as obtained by the method of logistic regression. Thus, the risk of developing a cardiac problem can also be alternatively estimated by using the technique of density estimation.

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Table 1. Estimates of Odds Ratio as obtained by the application of Epanechnikov kernel in Density Estimation and Logistic Regression

Method	Odds Ratio	95% C.I.
Logistic Model	1.0029	0.9984-1.0074
<u>Density Estimation:</u> Epanechnikov Kernel	1.0025	1.002-1.0031

Multinomial Logistic Regression Model for the Inferential Risk Age Groups for Infection Caused by *Vibrio cholerae* in Kolkata, India

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Multinomial Logistic Regression (MLR) modeling is an effective approach for categorical outcomes, as compared with discriminant function analysis and log-linear models for profiling individual category of dependent variable. To explore the yearly change of inferential age groups of acute diarrhoeal patients infected with *Vibrio cholerae* during 1996-2000 by MLR, systematic sampling data were generated from an active surveillance study. Among 1330 *V.cholerae* infected cases, the predominant age category was up to 5 years accounting for 478 (30.5%) cases. The independent variables *V.cholerae* O1 ($p < 0.001$) and non-O1 and non-O139 ($p < 0.001$) were significantly associated with children under 5 years age group. *V.cholerae* O139 inferential age group was > 40 years. The infection mediated by *V.cholerae* O1 had significantly decreasing trend Exp(B) year wise from 1996 to 2000 ($p < 0.001$, $p < 0.001$, $p < 0.001$, $p < 0.001$ and $p < 0.001$, respectively). MLR model showed that up to 5 year's age children are more vulnerable to infection caused by *V.cholerae* O1.

Key words: MLR, *Vibrio cholerae*, exp(B), explanatory, dependent, categorical

Introduction

Study design and data sources

Cholera is an epidemic disease in developing countries which has been the focus of intensive research for many years. This water borne disease is typified by severe watery diarrhea, vomiting and dehydration of the different serogroups of *V. cholerae*, serogroups O1, O139 and non-O1, non-O139 colonize in the small intestine and produce enterotoxin

responsible for watery diarrhea. Until 19th century, cholera was confined in the Indian sub-continent (Epstein, 1993; Islam et al., 1994) and from this region, it has spread to many parts of the world causing seven pandemics. (Codeco, 2001; Faruque et al., 1998; Banerjee & Hazra, 1974). In 1992, a newly described non-O1 serogroup of *V. cholerae* designated O139 Bengal, caused unusual cholera outbreaks in India (Ramamurthy et al., 1993). Total eradication of this organism is very unlikely because of its propensity and acquaintance in the coastal ecosystem (Sack et al., 2004). In cholera endemic regions, severe cholera affects one in every 10-50 individuals, the highest attack rates of disease being in children of two to four years age (Cash et al., 1974). About 5.5 millions cases of cholera occur annually in Asia and Africa, 8% severe enough to be hospitalized, and 20% of the severe cases resulting in deaths, totaling approximately 120000/year (Mahalanabis et al., 1992; Noah & Mahony, 1998).

Classification and prediction are the more common practices in applied medical research. Mathematical model is widely used for prediction of disease outcomes. Discriminate analysis is mainly used for classification and

The authors thank all the scientists and Research Fellows of National Institute of Cholera and Enteric Diseases, Kolkata for helping to generate the laboratory data, and Infectious Diseases Hospitals, Kolkata, for taking part in the active surveillance program. Comments or question about this article should be directed to the first author at: rajenk20@yahoo.com or rajenk20@hotmail.com, or Division of Epidemiology, National Institute of Cholera & Enteric Diseases, P-33, Scheme-XM, CIT.Road, Beliaghata, Kolkata 700 010, West Bengal, India.

logistic regression and the dependent variable is binary or strict with two category. In a few studies, the relative predictivity of these methods were employed as an outcome variable that had more than two groups with unequal sizes. These models have been investigated when reducing bias by promoting the efficiency of the parameter estimation when the dependent variable has more than two groups. In this study Multivariate Logistic regression model was employed to identify inferential age group at greatest risk for diarrhea.

Materials And Methods

During 1996 to 2000, systematic sampling was done from every 5th hospitalized diarrhea patients attending the Infectious Diseases Hospital, Kolkata, India in two randomly selected days of the week. Samples were collected in the form of stool or rectal swab and sent to the laboratory for the isolation of common enteric pathogens within 3 hrs. The enteric pathogens were isolated and identified by standard laboratory methods (World Health Organization, 1987; Garg et al., 2000).

Data Management

The pre-designed proforma describing case demographics, symptoms etc. were checked manually and sent to data management center. The data were entered into pre-designed format of the proforma in EPI-info (6.0 version) with inbuilt entry validation checking facilitated program, by two trained data entry professionals in two separate computers. Data were randomly checked and matched to derive consistency and validity. The edited data was exported to SPSS version 4.0, and the final analysis was done using the SPSS.10. In this study, the inferential age groups was explored for three different serogroups of *V.cholerae*, O1, O139 and non-O1, non-O139 among culture positive cases by MLR and also to know the year wise changing pattern by parametric estimation through Odds Ratio(OR) ((Exp(B)). The proposed objective of the study was to determine the likelihood of age to have infection by *V.cholerae* O1, O139 and non-O1, non-O139, serogroups.

The age groups were classified into 6 categories viz. up to 5 years , above 5-10 years,

above 10-20 years, above 20-30 years, above 30-40 years and more than 40 years and were coded as 1-6, respectively. The relationship between the risk dependent variable and each of the three categorical explanatory variables in the serogroup are shown in Table 1. Infection by any serogroup of *V.cholerae* was classified in numbers as 1 for organism present and 2 for its absence.

To describe categorical dependent variables and one or more categorical or dichotomous or continuous explanatory variables, Logistic regression was found suitable if dependent is strict with two categories. The conceptualized objective in this study was to employ MLR which may be more efficient and reliable to obtain the probability estimation of concerned patient population. In addition, MLR explores estimation of the net effects of a set of explanatory variables on the dependent variable (Cabrera, 1994; Demaris, 1992; Menard, 2000).

Data Analysis

The MLR model involves categorical dependent variable (more than two) Y. e.g. six categories of age group and 3 explanatory (*V.cholerae* serogroups) variables x_1 x_2 and x_3 ($x_1=O1$, $x_2=O139$ and $x_3=non-O1$, $non-O139$).

Let P_1 = the probability of up to 5 years age group at risk ($Y=1$), P_2 = the probability of above 5-10 years age group at risk ($Y=2$) P_3 = the probability of above 10-20 years age group at risk ($Y=3$), P_4 = the probability of above 20-30 years age group at risk ($Y=4$), P_5 = the probability of above 30-40 years age group at risk ($Y=5$) and P_6 = the probability of more than 40 years age group at risk ($Y=6$). The modality of MLR relates to the log of odds (or logit) of Y to the explanatory variable x_1 in linear form as

$$P_i = A + P x_i$$

$$\text{Probit}(P_i) = \text{intercept} + R. \text{ co-eff}(x_i) \quad (1)$$

The model explores

$$\text{Prob}(y=j) = \frac{e^{\sum_{jk} \beta_{jk} x_k}}{1 + \sum e^{\sum_{jk} \beta_{jk} x_k}} \quad (2)$$

Table 1: Distribution of *V.cholerae* O1, O139 and non-O1 , non-O139 among different age groups of patients during 1996-2000.

Age groups (in years)	<i>V.cholerae</i> serogroup	1996		1997		1998		1999		2000	
		No	%	No	%	No	%	No	%	No	%
Upto 5	(n=301) O1	70	23.3	43	14.3	93	30.9	54	17.9	41	13.6
	(n=55) O139	14	25.4	16	29.1	7	12.7	15	27.3	3	5.5
	(n=109) Non-O1 , Non-O139	8	7.3	13	11.9	29	26.6	38	34.9	21	19.3
>5-10	(n=90) O1	18	20.0	12	13.3	34	37.8	15	16.7	11	12.2
	(n=27) O139	6	22.2	12	44.4	2	7.5	3	11.1	4	14.8
	(n=14) Non-O1, Non-O139	2	14.3	3	21.4	5	5.7	2	14.3	2	14.3
>10-20	(n=87) O1	19	21.8	6	6.9	29	33.3	21	24.2	12	13.8
	(n=52) O139	8	15.4	24	46.1	6	11.5	11	21.2	3	5.8
	(n=39) Non-O1, Non-O139	6	15.4	15	38.4	12	30.8	3	7.7	3	7.7
>20-30	(n=100) O1	20	20.0	12	12.0	44	44.0	13	13.0	11	11.0
	(n=87) O139	20	23.0	29	33.3	18	20.7	18	20.7	2	2.3
	(n=59) Non-O1, Non-O139	15	25.4	18	30.5	14	23.7	7	11.9	5	8.5
>30-40	(n=40) O1	8	20.0	9	22.5	12	30.0	8	20.0	3	7.5
	(n=51) O139	11	21.6	19	37.2	8	15.7	7	13.7	6	11.8
	(n=29) Non-O1, Non-O139	7	24.1	6	20.7	7	24.1	5	17.2	4	13.8
>40	(n=63) O1	12	19.1	6	9.5	24	38.1	14	22.2	7	11.1
	(n=84) O139	20	23.8	25	29.8	18	21.4	16	19.0	5	6.0
	(n=43) Non-O1, Non-O139	7	16.3	9	20.9	13	30.2	11	25.6	3	7.0

$$P_{ij} = \log \frac{P(\Delta_i)}{P(\Delta_6)} = \text{intercept} + \text{parameter}(V_k) \quad (3)$$

$i, j, k > 0$ i = age1 to age5, j = 1996 to 2000, k = O1, O139 and non O1, non O139, V = *V. cholerae* and Δ_6 = age6.

The intercept (initial level) terms are simple logit for positive *V. cholerae* O1. The first intercept is the log of ratio of the probability of a positive in up to 5 years to the probability of a positive in > 40 years. Hence, co-efficient for positive cases reveal the relationship between the logits and *V. cholerae* O1. Because the co-efficient is positive and significantly different from 0 that *V. cholerae* O1 positives are more likely associated with upto5 years age group as compared to >40 years age group.

Result

During 1996-2000, a total of 1330 *V. cholerae* stool culture positive cases formed the test set in this analysis, of which 681 (51.20 %), 356 (26.8 %) and 293 (22%) were positive for *V. cholerae* O1, O139 and non-O1, non-O139 respectively. The age was coded as 6 categories in which 465 (35.0%), 131 (9.8%), 178 (13.4%), 246 (18.5%) 120 (9.0%) and 190 (14.3%) were in the age groups upto 5 years, >5-10 years, >10-20 years, >20-30 years, >30-40 years, >40 years respectively. The analysis was made to explore inferential age group. The predominant infected age category was upto 5 years age group. Overall, explanatory variables *V. cholerae* O1 ($p < 0.001$, OR=3.48, 95% confidence interval (CI): 2.44, 4.90) was highly significant with children under five years of age. *V. cholerae* O139 was detected for more than 40 years age group ($p < 0.001$, OR=2.99, 95% CI: 1.29, 4.98) and under five years old children were associated with *V. cholerae* non-O1, non-O139 ($p < 0.001$, OR=2.50, 95% CI: 1.38, 4.55). As per the above equation 3 the result shows

$$\text{Predicted logit (Y1} \leq 5 \text{ years)} = .302 + 1.247 \text{ (} V. \text{ cholerae O1)} \quad (4a)$$

$$\text{Predicted logit (Y1} \leq 5 \text{ years)} = 1.335 + (-)1.550 \text{ (} V. \text{ cholerae O139)} \quad (4b)$$

$$\text{Predicted logit (Y1} \leq 5 \text{ years)} = .898 + (-).055 \text{ (} V. \text{ cholerae non-O1, non-O139)} \quad (4c)$$

Similarly, a prediction can be made for other age groups.

Overall, the chi-square test of proportional odds assumption was significant (degrees of freedom(df) = 5: $p < 0.001$), indicating that the model is fit. Table 2 depicts only the predominantly affected age group with respective *V. cholerae* serogroup. Data on non-significant age group were not shown to avoid multiple tables. The explanatory variables are compared individually with dependent variable age. According to MLR models, the log of the Odds of an up to 5 years age group shows risk of infection positively related to the serogroup *V. cholerae* O1, in all years (Table 2). It was also shown a decreasing slope (rate of change) during the consecutive years. The respective years of OR for *V. cholerae* O139 has increased in 1998 and declined, though there was no significant association in all years with its inferential age group >40 years. In the case of *V. cholerae* non-O1, non-O139, year wise significance was not detected but the more vulnerable age group was <5 years.

Conclusion

Generally, Logistic Regression analysis (LR) is a common statistical technique which could be used to predict the likelihood of a categorical or binary or dichotomous outcome variables. In epidemiological studies, the dependent variable is presence or absence of a disease. The LR model has been applied in social science (Janik & Kravitz, 1994). Most of the microbiological laboratory generated data are not being utilized with proper statistical techniques owing to lack of appropriate guidelines for application. This study exploited the usefulness of MLR as a tool in statistical modeling and detecting the inferential risk age groups for *V. cholerae* mediated infection for 1330 culture positive cases from 1996-2000.

Table 2. Multinomial Logistic Regression Models exploring significant risk age group of cholera infection during 1996-2000.

<i>V.cholerae</i> (serogroup)	Years	Age group category(in year)						5 years age group (reference group (>40))		
		5	>5- 10	>10- 20	>20- 30	>30- 40	>40	P-values	OR	95%CI
O1	1996	70	18	19	20	8	12	<0.001	5.21	2.30, 11.78
	1997	43	12	6	12	9	6	0.002	4.43	1.70, 11.51
	1998	93	34	29	44	12	24	0.001	2.96	1.50, 05.64
	1999	54	15	21	13	8	14	0.007	2.89	1.33, 06.25
	2000	41	11	12	11	3	7	0.019	4.26	1.27, 14.33
>40 years age group (reference group (>5-10))										
O139	1996	14	6	8	20	11	20	0.027	3.52	1.15, 10.75
	1997	16	12	15	29	19	25	0.147	2.08	.77, 5.62
	1998	7	2	6	18	8	18	0.005	9.00	1.95, 41.50
	1999	15	3	11	18	7	16	0.067	3.63	.91, 14.39
	2000	3	4	3	2	6	5	0.540	1.62	.31, 7.67

The MLR requires the dependent variables to be non-metric, dichotomous, nominal and ordinal, satisfy the level of measurement and independent variable to be metric or dichotomous. The minimum number of cases per independent variable is 10 using a guideline provided by Homen and Lameshow (2000), in which the MLR predicts and provides a set of co-efficient for each of the two comparisons. The co-efficient for the reference group are all zeros, similar to the co-efficient of the reference group for a dummy-coded variable. Dependent variable will be defined as groups, where the equations can be used to compute the probability and predict the groups associated with the highest probability. The predicted group membership can then be compared to the actual

group membership to obtain a measure of classification accuracy.

The emphasis is given on MLR utility because (a) application for categorical outcomes in multivariate techniques are very few, including Logistic Regression, discriminant function analysis and log-linear models, (b) the MLR does not make any assumptions of normality, linearity, and homogeneity of variance for the independent variables (Hosmer & Lemeshow, 2000; Peng & Nichols, 2003; Clayton & Hills, 1993). (c) MLR does not impose these requirements, it is preferable to use discriminant analysis when the data does not satisfy these assumptions. (d) a more useful measure to assess the utility of MLR is classification accuracy and (e) because the laboratory data generally exist either in

dichotomous or an ordinal form of variable that can be explored in the form of Odds Ratio. The LR and MLR are best methods for the above format of data structure.

This study explained how effectively the MLR models are useful in the epidemiology of cholera and overall model evaluations. The likelihood Ratio was examined to improve the MLR model over null models. An intercept is the only model that serves as a good baseline with no predictors. According to MLR model, the test yielded significance and was more effective than the null model.

In the tests of individual predictors, the Wald chi-square statistic was tested using individual B coefficients to inclined relationship with dependent variables. The goodness of fit statistics assess fitness of logistic model against actual classification i.e. six levels of age group category in the MLR model. The two measures were almost similar in overall estimation, which is similar to Ordinary Least Square (OLS) regression. No equivalents of this concept for MLR explains variance, and for this reason the Pseudo R-Square reported to be complementary to others, which has more useful evaluative indices such as tests of individual regression coefficients (Peng et al., 2001).

The advantage of inferential test of the goodness of fit was suggested by Begg and Gray (1984) for multinomial logistic models. In the validation of predicted probabilities, the MLR model predicts the logit of levels of degrees of inferential risk age group from independent variables. The logit is probability/1-probability, which can be transformed later to the probability scale according to the equation 2 (Rabins & Dickinson, 1985; Peterson & Harrell, 1990; Greenland, 1987; Savitz, 1992). The predicted probability of inferential risk age group is evaluated and compared with actual risk age to determine various levels of age groups.

Reference category was fixed based on the occurrence of positive cases in the age groups in which the cases were low. The main aim of the selection of reference category was to interrogate the age group favored by the pathogen. In *V.cholerae* O1, greater than 40 years age was selected as reference category owing to less incidence rate. The interesting trend of *V.cholerae* O139 was higher incidence

rate in older age group and lower in >5-10 years age group that served as reference category to explore existing relation. The parameter estimation of all age groups with different serogroups of *V.cholerae* was newly conceptualized by comparing reference category of age group with positive cases of respective serogroups. The above equation gives the ratio of comparing categories with reference category in the intercept.

The MLR supported the statistical significance of the three independent variables in different age groups for five consecutive years (1996-2000). Importantly, *V.cholerae* O1 infection mostly occurs upto 5 years age group, which is highly significant. Infection caused by *V.cholerae* O139 showed the significant risk age group was >40 years, which is a more interesting trend. *V.cholerae* non-O1, non-O139 was not significantly associated with any age group, but the highest risk age group was less than 5 years age. The effectiveness of MLR model was supported by multiple indices, including models for overall test of all explanatory variables and significance test of each explanatory variables. In the categorical outcomes, logistic regression is more flexible and less restrictive than discriminant function analysis and log-linear models (Wacholder, 1986; Peng et al., 2002).

Few studies describes the application of Multinomial logistic regression methods. In this finding, we found that MLR is an effective model for profiling greatest risk age groups due to infection caused by different serogroups of *V.cholerae*. Microbiologists and epidemiologists can employ this model for laboratory data.

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Early Scholars A Comparison of Two Rank Tests for Repeated Measures Designs

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This article compares the small-sample properties of the Agresti-Pendergast and the ATS rank-based method, as described in Brunner, Domh, and Langer (2002), for comparing J dependent groups. The results indicate that the Type I error of the Agresti-Pendergast method is more conservative when $J = 2$, but under most conditions, the ATS method performs best in terms of both Type I errors and power.

Key words: rank tests, repeated measures

Introduction

The classic rank-based method for comparing J dependent groups is Friedman's test. Consider a random sample of n vectors from some J -variate distribution. As is well-known, Friedman's test assigns ranks to the values within each vector and is based on a compound symmetry assumption under the hypothesis of no treatment effect (e.g., Brunner, Domhof, & Langer, p. 68). That is, the distribution is assumed to be invariant under all permutations, which implies that the variances and covariances are equal. Two attempts at improving test between Friedman's and are based in part by assigning ranks to the pooled data instead (Iman, 1974; Quade, 1979). Subsequently, Agresti and Pendergast (1986) proposed a rank-based test that was found to provide better control over the probability of a Type I error and better power. (For relevant theoretical results, see Kepner & Robinson, 1988.) Two alternative methods are

described by Brunner, Domhof and Langer (2002, section 7.2.2). The first, based on a Wald-type statistic, is known to be rather unsatisfactory when the sample size is relatively small. The second is an ANOVA-type statistic (ATS) that was found to be preferable to the Wald-type statistic, but no results were provided about how it compares to the Agresti-Pendergast technique. The goal in this article is to compare their small-sample properties via simulations. The results indicate that the ATS method performs better than the Agresti-Pendergast technique for most of conditions.

Description of the Methods

Let $\mathbf{X}_1, \dots, \mathbf{X}_n$, where $\mathbf{X}_k = (X_{k1}, \dots, X_{kJ})'$, $k = 1, \dots, n$, be a random sample from a J -variate distribution with distribution $\mathbf{F} = (F_1, \dots, F_J)'$. In the event sampling is from a discrete distribution, the j^{th} marginal distribution is taken to be $F_j(x) = \frac{1}{2}[F_j^+(x) + F_j^-(x)]$, where F_j^+ and denote F_j^- are the right continuous and the left continuous version of the distribution function, respectively. That is, $F_j^-(x) = P(X_j < x)$ and $F_j^+(x) = P(X_j \leq x)$. The total number of observations is $N = n \times J$ and the null hypothesis is $H_0: F_1 = \dots = F_J$.

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Agresti-Pendergast Test

Let R_{ij} be the midrank of X_{ij} among all N observations. The midrank is determined by means of the so-called counting functions

$$c^-(x) = \begin{cases} 0, & x \leq 0 \\ 1, & x > 0 \end{cases},$$

$$c^+(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0 \end{cases},$$

and

$$c(x) = \frac{1}{2}[c^+(x) + c^-(x)].$$

The midrank of X_{ij} among the N random variables in the i^{th} row and the j^{th} column can be written as $R_{ij} = \frac{1}{2} + \sum_{k=1}^n \sum_{l=1}^J c(X_{ij} - X_{kl})$. Let

$\bar{\mathbf{R}}_j = \frac{1}{n} \sum_{i=1}^n R_{ij}$ for $1 \leq j \leq J$. The estimated covariance matrix $\mathbf{S}$ of the ranks, which has entries s_{ij} , is

$$s_{ij} = \frac{1}{n-J+1} \sum_{i=1}^n (\mathbf{R}_{ij} - \bar{\mathbf{R}}_j)(\mathbf{R}_{ij} - \bar{\mathbf{R}}_k).$$

Under general conditions, the asymptotic distribution of $\mathbf{R}' = (\bar{\mathbf{R}}_1, \dots, \bar{\mathbf{R}}_J)$ is multivariate normal. Let $\nu = E(\mathbf{R})$ and

$$\mathbf{C}_1 = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -1 \end{pmatrix}$$

The null hypothesis $H_0 : F_1 = \dots = F_J$ implies that $\mathbf{C}_1 \nu = 0$ and the test statistic is

$$F = \frac{n}{J-1} (\mathbf{C}_1 \mathbf{R})' (\mathbf{C}_1 \mathbf{S} \mathbf{C}_1')^{-1} \mathbf{C}_1 \mathbf{R},$$

which has, approximately, an F distribution with degrees of freedom $J-1$ and $(J-1)(n-1)$ when null hypothesis is true.

ATS

Following the notation in Brunner et al. (2002), let $\mathbf{I}_J = \text{diag}\{1, \dots, 1\}$ be the J -dimensional identity matrix, let $\mathbf{J}_J$ denote the J -by- J matrix of 1s, and let

$$\mathbf{C}_2 = \mathbf{I}_J - \frac{1}{J} \mathbf{J}_J = \begin{pmatrix} 1 & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & 1 \end{pmatrix}_{J \times J} - \frac{1}{J} \begin{pmatrix} 1 & \dots & 1 \\ \dots & \dots & \dots \\ 1 & \dots & 1 \end{pmatrix}_{J \times J}.$$

The null hypothesis $H_0 : F_1 = \dots = F_J$ is equivalent to

$$H_0 : \mathbf{C}_2 \mathbf{F} = \begin{pmatrix} F_1 - \bar{F} \\ \dots \\ F_J - \bar{F} \end{pmatrix} = \begin{pmatrix} 0 \\ \dots \\ 0 \end{pmatrix} = 0.$$

Let

$$\mathbf{R}_i = (R_{i1}, \dots, R_{iJ}), \quad \bar{\mathbf{R}} = \frac{1}{n} \sum_{i=1}^n \mathbf{R}_i,$$

and let

$$\hat{\mathbf{V}}_n = \frac{1}{N^2(n-1)} \sum_{i=1}^n (\mathbf{R}_i - \bar{\mathbf{R}})(\mathbf{R}_i - \bar{\mathbf{R}})'$$

denote an estimate of the covariance matrix V_n . For the ATS method, the test statistic is

$$F_n(\mathbf{C}_2) = \frac{n}{N^2 \text{trace}(\mathbf{C}_2 \hat{\mathbf{V}}_n)} \sum_{j=1}^J (\bar{\mathbf{R}}_j - \frac{N+1}{2})^2.$$

Under $H_0 : \mathbf{C}_2 \mathbf{F} = 0$, the distribution of F_n can be approximated by an F distribution with

degrees of freedom $\hat{f} = \frac{[\text{trace}(\mathbf{C}_2 \hat{\mathbf{V}}_n)]^2}{\text{trace}(\mathbf{C}_2 \hat{\mathbf{V}}_n \mathbf{C}_2 \hat{\mathbf{V}}_n)}$

and ∞ .

Simulation Results

This section reports simulation results on the small-sample properties of the Agresti-Pendergast and ATS methods. The simulations were run with MATLAB 7.1. A correlation matrix with a common correlation ρ was used and observations were generated from J -variate normal distribution ($J = 2, 3, 4$). Because any order preserving transformation of the data does not alter the results, the simulation results apply

to a wide range of non-normal distributions. The sample sizes were taken to be $n = 10, 20$, and 30 and correlations used were $\rho = 0, 0.2, 0.5, 0.8$ resulting in 36 conditions. A total of 1,000 replications were used to estimate the Type I error probabilities, denoted by $\hat{\alpha}$, and estimated power, which is denoted by $\hat{\gamma}$. When studying power, the mean of the marginal distribution of the first group was increased from zero to one. The results are given in Table 1.

Table 1. Estimated Type I error probabilities and powers for the ATS and Agresti-Pendergast methods, based on 1,000 replications

n	J		$\rho = 0$		$\rho = 0.2$		$\rho = 0.5$		$\rho = 0.8$	
			$\hat{\alpha}$	$\hat{\gamma}$	$\hat{\alpha}$	$\hat{\gamma}$	$\hat{\alpha}$	$\hat{\gamma}$	$\hat{\alpha}$	$\hat{\gamma}$
10	2	ATS	0.095	0.595	0.085	0.688	0.081	0.843	0.082	0.989
		Agresti-Pendergast	0.064	0.495	0.050	0.593	0.050	0.775	0.053	0.975
	3	ATS	0.062	0.585	0.069	0.669	0.065	0.853	0.062	0.998
		Agresti-Pendergast	0.092	0.581	0.080	0.641	0.084	0.813	0.074	0.994
	4	ATS	0.072	0.579	0.065	0.646	0.066	0.849	0.047	0.996
		Agresti-Pendergast	0.111	0.611	0.116	0.671	0.107	0.814	0.107	0.988
20	2	ATS	0.065	0.862	0.072	0.913	0.059	0.994	0.067	1
		Agresti-Pendergast	0.053	0.833	0.053	0.895	0.046	0.990	0.050	1
	3	ATS	0.058	0.885	0.052	0.949	0.063	0.997	0.066	1
		Agresti-Pendergast	0.065	0.883	0.056	0.936	0.070	0.993	0.067	1
	4	ATS	0.052	0.900	0.056	0.936	0.054	0.993	0.058	1
		Agresti-Pendergast	0.070	0.897	0.088	0.921	0.072	0.992	0.072	1
30	2	ATS	0.060	0.963	0.071	0.975	0.065	1	0.050	1
		Agresti-Pendergast	0.050	0.954	0.060	0.971	0.051	1	0.042	1
	3	ATS	0.058	0.984	0.063	0.995	0.049	0.999	0.060	1
		Agresti-Pendergast	0.062	0.973	0.062	0.988	0.051	0.999	0.064	1
	4	ATS	0.045	0.991	0.058	0.994	0.057	1	0.043	1
		Agresti-Pendergast	0.057	0.986	0.076	0.990	0.068	1	0.059	1

Figure 1 Plots of Power vs. Sample size for ATS test and Agresti-Pendergast test (multinormal)

As can be seen, for $n \geq 20$, the $\hat{\alpha}$ values are reasonably close to the nominal value of 0.05 for both the Agresti-Pendergast and ATS methods. With a fixed n and ρ , $\hat{\alpha}$ decreases with J increasing when using ATS, while $\hat{\alpha}$ increases for the Agresti-Pendergast test. For instance, when $\rho = 0.2$ and $n = 30$, the $\hat{\alpha}$ values are 0.071 ($J = 2$), 0.062 ($J = 3$), and 0.058 ($J = 4$) for ATS, and for the Agresti-Pendergast test $\hat{\alpha}$ values are 0.060 ($J = 2$), 0.062 ($J = 3$), and 0.076 ($J = 4$). For $n = 10$ and $J = 2$, the ATS method can be unsatisfactory in terms of Type I errors, the estimate exceeding .075. Otherwise, ATS is generally preferable to the Agresti-Pendergast test. Also, for $n = 10$ and $J > 2$, now the Agresti-Pendergast method performs poorly in terms of Type I errors; the ATS method is preferable.

Table 2 gives the basic descriptive statistics of estimated the Type I errors and power for the two methods. As can be seen from the table, the Type I errors for ATS have smaller variances.

Table 2 Descriptive statistics of estimated Type I errors and powers for Agresti-Pendergast test and ATS

	Type I error $\hat{\alpha}$		Power $\hat{\gamma}$	
	mean	STD	Mean	STD
ATS	0.0625	0.0112	0.9061	0.1370
Agresti-Pendergast	0.0681	0.0192	0.8931	0.1485

Figure 2 Plots of Power vs. Sample size for Brunner-Puri test and Agresti-Pendergast test (Bin(10, 0.4))

Figure 1 contains the estimated powers for all of the conditions. To make it clear, the four ρ s are listed separately. As indicated, ATS is generally preferable.

The discrete case, where tied values occur, was also considered. For the goal of creating a reasonable number of tied values, the distribution used here is Binomial (10, 0.4). Figure 2 gives the plots of power vs. sample size in this case. As can be seen, ATS has higher power than Agresti-Pendergast for $\rho = 0.5$. For the independent case, the choice of method is less clear, with the Agresti-Pendergast offering a bit of an advantage in some instances.

Conclusion

In summary, the simulations show that in many situations, there is little separating ATS and Agresti-Pendergast. However, there are situations where ATS is preferable to Agresti-Pendergast in terms of both Type I errors and power. The main exception is the case $J = 2$ and $n = 10$, where the Agresti-Pendergast performs reasonably well in terms of Type I errors, while ATS does not.

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Algorithms and Code

JMASM26: Hettmansperger and McKean Linear Model Aligned Rank Test for the Single Covariate and One-Way ANCOVA Case (SAS)

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A SAS program (SAS 9.1.3 release, SAS Institute, Cary, N.C.) is presented to implement the Hettmansperger and McKean (1983) linear model aligned rank test (nonparametric ANCOVA) for the single covariate and one-way ANCOVA case. As part of this program, SAS code is also provided to derive the residuals from the regression of Y on X (which is step 1 in the Hettmansperger and McKean procedure) using either ordinary least squares regression (proc reg in SAS) or robust regression with MM estimation (proc robustreg in SAS).

Key words: Aligned ranks, ANCOVA, SAS, nonparametric

Introduction

Parametric analysis of covariance (ANCOVA) was introduced by Sir Ronald A. Fisher in 1932. The design goal of ANCOVA is to use the relationship between a dependent variable and covariate to adjust the dependent variable scores in order to reduce unexplained error variance (error variance in the dependent variable is reduced by an amount that can be accounted for by a covariate) and, hence, to provide a more precise estimate of treatment effects and a more powerful test of the hypothesis (Fisher, 1932; Harwell & Serlin, 1988; Maxwell & Delaney, 1990).

In order to provide a more sensitive test of the hypothesis, parametric ANCOVA must satisfy a set of underlying statistical assumptions (Elashoff, 1969; Huitema, 1980), which include (a) a linear relationship between the covariate (X) and the dependent variable (Y), (b) covariate independent of treatment, (c) equality of group

conditional variances (homogeneity of variance), (d) equality of group regression slopes (homogeneity of regression slopes), (e) normality of the distribution of Y scores for each X value within each group (conditional normality), and (f) independence of errors. However, in practical research settings, such as field experiments, it is not always possible to satisfy all of these statistical assumptions. If these underlying statistical assumptions are not tenable, then robustness and power of the parametric ANCOVA model could be threatened, and a nonparametric ANCOVA procedure should be considered.

Nonparametric ANCOVA models, which are less restrictive in their statistical assumptions, represent an alternative to the usual parametric ANCOVA. A variety of nonparametric ANCOVA models have been proposed, including those procedures developed by (1) Quade (1967); (2) McSweeney and Porter (1971); (3) Burnett and Barr (1977); (4) Rogosa (1980); (5) Conover and Iman (1982); (6) Hettmansperger and McKean (1983); and (7) Puri-Sen-Harwell-Serlin (1989). The nonparametric ANCOVA models are similar in that each model involves a ranking procedure to transform the original scores. Each model, however, is not similar with respect to robustness and power (Olejnik & Algina, 1984, 1985; Harwell & Serlin, 1988; Rheinheimer & Penfield, 2001).

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Previous Monte Carlo studies that have examined the robustness and power of the nonparametric ANCOVA models have, in general, found that the Hettmansperger and McKean (1983) method (which is an aligned rank test) is robust and powerful when the underlying statistical assumptions of the parametric ANCOVA are not tenable (such as conditional non-normality, unequal regression slopes, and variance heterogeneity—even in the presence of unequal group sample sizes) (Harwell & Serlin, 1988; Rheinheimer & Penfield, 2001).

A SAS program (SAS 9.1.3 release, SAS Institute, Cary, N.C.) is presented for implementing the Hettmansperger and McKean (1983) linear model aligned rank test for the single covariate and one-way ANCOVA case. The SAS program is presented in Appendix A.

Hettmansperger and McKean (1983) Nonparametric ANCOVA Method

A brief description of the Hettmansperger and McKean (1983) nonparametric linear model ANCOVA method is presented. For a single covariate and grouping variable, the hypothesis tested based on ranks in the linear model (for the omnibus between-subjects main effect of group) is:

$$H_0: \rho_{YD_1, \dots, D_{K-1} \cdot X} = 0, \quad (1)$$

where group K and $\rho_{YD_1, \dots, D_{K-1} \cdot X}$ is the rank correlation between the dependent variable Y and the $K-1$ group membership variables D_K with the effects of the covariate X removed. Under this null hypothesis, all groups are assumed to possess identical expected covariate-adjusted mean ranks.

Hettmansperger and McKean (1983) proposed an aligned rank test (of the hypothesis specified in Equation 1) that involves the following steps: (a) calculate the least squares residuals from the regression of Y on X , where Y is the single dependent variable and X is the covariate; (b) rank the raw score residuals from low to high (1 to N); (c) weight the ranked residuals (R'_i) using $R'_i = \sqrt{12} [R_i / (N+1) - 0.5]$, where R_i is the ranked

raw score residuals, N is the total number of observations, 12 and 0.5 are constants; and (d) perform a parametric ANOVA (with least squares estimation) on the weighted ranked residuals (R'_i), while maintaining the original group membership.

The sum of squares between groups, SS_{Between} , from the parametric ANOVA on R'_i is the aligned rank *Test Statistic*, which is asymptotically distributed as a central χ^2 with $K-1$ degrees of freedom. Hettmansperger and McKean (1983) originally proposed the use of least squares residuals from the regression of Y on X (step 1 in their procedure). If outliers are present in the data, however, then the residuals from the regression of Y on X (step 1 in the procedure) should be derived using robust regression. The current article, therefore, provides SAS code to derive the residuals using either ordinary least squares regression (proc reg in SAS) or robust regression with MM estimation (proc robustreg in SAS). The reader is referred to Rousseeuw and Leroy (1987) and Yohai (1987) for a discussion of robust estimates for regression.

Although the SAS program in the current article only addressed the single covariate and one-way ANCOVA case (for the one-tailed test of the omnibus between-subjects main effect of group), the Hettmansperger and McKean (1983) aligned rank test can be extended to the multiple covariate case and two-way/higher-order factorial ANCOVA case. A separate aligned rank test, however, is required for each main effect and interaction effect tested. The reader is referred to Adichie (1978), Hettmansperger and McKean (1983), and Hettmansperger (1984) for an expanded discussion of the aligned rank test.

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Appendix A

The following SAS program (SAS 9.1.3 release) can be used to perform the Hettmansperger and McKean (1983) aligned rank test for the single covariate and one-way ANCOVA case (one-tailed test of the omnibus between-subjects main effect of group).

/* Step 1: Read internal data into SAS data set hett */

/* Note. You may also read data from an external file into a SAS data set using Proc Import */

```
data hett;
input subject group X Y;
cards;
<your data>
;
```

/* Step 2: Use Proc Reg to compute and output the **least squares** residuals from the regression of Y on X , where Y is the dependent variable and X is the single covariate */

```
proc reg;
  model Y=X;
  output out=res r=residual;
run;
proc print data=res;
```

/* Alternative Step 2: If outliers are present in the data, then the residuals should be derived using robust regression. Use Proc Robustreg to compute and output the **robust** residuals, with MM estimation, from the regression of Y on X */

```
proc robustreg method=mm;
  model Y=X;
  output out=res r=residual;
run;
proc print data=res;
```

/* Step 3: Use Proc Rank to rank the raw score residuals from low to high (1 to N) */

```
proc rank data=res out=rank; var residual;
```

/* Step 4: Weight the ranked residuals (R'_i) using $R'_i = \sqrt{12} [R_i / (N + 1) - 0.5]$, where R_i is the ranked raw score residuals and N is the total number of observations */

```
data weight; set rank nobs=n;
  rename residual=RankedResiduals;
  weight=12** .5*(residual/(n+1)-.5);
run;
proc print data=weight;
```



```
/* Step 5: Perform a parametric ANOVA on the weighted ranked residuals ( $R'_i$ ), while
maintaining the original group membership */

proc glm; class group;
  model weight=group;
  ods output modelanova=ma(where=(hypothesistype=3));
run;

/* Step 6: One-tailed test of the omnibus between-subjects main effect of group
  Dependent = dependent variable = weighted ranked residuals ( $R'_i$ )
  Source = omnibus main effect of group
  DF = K-1 degrees of freedom
  HettMcKeanChisqValue = aligned rank test statistic (which is the  $SS_{\text{Between}}$ )
  ProbChisq = p-value of the obtained test statistic
  CriticalValueChisq = chi-square critical value with K-1 degrees of freedom,  $\alpha = .05$  */

data ma;
  set ma;
  rename ss=HettMcKeanChisqValue;
  ProbChisq=sdf('chisquare',ss,df);
  CriticalValueChisq=quantile('chisquare',.95,df);
run;

title 'The Hettmansperger and McKean Nonparametric One-Way ANCOVA (aligned rank test)
Procedure';
proc print data=ma noobs; var Dependent Source DF HettMcKeanChisqValue ProbChisq
CriticalValueChisq;
run;
```

JMASM27: An Algorithm for Implementing Gibbs Sampling for 2PNO IRT Models (Fortran)

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A Fortran 77 subroutine is provided for implementing the Gibbs sampling procedure to a normal ogive IRT model for binary item response data with the choice of uniform and normal prior distributions for item parameters. The subroutine requires the user to have access to the IMSL library. The source code is available at <http://www.siu.edu/~epse1/sheng/Fortran/>, along with a stand alone executable file.

Key words: IRT, two-parameter normal ogive model, MCMC, Gibbs sampling, Fortran.

Introduction

Item response theory (IRT) describes a probabilistic relationship between correct responses on a set of test items and a latent variable, where the influence of items and persons on the responses is modeled by distinct sets of parameters. Common IRT models include the two-parameter normal ogive (2PNO; Lawley, 1943, 1944; Lord, 1952, 1953a, 1953b) model such that the probability of person i obtaining a correct response for item j , where $i = 1, \dots, n$ and $j = 1, \dots, k$, is defined as

$$P(y_{ij} = 1) = \Phi(\alpha_j \theta_i - \gamma_j) \\ = \int_{-\infty}^{\alpha_j \theta_i - \gamma_j} \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}} dt, \quad (1)$$

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where γ_j and α_j denote item parameters and θ_i denotes the continuous person trait. In the model, items are assumed to vary in terms of location, γ_j , as well as slope, α_j . Simultaneous estimation of both item and person parameters results in statistical complexities in the estimation task of IRT models, which have made estimation procedures a primary focus of psychometric research over decades (e.g., Birnbaum, 1969; Bock & Aitkin, 1981; Molenaar, 1995). Recent attention has been focused on Markov chain Monte Carlo (MCMC; e.g., Chib & Greenberg, 1995) techniques, which have demonstrated to be useful for complex estimation problems in many areas of applied statistics. Albert (1992) was the first to apply an MCMC algorithm, known as Gibbs sampling (Casella & George, 1992; Gelfand & Smith, 1990; Geman & Geman, 1984), to the 2PNO model, where he adopted non-informative priors for item parameters.

As Albert's (1992) focus was on investigating the applicability of Gibbs sampling to IRT, he did not specifically consider the situations where informative priors are adopted for item parameters. However, in some applications, they are more preferred than vague priors. For example, when comparing several candidate models, Bayes factors are commonly adopted in the Bayesian framework, but they are not defined with non-informative priors (Gelman et al., 2003). In this case, the program given by Albert (1992) does not provide a solution. Moreover, given that MCMC is computationally

demanding in drawing a sufficiently long chain to ensure convergence, a major problem in applied IRT is the accessibility of efficient MCMC programs. Researchers have either used WinBUGS (e.g., Bazán, Branco & Bolfarine, 2006; DeMars, 2005) to implement MCMC for IRT models, or coded the sampler in S-Plus (e.g., Patz & Junker, 1999) or MATLAB (e.g., Albert, 1992). They noted that each execution consumed many hours, and hence was computationally expensive. This fact makes it impractical for users to utilize these programs for various applications of IRT. They further limit researchers in conducting Monte Carlo studies, or developing more complicated IRT models. It is then anticipated that Fortran will provide a better solution, as it is the fastest programming language for numerical computing (Brainerd, 2003).

In view of the above, the purpose of this article is to provide a Fortran subroutine that obtains the posterior estimates (and their associated standard errors) of item and person parameters in the 2PNO IRT model. The subroutine will have the option of specifying non-informative and informative priors for item parameters.

Methodology

The Gibbs Sampling Procedure

To implement Gibbs sampling to the 2PNO model defined in (1), a latent continuous random variable Z is introduced so that $Z_{ij} \sim N(\alpha_j \theta_i - \gamma_j, 1)$ (Albert, 1992; Tanner & Wong, 1987). With prior distributions assumed for θ_i and ξ_j , where $\xi_j = (\alpha_j, \gamma_j)'$, the joint posterior distribution of (θ, ξ) is hence

$$p(\theta, \xi | \mathbf{y}) \propto f(\mathbf{y} | \mathbf{Z}) p(\mathbf{Z} | \theta, \xi) p(\theta) p(\xi), \quad (2)$$

where $f(\mathbf{y} | \mathbf{Z})$ is the likelihood function.

With a normal prior for θ_i and non-informative priors for α_j and γ_j so that $\theta_i \sim N(\mu, \sigma^2)$, $\alpha_j > 0$ and $p(\gamma_j) \propto 1$, the full conditional distributions of Z_{ij} , θ_i , and ξ_j can be derived in closed forms as follows:

$$Z_{ij} | \bullet \sim \begin{cases} N_{(0, \infty)}(\alpha_j \theta_i - \gamma_j, 1), & \text{if } y_{ij} = 1 \\ N_{(-\infty, 0)}(\alpha_j \theta_i - \gamma_j, 1), & \text{if } y_{ij} = 0 \end{cases} \quad (3)$$

$$\theta_i | \bullet \sim N \left(\frac{\sum_j (Z_{ij} + \gamma_j) \alpha_j + \mu}{\frac{1}{\sigma^2} + \sum_j \alpha_j^2}, \frac{1}{\frac{1}{\sigma^2} + \sum_j \alpha_j^2} \right) \quad (4)$$

$$\xi_j | \bullet \sim N((\mathbf{x}' \mathbf{x})^{-1} \mathbf{x}' \mathbf{Z}_j, (\mathbf{x}' \mathbf{x})^{-1}) I(\alpha_j > 0), \quad (5)$$

where $\mathbf{x} = [\theta, -1]$. Alternatively, informative conjugate priors can be assumed for α_j and γ_j so that $\alpha_j \sim N_{(0, \infty)}(\mu_\alpha, \sigma_\alpha^2)$, $\gamma_j \sim N(\mu_\gamma, \sigma_\gamma^2)$. In this case, the full conditional distribution of ξ_j is derived as

$$\xi_j | \bullet \sim N((\mathbf{x}' \mathbf{x} + \Sigma_\xi^{-1})^{-1} (\mathbf{x}' \mathbf{Z}_j + \Sigma_\xi^{-1} \boldsymbol{\mu}_\xi), (\mathbf{x}' \mathbf{x} + \Sigma_\xi^{-1})^{-1}) I(\alpha_j > 0) \quad (6)$$

where $\boldsymbol{\mu}_\xi = (\mu_\alpha, \mu_\gamma)'$ and $\Sigma_\xi = \begin{pmatrix} \sigma_\alpha^2 & 0 \\ 0 & \sigma_\gamma^2 \end{pmatrix}$.

Hence, with starting values $\theta^{(0)}$ and $\xi^{(0)}$, observations $(Z^{(l)}, \theta^{(l)}, \xi^{(l)})$ can be simulated from the Gibbs sampler by iteratively drawing from their respective full conditional distributions specified in (3), (4) and (5) (or equations 3, 4, and 6). To go from $(Z^{(l-1)}, \theta^{(l-1)}, \xi^{(l-1)})$ to $(Z^{(l)}, \theta^{(l)}, \xi^{(l)})$, it takes three transition steps:

1. Draw $Z^{(l)} \sim p(Z | y, \theta^{(l-1)}, \xi^{(l-1)})$;
2. Draw $\theta^{(l)} \sim p(\theta | Z^{(l)}, \xi^{(l-1)})$;
3. Draw $\xi^{(l)} \sim p(\xi | Z^{(l)}, \theta^{(l)})$.

This iterative procedure produces a sequence of $(\theta^{(l)}, \xi^{(l)})$, $l = 0, \dots, L$. To reduce the effect of the starting values, early iterations in the Markov chain are set as burn-ins to be discarded. Samples from the remaining iterations are then used to summarize the posterior density of item

parameters ξ and ability parameters θ . As with standard Monte Carlo, with large enough samples, the posterior means of ξ and θ are considered as estimates of the true parameters. However, their standard deviations tend to underestimate the posterior standard deviations, as subsequent samples in Gibbs sampler are autocorrelated (e.g., Albert, 1992; Patz & Junker, 1999). One approach to calculating them is through batching (Ripley, 1987). That is, with a long chain of samples being separated into contiguous batches of equal length, the posterior mean and standard deviation for each parameter are then estimated to be the sample mean and standard deviation of these batch means respectively. Thus, the standard error of the estimate is a ratio of the standard deviation and the square root of the number of batches.

The Fortran Subroutine

The subroutine initially sets the starting values for the parameters, so that $\theta_i^{(0)} = 0$, $\alpha_i^{(0)} = 2$ and $\gamma_i^{(0)} = -\Phi^{-1}(\sum_j y_{ij} / n) \sqrt{5}$ (Albert, 1992). It then iteratively draws random samples for Z and θ from their respective full conditional distributions specified in (3) and (4) with $\mu = 0$ and $\sigma^2 = 1$. Samples for ξ_j are simulated either from (5), where uniform priors are assumed for ξ_j , or from (6), where normal priors are adopted with $\mu_\alpha = \mu_\gamma = 0$ and $\sigma_\alpha^2 = \sigma_\gamma^2 = 1$. The algorithm continues until all the L samples are simulated. It then discards the early burn-in samples, and computes the posterior estimates and standard errors for the model parameters, θ , α and γ , using batching.

For example, for a 2000-by-10 (i.e., $n = 2,000$ and $k = 10$) dichotomous (0-1) data matrix simulated using the item parameters shown in the first two columns of Table 1, the Gibbs

sampler was implemented so that 10,000 samples were simulated with the first 5,000 taken to be burn-in. The remaining 5,000 samples were separated into 5 batches, each with 1,000 samples. Two sets of the posterior means for α and γ , as well as their standard errors, were obtained assuming the uniform or normal prior distributions described previously, and are displayed in the rest of the table. It is noted that the item parameters were estimated with enough accuracy and the two sets of posterior estimates differ only slightly from each other, signifying that the results are not sensitive to the choice of priors for ξ . For this example, each implementation took less than 13 minutes. Although 10,000 iterations are long enough for the Markov chain to reach the stationary distribution, one may easily increase the length of the chain to be as long as 50,000, which takes about 60-90 minutes for each execution.

Conclusion

This Fortran subroutine leaves it to the user to choose between uniform and normal priors for the item parameters, α and γ . In addition, the user can change the source code so that the prior distribution for θ_i assumes different location, μ and scale, σ^2 . Similarly, μ_α , σ_α^2 , and μ_γ , σ_γ^2 can be modified to reflect different prior beliefs on the distributions for the item parameters. It is noted that convergence can be assessed by comparing the marginal posterior mean and standard deviation of each parameter computed for every 1,000 samples after the burn-ins. Similar values provide a rough indication of similar marginal posterior densities, which further indicates possible convergence of the Gibbs sampler (Gelfand, Hills, Racine-Poon & Smith, 1990; Hoijtink & Molenaar, 1997).

Table 1. Posterior estimates and their standard errors for α and γ with uniform priors and normal priors.

Parameters	γ	Posterior estimates			
		uniform priors		normal priors	
		$\hat{\alpha}$ (SE)	$\hat{\gamma}$ (SE)	$\hat{\alpha}$ (SE)	$\hat{\gamma}$ (SE)
0.0966	-0.7997	0.1147 (.0009)	-0.8258 (.0010)	0.1120 (.0012)	-0.8223 (.0006)
0.0971	-0.5321	0.1291 (.0003)	-0.5441 (.0006)	0.1285 (.0022)	-0.5449 (.0004)
0.4589	0.8583	0.4412 (.0031)	0.9289 (.0021)	0.4416 (.0031)	0.9278 (.0017)
0.9532	0.7237	1.1335 (.0088)	0.8906 (.0032)	1.1124 (.0074)	0.8801 (.0041)
0.0771	-0.8184	0.0517 (.0005)	-0.8063 (.0005)	0.0510 (.0007)	-0.8056 (.0007)
0.4891	-0.5834	0.4761 (.0023)	-0.6186 (.0006)	0.4726 (.0023)	-0.6188 (.0004)
0.8599	0.3629	0.7960 (.0028)	0.3484 (.0013)	0.8015 (.0036)	0.3501 (.0022)
0.9427	-0.9010	0.9230 (.0060)	-0.8661 (.0017)	0.9189 (.0083)	-0.8618 (.0049)
0.2727	-0.9339	0.3981 (.0027)	-0.9497 (.0018)	0.3948 (.0028)	-0.9465 (.0023)
0.6532	-0.3978	0.6562 (.0016)	-0.3785 (.0008)	0.6544 (.0015)	-0.3781 (.0009)

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Appendix

```
SUBROUTINE GSU2(Y, N, K, L, BURNIN, BN, UNIF, ITEM, PERSON)
C*****
C Y is the n-by-k binary item response data
C N is the number of subjects
C K is the test length (number of items)
C L is the number of iterations using Gibbs sampling
C BURNIN is the first number of iterations that are to be discarded
C BN is the number of batches
C UNIF is a 0-1 indicator with 0 specifying normal priors for item
C   parameters and 1 specifying uniform priors for them
C ITEM is a k-by-4 matrix of posterior estimates and standard errors
C   for item parameters
C PERSON is a n-by-2 matrix of posterior estimates and standard errors
C   for person abilities
C*****
```

```

      INTEGER      L, COUNT, IRANK, BURNIN, UNIF, INDX(2), BN,
&      BSIZE, Y(N, K)
      REAL  A(K), G(K), TH(N), LP, MU, VAR, AV(L,K), GV(L,K), THV(N,L),
&      PHAT(K), U, Z(N,K), V, MN, MSUM, PVAR, PMEAN, TT, X(N,2),
&      XX(2,2), IX(2,2), ZV(N,1), XZ(2,1), AMAT(2,2), BZ(2,1), AMU,
&      GMU, AVAR, GVAR, AGMU(2,1), AGVAR(2,2), SIGMA(2,2), BETA(1,2),
&      BI(1,2), ITEM(K,4), PERSON(N,2), SUM1, SUM2, SUM3,
&      M1, M2, M3, TOT1, TOT2, TOT3, SS1, SS2, SS3
      DOUBLE PRECISION  BB, TMP
C*****
C Connect to external libraries for normal (RNNOR) and uniform (RNUN)
C random number generator, inverse (ANORIN, DNORIN) and CDF (ANORDF,
C DNORDF) for the standard normal distribution, and Cholesky
C factorization (CHFAC) routines
C*****
      EXTERNAL  RNNOR, RNSET, RNUN, ANORDF, ANORIN, CHFAC, DNORDF, DNORIN
C*****
C Set initial values for item parameters a, g, and person ability theta so
C that a = 2, g =  $-\Phi^{-1}(\sum_i y_{ij}/n)\sqrt{5}$  for all k items, and theta = 0 for all n
C persons.
C*****
      PHAT = SUM(Y, 1)
      DO 10 I = 1, K
        A(I) = 2.0
        G(I) = -ANORIN(PHAT(I)/N)*SQRT(5.0)
10  CONTINUE
      DO 20 I = 1, N
        TH(I) = 0.0
20  CONTINUE
C*****
C MU and VAR are the mean and the variance for the prior distribution of
C theta.
C*****
      MU = 0.0
      VAR = 1.0
C*****
C Start iteration
C*****
      COUNT = 0
      DO 30 IT = 1, L
        COUNT = COUNT + 1
C*****
C Update samples for Z from its normal posterior distributions
C*****
      DO 40 I = 1, N
        DO 40 J = 1, K
          LP = TH(I) * A(J) - G(J)
          BB = ANORDF((0.0 - LP))
          CALL RNUN (1, U)
          TMP = BB*(1 - Y(I, J)) + (1 - BB)*Y(I, J) * U + BB*Y(I, J)
          Z(I, J) = DNORIN(TMP) + LP
40  CONTINUE

```

```

C*****
C Update samples for theta from their normal posterior distributions
C*****
      V = 1/SUM(A*A)
      PVAR = 1/(1/V + 1/VAR)
      DO 50 I = 1, N
        MSUM = 0.0
        DO 60 J = 1, K
          MSUM = MSUM+A(J)*(Z(I, J) + G(J))
60      CONTINUE
      MN = MSUM*V
      PMEAN = (MN/V + MU/VAR)*PVAR
      CALL RNNOR(1,TT)
      TH(I) = TT*SQRT(PVAR) + PMEAN
      THV(I, COUNT) = TH(I)
50      CONTINUE
C*****
C Update samples for item parameters, a and g from their multivariate
C normal posterior distributions
C*****
      DO 70 J = 1, 1
        DO 70 I = 1, N
          X(I, J) = TH(I)
70      CONTINUE
      DO 80 J = 2, 2
        DO 80 I = 1, N
          X(I, J) = -1
80      CONTINUE
      IF (UNIF == 0) THEN
C*****
C Specify the prior means (AMU, GMU) and variances (AVAR, GVAR)
C for a and g.
C*****
      AMU = 0.0
      GMU = 0.0
      AVAR = 1.0
      GVAR = 1.0
C*****
C Put the means and variances in vector and matrix format
C*****
      AGMU(1, 1) = AMU
      AGMU(2, 1) = GMU
      AGVAR(1, 1) = AVAR
      AGVAR(2, 2) = GVAR
C*****
C Call the matrix inversion routine.

```



```

C Invert matrix AGVAR with the inverse stored in SIGMA
C*****
      CALL MIGS(AGVAR, 2, SIGMA, INDX)
      XX = MATMUL(TRANPOSE(X), X) + SIGMA
      ELSE IF (UNIF == 1) THEN
        XX = MATMUL(TRANPOSE(X), X)
      END IF
C*****
C Call the matrix inversion routine.
C Invert matrix XX with the inverse stored in IX
C*****
      CALL MIGS(XX, 2, IX, INDX)
C*****
C Call the Cholesky factorization routine. Compute the Cholesky
C factorization of the symmetric definite matrix IX and store the
C result in AMAT
C*****
      CALL CHFAC (2, IX, 2, 0.00001, IRANK, AMAT, 2)
      DO 90 J = 1, K
        DO 100 I = 1, N
          ZV(I, 1)=Z(I, J)
100      CONTINUE
          IF (UNIF == 0) THEN
            XZ = MATMUL(SIGMA, AGMU)+MATMUL(TRANPOSE(X), ZV)
          ELSE IF (UNIF == 1) THEN
            XZ = MATMUL(TRANPOSE(X), ZV)
          END IF
          BZ = MATMUL(IX, XZ)
          A(J) = 0
          DO WHILE (A(J).LE.0)
            CALL RNNOR (2, BI)
            BETA = MATMUL(BI, AMAT)+TRANPOSE(BZ);
            A(J) = BETA(1, 1)
            G(J) = BETA(1, 2)
          END DO
          AV(COUNT, J) = A(J)
          GV(COUNT, J) = G(J)
        90      CONTINUE
      30 CONTINUE
C*****
C Calculate the posterior means and SEs for a, g and theta and store them
C in ITEM and PERSON
C*****
      BSIZE=(L-BURNIN)/BN
      DO 110 J = 1, K
        COUNT = BURNIN
        TOT1 = 0.0
        TOT2 = 0.0
        SS1 = 0.0
        SS2 = 0.0
        DO 120 M = 1, BN
          SUM1 = 0.0
          SUM2 = 0.0
          DO 130 I = 1, BSIZE
            COUNT = COUNT + 1
            SUM1 = SUM1 + AV(COUNT, J)
            SUM2 = SUM2 + GV(COUNT, J)

```

```
130      CONTINUE
        M1 = SUM1/BSIZE
        M2 = SUM2/BSIZE
        TOT1 = TOT1 + M1
        TOT2 = TOT2 + M2
        SS1 = SS1 + M1*M1
        SS2 = SS2 + M2*M2
120  COUNTINE
        ITEM(J, 1) = TOT1/BN
        ITEM(J, 2) = SQRT((SS1 - (TOT1*TOT1/BN))/(BN - 1))/SQRT(FLOAT(BN))
        ITEM(J, 3) = TOT2/BN
        ITEM(J, 4) = SQRT((SS2 - (TOT2*TOT2/BN))/(BN - 1))/SQRT(FLOAT(BN))
110 CONTINUE

        DO 140 J = 1,N
          COUNT = BURNIN
          TOT3 = 0.0
          SS3 = 0.0
          DO 150 M = 1, BN
            SUM3 = 0.0
            DO 160 I = 1, BSIZE
              COUNT = COUNT + 1
              SUM3 = SUM3 + THV(J, COUNT)
160          CONTINUE
            M3 = SUM3/BSIZE
            TOT3 = TOT3 + M3
            SS3 = SS3 + M3*M3
150        CONTINUE
          PERSON(J, 1) = TOT3/BN
          PERSON(J, 2) = SQRT((SS3 - (TOT3*TOT3/BN))/(BN - 1))/SQRT(FLOAT(BN))
140        CONTINUE

        RETURN
        END
```

Translations, Ephemerals, & Biographies Mathematics in Volume I of *Scripta Universitatis*

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Immanuel Velikovsky's journal, *Scripta Universitatis*, edited by Albert Einstein and first published in 1923, played a significant role in the establishment of the library, and hence, Hebrew University in Jerusalem. The inaugural issue contained an article by the French mathematician Jacques Hadamard. Excerpts from Velikovsky's diary pertaining to the rationale for the creation of the journal, and the interest in Jewish scholars such as Hadamard, are translated here.

Key words: *Scripta Universitatis*, Velikovsky, Hadamard, Hebrew University

Introduction

Immanuel Velikovsky (June 10, 1895 - November 17, 1979) studied medicine intermittently from 1913 through 1918 at various universities (Montpelier, Edinburgh, & Kharkov), eventually receiving the M. D. in 1921 from the University of Moscow. He was the author of *Worlds in Collision* (1950), *Ages in Chaos* (1952), *Earth in Upheaval* (1956), *Oedipus and Akhnaton* (1960), *Peoples of the Sea* (1977), *Ramses II and His Times* (1978), *Mankind in Amnesia* (1982, posthumously by his wife, Elisheva Kramer Velikovsky), and *Stargazers and Gravediggers* (1983, also posthumously).

While doing post-doctoral work at Charité and the Kaiser Wilhelm Akademie in Berlin in 1922 - 1923, he founded the journal *Scripta Universitatis*. This scholarly work comprised of two parts: (1) Mathematics and Physics, and (2) Judaica and Orientalia. It has been considered the impetus leading to the establishment of Hebrew University in Jerusalem. Jewish authors of note from around the world contributed articles in their native tongue, which were published in one side of the

Journal, while the other side of the journal contained a Hebrew translation of their work. A scan of the Hebrew cover of the first issue is presented in Figure 1, and the English cover of the same issue in Figure 2.

Velikovsky appointed Albert Einstein (March 14, 1879 – April 18, 1955) to serve as Editor. Einstein also contributed an article, with co-author Jacob Gommer from the University of Berlin, titled "Beweis der Nichtexistenz eines überall regulären zentrisch symmetrischen Feldes nach der Feld-Theorie von Th. Kaluza." Velikovsky relied on Einstein to recruit other notable Jewish scholars to submit to the journal.

Unfortunately, the two of them later parted ways. On July 5, 1946, Velikovsky met with Einstein in Princeton to discuss the extraterrestrial role of Venus in Earth's catastrophic planetary development that would become the premise of his *Worlds in Collision* (1950). Einstein found the theory to be preposterous, canceled further meetings with Velikovsky, and written communication between them was subsequently strained.

His elder daughter, Shulamit Velikovsky Kogan (b. 1925), gifted a copy of *Scripta* to a cataloger of her father's archives. She also included typeset excerpts from Velikovsky's letters written in the 1920s to his father (Figure 3) who lived in Israel. The excerpts are in diary format and pertain to the development of *Scripta*, written while Velikovsky was in Berlin and Leipzig. Autobiographical information in

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English pertaining to *Scripta* may also be found in Velikovsky (1978).

Among these excerpts, material regarding Albert Einstein and the mathematician Jacques Salomon Hadamard (December 8, 1865 – October 17, 1963) is translated below from Hebrew to (flowing American) English. A translation of Hadamard's contributed article in Volume 1 of *Scripta* will appear in the next issue

of the *Journal of Modern Applied Statistical methods*.

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August 20, 1922

Yesterday I visited Prof. Einstein, the purpose of which was to invite him to be the Editor of the [Physics and] Mathematics section [of *Scripta Universitatis*]. We spent a long time in conversation. He accepted upon himself to write to two important Jewish scholars, both close personal friends, who had yet to join us in this endeavor. They are the greatest mathematician in France, Hadamard, and the greatest biologist in America, Jacques Loeb. Because Einstein is now the Editor, I will bring to him, in the coming days, the hand written manuscripts in Mathematics [and Physics] to determine which to accept for publication. Afterward, I will invite editors for other sections. For Biology, I would like Wasserman.

December 17, 1922

In a few weeks, we will send as many as 500 circulars to a large number of scholars. I hope we will be able to thereby increase the number of participants, specifically Jewish scholars with international reputations, such as Volterra and Enriques (Italian mathematicians), Hadamard (French mathematician), Bergson (French philosopher), L. R. Flexner and J. Loeb (American biologists), and A. Michelson (American physicist). If these seven scholars will agree participate, it will become apparent to the Jewish world, and throughout the world for that matter, that the Jewish people have made important contributions to science, despite the fact that we are scattered all over the world.

January 2, 1923

There was a very important event that happened in our work this week. We were joined by the French scholar Hadamard, a famous mathematician. Einstein and I wrote him a letter of invitation to submit. In his answer he agreed, and attached a hand-written manuscript. Based on this, I will now have a much easier time to get other scholars in France to participate. Everyone knows that Einstein contributes to projects that promote Zionism, but when Hadamard joined us, this is something entirely new. Thus, getting such scholars to participate in the [Hebrew University] Jerusalem project was a worthwhile effort.*

[Footnote material added by Velikovsky much later] *Indeed, from that time, Hadamard became an active participant in Zionist activities, giving assistance to different projects in Israel. Many scholars who later became members of the board of directors of the Jerusalemite [Hebrew] University were initially attracted by their participation with *Scripta Universitatis*.

Figure 1. Cover of the Hebrew side of Volume I of *Scripta Universitatis*, indicating the Editor as Albert Einstein, and the journal was published in Jerusalem in the Jewish year 5684 (1923-1924).
From the private collection of Shlomo S. Sawilowsky.

Figure 2. Cover of the English side of Volume I of *Scripta Universitatis*.
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Figure 3. Two hand written notes with signature from Shulamit Velikovsky Kogan.
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Box Plots
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Dot Plots
Error Bar Charts
Histograms
Histograms: Combined*
Percentile Plots
Pie Charts
Probability Plots
ROC Curves*
Scatter Plots
Scatter Plot Matrix
Surface Plots
Violin Plots

Experimental Designs

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Box-Behnken
Central Composite
D-Optimal Designs
Fractional Factorial
Latin Squares
Plackett-Burman
Response Surface
Screening
Taguchi

Regression / Correlation

All-Possible Search
Canonical Correlation
Correlation Matrices
Cox Regression
Kendall's Tau Correlation
Linear Regression
Logistic Regression
Multiple Regression
Nonlinear Regression
PC Regression
Poisson Regression
Response-Surface
Ridge Regression
Robust Regression
Stepwise Regression
Spearman Correlation
Variable Selection

Quality Control

Xbar-R Chart
C, P, NP, U Charts
Capability Analysis
Cusum, EWMA Chart
Individuals Chart
Moving Average Chart
Pareto Chart
R & R Studies

Survival / Reliability

Accelerated Life Tests
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Bootstrap C.I.'s*
Built-In Models
Group Fitting and Testing*
Model Searching
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Miscellaneous

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Bootstrapping
Chi-Square Test
Confidence Limits
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  IF ( .NOT. PRESENT
    NULLIFY ( p%coef
  ELSE
    m = UBOUND(v,l)
    IF ( max_degree
      ALLOCATE ( p%
      p%coeffs
    ELSE
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      p%coeffs
    END IF
  END IF
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