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Journal Of Modern Applied Statistical Methods

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Editorial Assistant: **Julie M. Smith, Ph. D.**

Regular Articles

Underlying Distributions in Loglinear Models of Discrete Data

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The implications of loglinear models based on underlying uniform and binomial distribution are assessed with respect to modeling eight distributions. Regarding statistical selection of the loglinear models' parameterizations, results indicate that better fitting models are obtained when the distribution being modeled is dissimilar to the underlying distribution used. For loglinear models with predetermined numbers of parameters, results suggest that better fitting models can be obtained when the distribution being modeled is similar to the underlying distribution.

Key words: Loglinear models, uniform distribution, binomial distribution.

Introduction

Loglinear models are used to estimate the distributions of discrete data that occur in applied research involving political questionnaires, biomedical data and psychometric testing (Agresti, 2002; Bishop, Fienberg & Holland, 1975; Holland & Thayer, 2000; Kolen & Brennan, 2004). The choice of most interest when selecting a plausible loglinear model for a particular discrete distribution is usually the number of moments of the observed distribution to preserve in the modeled distribution. A less familiar choice pertains to the distribution that underlies the loglinear model, which is obtained when most or all of the loglinear model's parameters are set to zero. This study considers the implications of using different underlying distributions – specifically uniform and binomial distributions – for loglinear models of discrete distributions.

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Loglinear Models of Discrete Distributions

Loglinear models of discrete distributions relate the log of a model's expected probabilities, ρ , to a linear function of a categorical variable's values, for example the scores of a psychometric test,

$$\log_e(\rho) = \alpha + \mu + \mathbf{X}\beta \quad (1)$$

where ρ is an I -by-1 column vector of the probabilities, α is a normalizing constant which ensures that the sum of the entries of ρ is 1, $\sum_i \rho_i = 1$, μ is an I -by-1 column vector of known constants, $\mathbf{X}$ is an I -by- K design matrix containing K functions of categorical variable X , and β is a K -by-1 column vector of free parameters. The $k = 1$ to K columns of $\mathbf{X}$ give the first through K^{th} degrees of the X values that can be expressed as power functions, x_i^k , or as used in this study, the more numerically stable and less collinear orthogonal polynomials. When maximum likelihood estimation is used for model 1 then the estimation results in the first derivative of the log-likelihood being set to zero, or,

$$\sum_i \hat{\rho}_i x_i^k = \sum_i \frac{n_i}{N} x_i^k, \quad (2)$$

where n_i is the observed frequency of the i^{th} category value of X and N is the total sample size. Equation 2 implies that the first K moments of X 's observed distribution will be preserved in the loglinear model's distribution (Agresti, 2002; Holland & Thayer, 2000).

Loglinear Models' Underlying Distributions

Specific values of μ can result in loglinear models such as model 1 reflecting different underlying distributions. When μ is a vector of zeros or of any constant and β is also zero the loglinear model resolves into a uniform distribution, $\log_e(\rho) = \alpha$. The loglinear model that produces a uniform distribution reflects the notion that the i -level probabilities are all equal and independent of X .

Another choice for the loglinear model's underlying distribution is available when μ is defined as I constants that vary by the categories of X , μ_i . Holland and Thayer (2000, pp. 139-140) showed that when model 1 has a μ with entries

$$\mu_i = \log_e \binom{x_I}{x_i},$$

where $\binom{x_I}{x_i}$ denotes the binomial coefficient,

" x_I choose x_i ," then a binomial distribution can be produced by defining β as β_1 and defining $\mathbf{X}$ as a single column of values for fitting the first degree of X , $(x_1^1, x_2^1, \dots, x_I^1)'$. With these definitions model 1 can be expressed as,

$$\rho_i = \binom{x_I}{x_i} \pi^{x_i} (1 - \pi)^{x_I - x_i} \quad (3)$$

where π is a function of the mean of X ,

$$\pi = \frac{1}{x_I} \sum_i \rho_i x_i = \frac{1}{x_I} \bar{x},$$

and a function of β_1 ,

$$\pi = \frac{\exp(\beta_1)}{1 + \exp(\beta_1)}.$$

Thus, equation 3 implies that for fixed value, x_I , and a parameter based on the mean, π , the probability of obtaining a particular value of X is a variate from a binomial distribution based on x_I trials and success probability π .

Assessing the Role of the Loglinear Model's Underlying Distribution in Models of Population Distributions

The role of the underlying distribution used in loglinear models has not been extensively studied. The focus of loglinear modeling applications to psychometric test score distributions tends to be on fitting several of the observed distributions' moments – that is, more than three (Holland & Thayer, 2000; Kolen & Brennan, 2004); thus, the relatively simple uniform and binomial distributions underlying the fitted distributions have not received much attention. It is possible, however, that the uniform and binomial distributions underlying the models that fit observed distributions have subtle influences on the overall fit of the loglinear model.

To illustrate the influence of uniform and binomial distributions, consider how loglinear models based on each distribution fit eight different population distributions. Table 1 shows the eight population distributions of X variables with 10 categories. Six of the population distributions were obtained from Steele and Chasling's (2006) study: the decreasing, step, triangular, platykurtic and leptokurtic distributions. Two other population distributions are based on both considered underlying distributions (the uniform distribution and the binomial distribution with $\pi = 0.5$). An additional under-dispersed binomial distribution was created to be similar to the binomial distribution, but with a relatively small variance.

For each of the eight distributions, loglinear models similar to model 1 were fit based on the uniform distribution ($K=0$, $\mu_i=0$), and on fitting $K = 1, 2, 3$ and 4 moments with the loglinear model based on the uniform

UNDERLYING DISTRIBUTIONS IN LOGLINEAR MODELS OF DISCRETE DATA

distribution (equation 1 where μ is a vector of zeros). Other loglinear models comparable to model 1 were fit based on the binomial distribution, $K = 1$, $\mu_i = \log_e \left(\frac{x_i}{x_i} \right)$, and on fitting $K = 2, 3$ and 4 moments with the loglinear model based on the binomial distribution (equation 1 where μ has entries

$$\mu_i = \log_e \left(\frac{x_i}{x_i} \right).$$

Table 1's population distributions and the fits of the loglinear models to the population distributions for a hypothetical sample size of $N = 100$ are illustrated in Figures 1-16. These figures show the fits of the considered models in terms of individual score values and each model's summarized likelihood ratio Chi-square statistic:

$$G^2 = 2 \sum_i n_i \log_e \left(\frac{n_i}{N \hat{\rho}_i} \right).$$

Table 1: Population Distributions

X 's Categories & Moments	Uniform	Decreasing	Step	Triangular	Platykurtic	Leptokurtic	Binomial	Under- Dispersed Binomial
1	0.10	0.32	0.05	0.17	0.04	0.05	0.01	0.00
2	0.10	0.13	0.05	0.13	0.11	0.05	0.04	0.03
3	0.10	0.10	0.05	0.10	0.11	0.05	0.12	0.13
4	0.10	0.08	0.05	0.07	0.12	0.05	0.21	0.22
5	0.10	0.07	0.05	0.03	0.12	0.30	0.25	0.26
6	0.10	0.07	0.15	0.03	0.12	0.30	0.21	0.21
7	0.10	0.06	0.15	0.07	0.12	0.05	0.12	0.12
8	0.10	0.06	0.15	0.10	0.11	0.05	0.04	0.04
9	0.10	0.05	0.15	0.13	0.11	0.05	0.01	0.00
10	0.10	0.05	0.15	0.17	0.04	0.05	0.00	0.00
Mean	5.50	3.86	6.75	5.50	5.50	5.50	5.00	5.00
Std. Dev.	2.87	2.91	2.59	3.41	2.51	2.06	1.57	1.41
Skew	0.00	0.69	-0.68	0.00	0.00	0.00	0.02	0.04
Kurtosis	1.78	2.17	2.56	1.38	1.91	3.35	2.75	2.40

Figures 1-16 suggest that model fit is a function of the number of moments fit in the model and also show how closely the underlying distribution reflects the distribution being modeled. Loglinear models that fit $K = 3$ and 4 moments tend to have better fits (lower G^2 values) compared to models that fit $K = 0, 1$ and 2 moments, however, the loglinear model's underlying distribution appears to moderate the influence of K .

For population distributions more similar to the uniform distribution (i.e., the uniform, decreasing, step, triangular and platykurtic population distributions), models based on an underlying uniform distribution can closely fit the population distributions with fewer moments than those required by models based on an underlying binomial distribution (Figures 1, 3, 5, 7 & 9 vs. Figures 2, 4, 6, 8 & 10). For population distributions similar to the binomial distribution (i.e., the leptokurtic, binomial and under-dispersed binomial population distributions), models based on an underlying binomial distribution can closely fit the population distributions with fewer moments than those required by models based on an underlying uniform distribution (Figures 11, 13 & 15 vs. Figures 12, 14 & 16).

Methodology

To better understand the implications of results shown in Figures 1-16, a series of simulations was conducted. For the simulations of interest, 1,000 datasets of sample sizes 30, 100 and 1,000 were drawn from each of Table 1's population distributions. For each of the randomly drawn datasets, loglinear models were fit based on an underlying uniform distribution with $K = 0-4$, and also based on an underlying binomial distribution with $K = 1-4$. For models reflecting one of the two underlying distributions, the K values were selected based on nested Chi-square tests for differences in models' G^2 statistics (Haberman, 1974) and also on minimizing models' AIC statistics (Akaike, 1981).

To consider the influence of the underlying distribution for situations similar to what might be encountered in psychometric testing practice, where the moments to be fit in a test score distribution might be predetermined rather than statistically selected, modeling

results were also produced by always fitting $K = 4$ moments based on the both the uniform and the binomial distributions. The results of interest for each combination of sample size, underlying distribution and moment selection method were the percentages of datasets where specific K values were selected, the mean K values across all 1,000 datasets and the average model fit (i.e., mean G^2 values) across all 1,000 datasets.

Results

Simulation results are summarized in Tables 2-9. Each table presents the simulation results for one of Table 1's eight population distributions; rows show the simulation results for a specific combination of sample size (30, 100 or 1,000), underlying distribution (the uniform or binomial distribution) and selection method for K (G^2 , AIC , or $K = 4$). Each row's results show the percentage of moments (K) selected in the 1,000 simulated datasets, the mean of the selected K 's and the mean model fit (mean G^2). Because the percentages in Tables 2-9 are presented in rounded form, they do not always sum to exactly 100% within each row.

Some results shown in Tables 2-9 have been shown elsewhere (Moses & Holland, 2010). K selections based on the AIC result in larger K values than selections based on the G^2 . Selections based on sample sizes of 1,000 result in larger K values than selections based on smaller sample sizes. Models with larger K values fit the sample distributions more closely; that is, they result in smaller G^2 .

Tables 2-9 show that the influences of the G^2 and AIC selection strategies and the sample sizes are moderated by how closely the loglinear model's underlying distribution reflects the population distribution. For population distributions that closely reflect the uniform distribution (i.e., the uniform and decreasing population distributions, Tables 2-3), using the uniform distribution results in AIC and G^2 model selections with smaller mean K values and larger mean G^2 values than using the binomial distribution. These results were also partially obtained for the step population distribution (Table 4, $N = 30$ and 100), the triangular population distribution (Table 5, $N = 30$), and the leptokurtic population distribution (Table 7, $N = 30$ and 100).

UNDERLYING DISTRIBUTIONS IN LOGLINEAR MODELS OF DISCRETE DATA

Figure 1: Uniform Population Distribution Modeling Results
Based on an Underlying Uniform Distribution

Figure 2: Uniform Population Distribution Modeling Results
Based on an Underlying Binomial Distribution

Figure 3: Decreasing Population Distribution Modeling Results
Based on an Underlying Uniform Distribution

Figure 4: Decreasing Population Distribution Modeling Results
Based on an Underlying Binomial Distribution

UNDERLYING DISTRIBUTIONS IN LOGLINEAR MODELS OF DISCRETE DATA

Figure 5: Step Population Distribution Modeling Results
Based on an Underlying Uniform Distribution

Figure 6: Step Population Distribution Modeling Results
Based on an Underlying Binomial Distribution

Figure 7: Triangular Population Distribution Modeling Results
Based on an Underlying Uniform Distribution

Figure 8: Triangular Population Distribution Modeling Results
Based on an Underlying Binomial Distribution

UNDERLYING DISTRIBUTIONS IN LOGLINEAR MODELS OF DISCRETE DATA

Figure 9: Platykurtic Population Distribution Modeling Results
Based on an Underlying Uniform Distribution

Figure 10: Platykurtic Population Distribution Modeling Results
Based on an Underlying Binomial Distribution

Figure 11: Leptokurtic Population Distribution Modeling Results
Based on an Underlying Uniform Distribution

Figure 12: Leptokurtic Population Distribution Modeling Results
Based on an Underlying Binomial Distribution

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Figure 13: Binomial Population Distribution Modeling Results
Based on an Underlying Uniform Distribution

Figure 14: Binomial Population Distribution Modeling Results
Based on an Underlying Binomial Distribution

Figure 15: Under-Dispersed Binomial Population Distribution Modeling Results
Based on an Underlying Uniform Distribution

Figure 16: Under-Dispersed Binomial Population Distribution Modeling Results
Based on an Underlying Binomial Distribution

UNDERLYING DISTRIBUTIONS IN LOGLINEAR MODELS OF DISCRETE DATA

Table 2: Simulation Results for the Uniform Population Distribution

N	Underlying Distribution	Percentage of K Moments Selected (out of 1,000 replications)					Mean Moments (K)	Mean G^2
		0	1	2	3	4		
G^2 Selections of K								
30	Uniform	94%	1%	1%	2%	2%	0.16	9.37
	Binomial		0%	94%	3%	3%	2.08	7.75
100	Uniform	96%	1%	1%	1%	1%	0.11	8.97
	Binomial		0%	91%	4%	5%	2.15	7.56
1,000	Uniform	96%	2%	0%	1%	1%	0.08	8.38
	Binomial		0%	26%	25%	50%	3.24	7.11
AIC Selections of K								
30	Uniform	74%	12%	6%	4%	4%	0.52	8.35
	Binomial		0%	72%	16%	12%	2.41	6.80
100	Uniform	73%	13%	8%	4%	3%	0.51	7.84
	Binomial		0%	62%	21%	18%	2.56	6.28
1,000	Uniform	74%	13%	5%	5%	3%	0.49	7.28
	Binomial		0%	5%	13%	82%	3.77	5.22
Always Fit $K = 4$								
30	Uniform	0%	0%	0%	0%	100%	4.00	5.78
	Binomial	0%	0%	0%	0%	100%	4.00	5.78
100	Uniform	0%	0%	0%	0%	100%	4.00	5.22
	Binomial	0%	0%	0%	0%	100%	4.00	5.24
1,000	Uniform	0%	0%	0%	0%	100%	4.00	4.80
	Binomial	0%	0%	0%	0%	100%	4.00	4.96

Table 3: Simulation Results for the Decreasing Population Distribution

N	Underlying Distribution	Percentage of K Moments Selected (out of 1,000 replications)					Mean Moments (K)	Mean G^2
		0	1	2	3	4		
G^2 Selections of K								
30	Uniform	19%	62%	13%	5%	1%	1.08	10.62
	Binomial		0%	92%	5%	4%	2.12	8.21
100	Uniform	0%	35%	46%	16%	3%	1.86	9.55
	Binomial		0%	78%	9%	13%	2.35	8.17
1,000	Uniform	0%	0%	1%	69%	30%	3.29	8.61
	Binomial		0%	1%	3%	96%	3.96	6.84
AIC Selections of K								
30	Uniform	3%	36%	33%	21%	8%	1.96	7.58
	Binomial		0%	65%	22%	13%	2.49	7.09
100	Uniform	0%	6%	35%	40%	19%	2.72	6.35
	Binomial		0%	44%	21%	35%	2.91	6.38
1,000	Uniform	0%	0%	0%	27%	73%	3.73	6.84
	Binomial		0%	0%	0%	100%	4.00	6.67
Always Fit $K = 4$								
30	Uniform	0%	0%	0%	0%	100%	4.00	6.04
	Binomial	0%	0%	0%	0%	100%	4.00	6.04
100	Uniform	0%	0%	0%	0%	100%	4.00	5.43
	Binomial	0%	0%	0%	0%	100%	4.00	5.43
1,000	Uniform	0%	0%	0%	0%	100%	4.00	6.59
	Binomial	0%	0%	0%	0%	100%	4.00	6.67

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Table 4: Simulation Results for the Step Population Distribution

N	Underlying Distribution	Percentage of K Moments Selected (out of 1,000 replications)					Mean Moments (K)	Mean G^2
		0	1	2	3	4		
G^2 Selections of K								
30	Uniform	45%	44%	4%	6%	3%	0.78	11.57
	Binomial		1%	91%	3%	5%	2.13	8.95
100	Uniform	2%	72%	7%	17%	3%	1.48	12.34
	Binomial		0%	81%	4%	15%	2.33	10.90
1,000	Uniform	0%	0%	0%	69%	30%	3.30	37.72
	Binomial		0%	2%	1%	97%	3.95	38.01
AIC Selections of K								
30	Uniform	10%	50%	16%	17%	8%	1.63	8.65
	Binomial		0%	68%	16%	16%	2.48	7.91
100	Uniform	0%	35%	15%	34%	16%	2.32	9.68
	Binomial		0%	54%	12%	34%	2.81	9.50
1,000	Uniform	0%	0%	0%	30%	70%	3.70	36.16
	Binomial		0%	0%	0%	100%	4.00	37.84
Always Fit $K = 4$								
30	Uniform	0%	0%	0%	0%	100%	4.00	6.83
	Binomial	0%	0%	0%	0%	100%	4.00	6.89
100	Uniform	0%	0%	0%	0%	100%	4.00	8.32
	Binomial	0%	0%	0%	0%	100%	4.00	8.52
1,000	Uniform	0%	0%	0%	0%	100%	4.00	35.89
	Binomial	0%	0%	0%	0%	100%	4.00	37.84

Table 5: Simulation Results for the Triangular Population Distribution

N	Underlying Distribution	Percentage of K Moments Selected (out of 1,000 replications)					Mean Moments (K)	Mean G^2
		0	1	2	3	4		
G^2 Selections of K								
30	Uniform	46%	2%	44%	2%	7%	1.21	10.83
	Binomial		0%	93%	4%	3%	2.10	8.56
100	Uniform	1%	0%	75%	1%	22%	2.43	9.69
	Binomial		0%	88%	6%	6%	2.19	9.66
1,000	Uniform	0%	0%	0%	0%	100%	4.00	23.55
	Binomial		0%	14%	19%	66%	3.52	26.68
AIC Selections of K								
30	Uniform	17%	2%	50%	11%	19%	2.13	8.13
	Binomial		0%	71%	16%	12%	2.41	7.62
100	Uniform	0%	0%	46%	7%	46%	3.00	7.98
	Binomial		0%	56%	21%	23%	2.66	8.20
1,000	Uniform	0%	0%	0%	0%	100%	4.00	23.55
	Binomial		0%	2%	6%	92%	3.91	25.23
Always Fit $K = 4$								
30	Uniform	0%	0%	0%	0%	100%	4.00	6.50
	Binomial	0%	0%	0%	0%	100%	4.00	6.55
100	Uniform	0%	0%	0%	0%	100%	4.00	7.08
	Binomial	0%	0%	0%	0%	100%	4.00	7.24
1,000	Uniform	0%	0%	0%	0%	100%	4.00	23.55
	Binomial	0%	0%	0%	0%	100%	4.00	25.12

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Table 6: Simulation Results for the Platykurtic Population Distribution

N	Underlying Distribution	Percentage of K Moments Selected (out of 1,000 replications)					Mean Moments (K)	Mean G^2
		0	1	2	3	4		
G^2 Selections of K								
30	Uniform	74%	0%	17%	0%	9%	0.71	10.38
	Binomial		2%	91%	1%	6%	2.11	8.00
100	Uniform	26%	0%	50%	1%	24%	1.96	9.44
	Binomial		0%	86%	4%	10%	2.24	7.94
1,000	Uniform	0%	0%	0%	0%	100%	3.99	12.24
	Binomial		0%	16%	8%	76%	3.60	12.41
AIC Selections of K								
30	Uniform	44%	3%	29%	5%	19%	1.53	8.22
	Binomial		0%	70%	13%	16%	2.46	6.93
100	Uniform	7%	0%	41%	5%	47%	2.85	6.95
	Binomial		0%	60%	15%	26%	2.66	6.72
1,000	Uniform	0%	0%	0%	0%	100%	4.00	12.22
	Binomial		0%	2%	3%	96%	3.94	11.25
Always Fit $K = 4$								
30	Uniform	0%	0%	0%	0%	100%	4.00	5.88
	Binomial	0%	0%	0%	0%	100%	4.00	5.84
100	Uniform	0%	0%	0%	0%	100%	4.00	5.78
	Binomial	0%	0%	0%	0%	100%	4.00	5.67
1,000	Uniform	0%	0%	0%	0%	100%	4.00	12.22
	Binomial	0%	0%	0%	0%	100%	4.00	11.18

Table 7: Simulation Results for the Leptokurtic Population Distribution

N	Underlying Distribution	Percentage of K Moments Selected (out of 1,000 replications)					Mean Moments (K)	Mean G^2
		0	1	2	3	4		
G^2 Selections of K								
30	Uniform	11%	0%	42%	7%	41%	2.68	13.94
	Binomial		21%	16%	9%	54%	2.97	13.21
100	Uniform	0%	0%	3%	0%	97%	3.94	23.57
	Binomial		0%	1%	0%	99%	3.98	23.12
1,000	Uniform	0%	0%	0%	0%	100%	4.00	185.28
	Binomial		0%	0%	0%	100%	4.00	181.76
AIC Selections of K								
30	Uniform	3%	0%	21%	10%	66%	3.35	11.86
	Binomial		8%	11%	8%	73%	3.47	11.65
100	Uniform	0%	0%	1%	0%	99%	3.99	23.41
	Binomial		0%	0%	0%	100%	4.00	23.05
1,000	Uniform	0%	0%	0%	0%	100%	4.00	185.28
	Binomial		0%	0%	0%	100%	4.00	181.76
Always Fit $K = 4$								
30	Uniform	0%	0%	0%	0%	100%	4.00	11.17
	Binomial	0%	0%	0%	0%	100%	4.00	11.07
100	Uniform	0%	0%	0%	0%	100%	4.00	23.40
	Binomial	0%	0%	0%	0%	100%	4.00	23.05
1,000	Uniform	0%	0%	0%	0%	100%	4.00	185.28
	Binomial	0%	0%	0%	0%	100%	4.00	181.76

UNDERLYING DISTRIBUTIONS IN LOGLINEAR MODELS OF DISCRETE DATA

Table 8: Simulation Results for the Binomial Population Distribution

N	Underlying Distribution	Percentage of K Moments Selected (out of 1,000 replications)					Mean Moments (K)	Mean G^2
		0	1	2	3	4		
G^2 Selections of K								
30	Uniform	0%	0%	96%	1%	4%	2.08	6.09
	Binomial		94%	1%	1%	4%	1.15	6.86
100	Uniform	0%	0%	95%	1%	4%	2.09	6.89
	Binomial		94%	2%	1%	3%	1.13	7.62
1,000	Uniform	0%	0%	92%	1%	7%	2.14	7.46
	Binomial		96%	1%	1%	2%	1.10	7.69
AIC Selections of K								
30	Uniform	0%	0%	74%	9%	17%	2.43	5.11
	Binomial		72%	12%	6%	10%	1.53	5.82
100	Uniform	0%	0%	77%	10%	13%	2.36	6.12
	Binomial		75%	12%	6%	7%	1.46	6.70
1,000	Uniform	0%	0%	68%	11%	21%	2.53	6.31
	Binomial		76%	12%	7%	5%	1.42	6.78
Always Fit $K = 4$								
30	Uniform	0%	0%	0%	0%	100%	4.00	4.01
	Binomial	0%	0%	0%	0%	100%	4.00	3.99
100	Uniform	0%	0%	0%	0%	100%	4.00	4.99
	Binomial	0%	0%	0%	0%	100%	4.00	4.96
1,000	Uniform	0%	0%	0%	0%	100%	4.00	5.13
	Binomial	0%	0%	0%	0%	100%	4.00	5.08

Table 9: Simulation Results for the Under-Dispersed Binomial Population Distribution

N	Underlying Distribution	Percentage of K Moments Selected (out of 1,000 replications)					Mean Moments (K)	Mean G^2
		0	1	2	3	4		
G^2 Selections of K								
30	Uniform	0%	0%	91%	0%	9%	2.19	4.70
	Binomial		85%	5%	0%	10%	1.36	5.70
100	Uniform	0%	0%	79%	0%	21%	2.42	5.80
	Binomial		64%	18%	0%	18%	1.73	7.13
1,000	Uniform	0%	0%	0%	0%	100%	4.00	8.49
	Binomial		0%	0%	0%	100%	4.00	8.37
AIC Selections of K								
30	Uniform	0%	0%	71%	1%	27%	2.56	3.72
	Binomial		57%	24%	1%	18%	1.81	4.40
100	Uniform	0%	0%	49%	1%	50%	3.01	4.26
	Binomial		23%	40%	1%	36%	2.49	4.85
1,000	Uniform	0%	0%	0%	0%	100%	4.00	8.49
	Binomial		0%	0%	0%	100%	4.00	8.35
Always Fit $K = 4$								
30	Uniform	0%	0%	0%	0%	100%	4.00	2.56
	Binomial	0%	0%	0%	0%	100%	4.00	2.55
100	Uniform	0%	0%	0%	0%	100%	4.00	3.20
	Binomial	0%	0%	0%	0%	100%	4.00	3.18
1,000	Uniform	0%	0%	0%	0%	100%	4.00	8.49
	Binomial	0%	0%	0%	0%	100%	4.00	8.35

For population distributions that closely reflect the binomial distribution (i.e., the binomial and under-dispersed binomial population distributions, Tables 8-9), using the binomial distribution results in *AIC* and G^2 model selections with smaller mean K values and larger mean G^2 values than using the uniform distribution. Model selection results for the platykurtic population distribution were mixed (Table 6).

When loglinear models were fit with each underlying distribution using a predetermined $K = 4$, rather than a statistically selected K value, the results depended on how closely the underlying distribution reflected the population distribution. For the uniform, decreasing, step and triangular population distributions (Tables 2-5), the use of a predetermined K value of 4 resulted in slightly smaller mean G^2 values with the uniform distribution than the binomial distribution. For the platykurtic, leptokurtic, binomial and under-dispersed binomial population distributions (Tables 6-9), the use of a predetermined K value of 4 resulted in slightly smaller mean G^2 values with the binomial distribution than the uniform distribution.

Conclusion

The results of this study show that the loglinear model's underlying distribution has a small – but real – effect in modeling discrete distributions. This effect depends on the population distribution and on how the number of moments is determined. For models fitting a predetermined number of moments, this study shows that the use of a binomial underlying distribution can result in better fits for distributions that are similar to the binomial distribution, whereas the use of a uniform underlying distribution can result in better fits for distributions similar to the uniform distribution.

For the statistical selection of loglinear models in sample distributions, results suggest that using a distribution less similar to the distribution being modeled (e.g., using the binomial as the underlying distribution for uniformly distributed populations and samples)

results in more moments being chosen and slightly better model fit. The implications for modeling distributions more likely to resemble binomial distributions than uniform distributions (e.g., psychometric tests) are that better fitting models can be statistically selected when using an underlying uniform distribution, and better fitting models for a predetermined number of moments can be obtained using an underlying binomial distribution.

Results obtained herein are useful replications and extensions of other studies that have assessed statistical power for detecting departures from uniform distributions (Choulakian, Lockhart & Stephens, 1994; Pettitt & Stephens, 1977; Steele & Chaseling, 2006). This study also showed that the likelihood ratio (G^2) selection strategy had relatively moderate power levels and the *AIC* selection strategies had relatively high power levels compared to the strategies considered in Steele and Chaseling's study (i.e., the Kolmogorov-Smirnov, nominal Kolmogorov-Smirnov, Cramer-von Mises, Anderson-Darling, Pearson Chi-square and Watson's tests). Similar to the prior studies, this study found that power is higher when the underlying distribution is less similar to the distribution being modeled.

This study extends prior power studies by considering Type I error, where this study shows that Type I error rates were closer to 5% for the G^2 selection strategy than the *AIC* selection strategy. The more controlled Type I error rates of the G^2 selection strategy were observed both for the uniform distribution (underlying and population, Table 2) and also for the binomial distribution (underlying and population, Table 8). This study's findings that the G^2 and *AIC* selection strategies' Type I error and power tendencies for assessing binomial distributions are similar to those for assessing uniform distributions also extend prior studies that have primarily focused on detecting departures from uniform distributions. Results suggest that future studies considering loglinear models' underlying distributions would be useful for comparing other distributions and statistical selection strategies.

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The Impact of Violating Factor Scaling Method Assumptions On Latent Mean Difference Testing in Structured Means Models

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Type I error rates and power of the likelihood ratio test and bias of the standardized effect size measure associated with the latent mean difference in structured means modeling are examined when violating the assumptions underlying the two available factor scaling methods under various conditions. Implications and recommendations are discussed.

Key words: Structured means modeling, latent mean difference testing, non-invariant factor loadings, factor scaling methods, reference indicator.

Introduction

Many social science studies focus on comparing outcomes for groups categorized by observed variables such as gender, race or treatment group membership. Structural equation modeling (SEM) and, more specifically, structured means modeling (SMM; Sörbom, 1974) may be used to compare, for example, male and female high school students' latent variable means on math anxiety. The SMM approach is a multiple-group confirmatory factor analysis (MG-CFA) model in which the mean structure is incorporated into the model for testing the difference in latent variable means across groups.

As with traditional CFA techniques, each latent variable must be assigned a scale of measurement in SMM. This may be accomplished by either constraining one loading per factor to a value of one across groups or constraining each factor's variance to a value of one across groups (Kline, 2011). Both factor scaling methods require meeting certain assumptions. For example, the reference indicator (RI) strategy involves an assumption that the RI has invariant factor loadings across groups. The factor-variance scaling method, by contrast, is based on an assumption that the factor variances are equal across groups. To date, no published study has examined the effect on latent mean comparisons of constraining unequal factor loadings or unequal factor variances to a value of one across groups. The focus of this study is to investigate the impact of violating the assumptions underlying two factor scaling methods on the latent mean difference test and the standardized effect size measure associated with the latent mean difference in SMM.

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Structured Means Model and Testing Latent Mean Differences

A single-factor, p -indicator structured means model can be expressed in matrix notation using the following measurement equation:

$$\mathbf{x}_g = \mathbf{v}_g + \mathbf{\Lambda}_g \boldsymbol{\xi}_g + \boldsymbol{\delta}_g, \quad (1)$$

where g ($g = 1, 2, \dots, G$) represents group membership, $\mathbf{x}$ is a vector containing $p \times 1$ observed variable scores, $\mathbf{v}$ is a $p \times 1$ vector containing indicator variable intercepts, $\mathbf{\Lambda}$ is a $p \times 1$ vector of factor loadings that relates the observed indicator variables to the latent variable, ζ is a latent variable score and δ is a $p \times 1$ vector of normally distributed random measurement errors associated with the observed indicator variables.

In a structured means model (SMM), certain constraints are imposed in order to validly compare latent means across groups as well as to ensure model identification. The factor loadings and observed indicator variables' intercepts are constrained to be equal across groups in SMM. This allows latent mean differences detected between groups to be attributed to actual differences in the constructs as opposed to differences in the measurement of the constructs across the groups (Rock, Werts & Flaugher, 1978; Sörbom, 1974). In addition, it is not possible to estimate the intercepts of all observed indicator variables separately across groups as this would result in the under-identification of the means portion of the model (Sörbom, 1974).

Under the assumption of factor loading and intercept invariance, and assuming that the mean of the measurement errors within each group is equal to zero, the expected values of observed variables in each group can be expressed in matrix notation as:

$$E[\mathbf{x}_g] = \mu_g = \mathbf{v} + \mathbf{\Lambda}\kappa_g, \quad (2)$$

where κ_g is the latent variable mean for group g , $\mathbf{v}$ is a $p \times 1$ vector containing the observed variables' intercepts which are invariant across groups, and $\mathbf{\Lambda}$ represents a $p \times 1$ vector containing invariant factor loadings (Yoon & Millsap, 2007). In addition, assuming that the measurement errors are uncorrelated and that the measurement errors are uncorrelated with the latent variable in each group, g , the covariances among observed variables in each group can be expressed in matrix notation as:

$$\begin{aligned} E[(\mathbf{x}_g - \mu_g)(\mathbf{x}_g - \mu_g)'] &= \Sigma_g \\ &= \mathbf{\Lambda}\Phi_g\mathbf{\Lambda}' + \Theta_g \end{aligned} \quad (3)$$

where Φ is the latent variable variance, Θ is a $p \times p$ diagonal matrix containing p measurement error variances associated with the observed indicator variables and $\mathbf{\Lambda}$ represents a $p \times 1$ vector containing invariant factor loadings (Sörbom, 1974; Yoon & Millsap, 2007).

If factor loading and/or intercept invariance is not supported by means of model fit assessment and/or model comparisons, Byrne, Shavelson and Muthén (1989) suggested that some of the constraints may be relaxed and that partial invariance suffices when using the SMM approach to compare latent means across groups. It is important to note that there exists a debate concerning the issue of partial measurement invariance and the meaningful interpretation of latent mean differences in SMM. Some contend that strict invariance is required for valid interpretations of latent mean differences (Meredith, 1993), whereas others maintain that strong invariance is sufficient (Hancock, 1997; Thompson & Green, 2006). (In addition, some researchers have argued – and demonstrated – that meaningful interpretations of latent mean differences may be rendered under partial factor loading and partial intercept invariance; this debate is beyond the scope of this work but the interested reader is referred to: Byrne, Shavelson & Muthén, 1989; Muthén & Christofferson, 1981; Steenkamp & Baumgartner, 1998.)

The means portion of the model is estimated through use of a constant which is modeled to have direct effects on the latent and observed indicator variables. The constant's direct effect on a latent variable represents the latent variable mean and its effects on observed indicator variables represent observed variables' intercepts (Kline, 2011). An added constraint must also be imposed for identification of the means portion of the model. Namely, the latent mean in one group, treated as the reference group, must be constrained to zero whereas the latent means in the remaining $G - 1$ comparison groups are estimated. Therefore, the test of the latent mean of the $G - 1$ comparison groups

corresponds to a test of the latent mean difference between each of the $G - 1$ comparison group's and the reference group's latent mean (Hancock, 1997). For simplicity, a two-group comparison of the latent means in a single-factor model will be assumed for the ensuing discussion of latent mean comparisons in SMM.

Because the expected value of the latent variable is given by:

$$E(\xi_g) = \kappa_g, \quad (4)$$

the latent variable mean in the reference group for a two-group comparison of a single-factor model is:

$$E(\xi) = \kappa_1 = 0, \quad (5)$$

and the latent variable mean in the comparison group (group two) is:

$$E(\xi) = \kappa_2 - \kappa_1 = \kappa_2. \quad (6)$$

Accordingly, the null hypothesis tested in SMM is that the two groups' means are equal:

$$H_0 : \kappa_1 = \kappa_2. \quad (7)$$

The z test statistic is commonly used to evaluate the statistical significance of the latent mean difference estimate in SMM. If the z test statistic associated with the estimated latent mean difference is statistically significant, then it is inferred that there is a significant difference between the two groups' latent variable means. Unfortunately, the z test statistic is not invariant to the choice of factor scaling method. Consequently, the likelihood ratio test, LRT_κ , has been suggested to evaluate the statistical significance of the latent mean difference estimate in SMM because it is invariant to factor scaling procedures (Gonzalez & Griffin, 2001; Hancock, Lawrence & Nevitt, 2000).

When calculating the LRT_κ , two models must be estimated: The parameter of interest (the latent variable mean difference) is freely estimated in group two in one model but

is constrained to be equal to the reference group's latent variable mean value of zero in the second model. The LRT_κ is calculated as the difference between the two nested models' Chi-square (χ^2) statistics, and the LRT_κ is asymptotically distributed as a non-central χ^2 statistic:

$$LRT_\kappa = \Delta\chi^2 = \chi^2_{restricted} - \chi^2_{baseline\ model}, \quad (8)$$

where $\chi^2_{restricted}$ is the χ^2 statistic associated with the model in which the latent variable mean difference is constrained to a value of zero and $\chi^2_{baseline\ model}$ is the χ^2 statistic associated with the model in which the latent mean is freely estimated in group two. The LRT_κ has corresponding degrees of freedom equal to the difference in the degrees of freedom associated with each model and is calculated to evaluate whether there is a statistically significant drop in model fit when constraining a particular parameter (the latent variable mean difference) to zero. A significant LRT_κ indicates that the parameter of interest differs significantly from zero.

Although the LRT_κ may be used to evaluate whether there is a statistically significant difference between two groups' latent means, it does not provide any information about the practical significance of the latent mean difference. Hancock (2001) suggested using a standardized effect size measure, $\hat{\delta}_\kappa$, to describe the practical difference between two groups' latent means. When using the SMM approach, the standardized latent mean difference effect size, $\hat{\delta}_\kappa$, is estimated as follows:

$$\begin{aligned} \hat{\delta}_\kappa &= (\hat{k}_1 - \hat{k}_2) / \hat{\phi}^{1/2} = \hat{k}_2 / \hat{\phi}^{1/2}, \\ \hat{\delta}_\kappa &= |\hat{k}_1 - \hat{k}_2| / \hat{\phi}^{1/2} = \hat{k}_2 / \hat{\phi}^{1/2} \end{aligned} \quad (9)$$

where $\hat{k}_1$ and $\hat{k}_2$ represent groups one and two latent mean estimates, respectively. For model identification purposes, the latent mean of the reference group (group one) is typically constrained to a value of zero, but the latent mean of the comparison group (group two) is estimated (Hancock, 1997), resulting in the rightmost expression of Equation 9. The pooled factor variance estimate, $\hat{\phi}$, is determined as follows:

$$\hat{\phi} = (n_1\hat{\phi}_1 + n_2\hat{\phi}_2) / (n_1 + n_2) \quad (10)$$

where $\hat{\phi}_1$ and $\hat{\phi}_2$ are the estimated factor variances for groups one and two, respectively, and n_1 and n_2 represent the sample sizes for groups one and two, respectively. It is important to note that the calculation and use of the pooled factor variance involves an assumption of homogeneity of the two groups' factor variances. The interpretation of $\hat{\delta}_\kappa$ is similar to that in conventional univariate analyses. For example, $\hat{\delta}_\kappa = 0.5$ can be interpreted as indicating that the two groups' latent mean estimates differ by half a standard deviation (Hancock, 2001).

Factor Scaling Method Implications and Related Research

Both factor scaling methods may be used to scale the latent variable in a structured means model and both involve strict assumptions. For example, the factor-variance-based scaling method is grounded on the assumption that the factor variance is invariant across groups. If the factor variances are not equal across groups, the scale of the factor loadings will be changed, possibly making truly invariant factor loadings falsely appear non-invariant across groups. This could also make the metric invariance test less accurate (Cheung & Rensvold, 1999; Kline, 2011; Yoon & Millsap, 2007).

The reference indicator (RI) strategy is based on the assumption that the RI's loading is invariant across groups. If this assumption is violated, all other factor loadings in a structured

means model will be rescaled. Constraining the RI's non-invariant factor loadings to a value of one across groups will result in different metrics for the two groups' factor loadings and can lead to incorrect inferences about the changed loadings' invariance; therefore, it is important to select an item that has invariant factor loadings across groups to serve as the RI in a structured means model (Johnson, Meade & DuVernet, 2009).

Although assumptions associated with the two factor scaling methods are important, researchers have not examined the issue to a great extent. For example, Johnson, Meade and DuVernet (2009) conducted a literature review of studies published between 2005 and 2007 that involved measurement invariance (MI) tests; only 17 out of 153 studies referenced Cheung and Rensvold's (1999) study in which a new technique to select invariant item sets to serve as the RI was recommended. Most research simply assumed that the selected RI variable had invariant factor loadings across groups; consequently, it is essential that the impact of violating the assumptions associated with the two factor scaling methods be inspected in order to better inform applied users of SMM.

Previous studies germane to this study include those in which the effect of partial metric invariance on latent mean difference testing was assessed. For example, Kaplan and George (1995) conducted a population study to assess the power to detect latent mean differences between two groups in the SMM approach while manipulating the magnitude of the latent mean difference, group sample size ratio, frequency of non-invariant factor loadings, factor loading size, factor loading pattern and the number of observed indicators per factor. Because factor loadings were varied in the study, the determinant of the covariance matrix [$\det(\Sigma)$] was also varied. The determinant corresponds to the generalized variance, which indicates the amount of variance shared among a set of variables. Two combinations of ratios of larger sample size (n_{Larger}) to generalized variance [$\det(\Sigma)$] conditions were examined, including a positive, $n_{Larger}:\det(\Sigma)$, condition in which the group with the larger sample size was paired with the larger generalized variance, and

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a negative, $n_{Larger}:\det(\Sigma)$, condition in which the group with the larger sample size was paired with the smaller generalized variance.

The findings demonstrated that when the magnitude of the latent mean difference increased, the power of the latent mean difference test increased and the sample size ratio between the two groups tended to influence the power of the latent mean difference test. When the group sample sizes were equal, the power of the latent mean difference test was less affected by non-invariant factor loadings. However, when unequal sample sizes were present, the power associated with the latent mean difference test was low even though factor loading invariance held. A large drop in power was observed as the group sample size ratio increased which was observed in both positive and negative conditions. Nonetheless, higher power always occurred in the positive $n_{Larger}:\det(\Sigma)$ condition as compared to the negative $n_{Larger}:\det(\Sigma)$ condition. Finally, the power of the latent mean difference test increased when the model consisted of more indicator variables per factor.

Hancock, Lawrence and Nevitt (2000) conducted both a Monte Carlo simulation study and a population study investigating how partial metric invariance affected the Type I error rates and the power, respectively, of the latent mean difference test between two groups using SMM, multiple-indicator multiple-cause (MIMIC) modeling, and MANOVA approaches. Manipulated conditions included latent mean difference magnitude, total sample size, group sample size ratio, frequency of non-invariant factor loadings, factor loading size and factor loading pattern. Factor loading pattern manipulations resulted in four scenarios: (1) metric invariance with equal factor loadings across and within two groups; (2) metric invariance with equal factor loadings across two groups but unequal within groups; (3) metric non-invariance with approximately equivalent generalized variances for the two groups; and (4) metric non-invariance with different generalized variances for the two groups.

Type I error rates of the latent mean difference tests in all three approaches were well controlled under metric invariance, approximately equivalent group generalized

variance, and equal group sample size conditions. When both the sample size and the generalized variance were unequal between the two groups, however, Type I error rates of the latent mean difference test in the three approaches varied. The SMM approach was the only one in which Type I error rates were well controlled under all manipulated conditions. The Type I error rates when using the MIMIC approach were too low under the negative $n_{Larger}:\det(\Sigma)$ condition (larger sample size paired with smaller generalized variance) and were too high under the positive $n_{Larger}:\det(\Sigma)$ condition (larger sample size paired with larger generalized variance). The opposite pattern of Type I error rates were observed when using the MANOVA approach.

The power of the latent mean difference test in the three approaches increased when the sample size, magnitude of the factor loadings, and magnitude of the latent mean difference increased. When the sample size ratio between the two groups became larger, the power of the latent mean difference test in the three approaches decreased. Overall, the power of the latent mean difference test when using the MIMIC technique tended to be approximately equal to, or marginally higher than, the power when using the SMM technique, but the power associated with the MANOVA approach was the lowest. When different generalized variances were paired with unequal sample sizes, results indicated that the SMM approach had greater power in the negative $n_{Larger}:\det(\Sigma)$ condition whereas the MIMIC approach had greater power in the positive $n_{Larger}:\det(\Sigma)$ condition.

Hancock et al. (2000) reported that both SMM and MIMIC approaches were acceptable under equal group sample sizes. The SMM approach, however, was recommended under unequal group sample sizes. The choice of the SMM approach was based on its flexibility in accommodating non-invariant factor loadings. Additionally, the SMM approach had satisfactory power without sacrificing the Type I error rate. In contrast, the MIMIC approach's slightly higher power was marred by the potential cost of Type I error inflation (Hancock, et al., 2000).

Previous studies investigating the effects of partial measurement invariance on latent mean difference detection under various conditions have found that group sample size ratio, factor loading pattern, loading difference magnitude, and latent mean difference magnitude can affect both or either the Type I error rate and power of latent mean difference tests. However, previous simulation studies have not devoted much attention to the assumption underlying the RI strategy and – to the authors' knowledge – no published study has investigated the effect of violating the assumption underlying the factor-variance scaling method. The purpose of this Monte Carlo simulation study is to investigate the performance of the likelihood ratio test (LRT_{κ}) and the standardized latent mean difference effect size measure ($\hat{\delta}_{\kappa}$) when violating the assumptions fundamental to the two factor scaling methods and using the SMM approach to test latent mean differences.

Methodology

The impact of violating the assumptions associated with the two factor scaling methods on the performance of the LRT_{κ} and $\hat{\delta}_{\kappa}$ were examined under varied conditions, including group sample size ratio, factor loading pattern, loading difference magnitude, latent mean difference magnitude and group factor variance ratio. For each generated sample of data, two factor scaling methods (constraining one loading per factor to a value of one for both groups and assigning a value of one to each factor's variance for both groups) were implemented. The performance of the LRT_{κ} was evaluated via an assessment of its Type I error rates and power under specified conditions. The performance of the $\hat{\delta}_{\kappa}$ in terms of the parameter bias and relative parameter bias under certain conditions was also evaluated.

For simplicity, two groups' latent variable means were compared using the SMM approach. The model used for data generation and estimation was a simple, single-factor model with six observed indicator variables. The choice of the six observed indicator variables was based on designs of previous simulation studies (e.g.,

Kaplan & George, 1995) and reflects what has been found in applied research (Hinkin, 1995). The values of all invariant factor loadings were set to 0.4 to represent factor loadings commonly observed in applied studies (Enders & Finney, 2003) and because a relatively large loading difference value across groups was included and resulted in markedly large non-invariant factor loadings.

All observed variable intercepts were set to zero across groups in the generating models. Residual variances associated with the observed variables were calculated as one minus the squared condition-specific standardized factor loading. Error covariances were not modeled in the generating or estimating models. Total sample size was 500 and was not varied. This sample size was used because it is in the range of sample sizes utilized in previous simulation research in which adequate power was obtained (e.g., Hancock, et al., 2000) and permits the examination of reasonably disparate group sample sizes.

Manipulated Conditions: Group Sample Size Ratio

Three group sample size ratio conditions ($n_1: n_2$) were used when generating the data. The equal sample size condition (1:1) served as a baseline condition in which the sample size in each group was equal to 250. Two unequal sample size ratio conditions (1:4 and 4:1) were also used to generate the data: data in the 1:4 condition were generated such that the sample size was 100 and 400 in group one and in group two, respectively, and data in the 4:1 condition were generated in which the two groups' sample sizes were reversed.

Manipulated Conditions: Factor Loading Pattern

Five factor loading patterns were manipulated in this study. In the equal factor loading pattern condition, all factor loadings were generated to be invariant across groups to serve as a baseline condition. In the 1st loading unequal pattern condition, the RI's (here, the first observed indicator variable's) factor loading was set to be higher in group two than in group one by the condition-specific factor loading difference. In the 2nd loading unequal pattern condition, the factor loading of a non-RI

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variable (here, the second observed indicator variable) was set to be higher in group two than in group one by the condition-specific factor loading difference. In the all lower pattern condition and the mixed pattern condition, both the RI and the second observed indicator variable had non-invariant factor loadings across groups in the generating models. In the all lower pattern condition, both of the non-invariant factor loadings had lower true values in group one. In the mixed pattern condition, the true factor loading value for the RI was higher in group one and the true factor loading value for the second observed indicator variable was higher in group two.

Manipulated Conditions: Loading Difference Magnitude

Two factor loading difference values ($|\lambda_1 - \lambda_2| = 0.1$ and $|\lambda_1 - \lambda_2| = 0.4$) were investigated in the current simulation study to represent small and large differences. These two values are in the range of factor loading difference values investigated in previous simulation research (Hancock, et al., 2000; Kaplan & George, 1995). These factor loading differences were added to the invariant factor loading value of 0.4, resulting in factor loading non-invariance across groups (with loading values of 0.5 and 0.8, respectively).

Manipulated Conditions: Latent Mean Difference Magnitude

This study considered two latent mean difference values ($\kappa_2 - \kappa_1 = 0$ and $\kappa_2 - \kappa_1 = 0.5$). The condition of equal latent means ($\kappa_2 - \kappa_1 = 0$) across groups was included because this permits an assessment of the Type I error rates associated with the LRT_{κ} and the performance of the $\hat{\delta}_{\kappa}$ in terms of parameter bias. Scenarios with unequal latent means across groups were also investigated in order to assess the power of the LRT_{κ} and the performance of the $\hat{\delta}_{\kappa}$ in terms of relative parameter bias. A moderately large latent mean difference value ($\kappa_2 - \kappa_1 = 0.5$) was included because previous simulation studies found sufficient power with this latent mean difference value (Hancock, et al., 2000; Kaplan & George, 1995).

Manipulated Conditions: Group Factor Variance Ratio

In the simulation study, three factor variance ratio conditions ($\Phi_1 : \Phi_2$) were considered. In the first factor variance ratio condition, the factor variances for the two groups were set to be equal (1:1). In the second and third factor variance ratio conditions, the factor variances for the two groups were set to be unequal with a ratio of 0.8:1.2 and 1.2:0.8. These two unequal factor variance conditions represent a realistic yet moderate difference (Kim, Cramond & Bandalos, 2006) between the two groups' factor variances which provides a starting point for this line of research.

Data Generation

Raw data for the two groups were generated in SAS (Version 9.2; SAS Institute Inc., 2008) according to the specified population parameters for a single-factor, six-indicator CFA model using the Kaiser and Dickman (1962) matrix decomposition procedure (Fan & Fan, 2005). Thus, each generated sample of data consisted of $n_1 \times 6$ and $n_2 \times 6$ matrices for group one and group two, respectively, where n_1 and n_2 represent the condition-specific sample size for each of the two groups. One thousand (1,000) raw data sets were generated for each of the 162 combinations of manipulated conditions. After raw data for the two groups were generated, SAS 9.2 was programmed to call DOS to run *Mplus* (Version 6.1; Muthén & Muthén, 2010), as described by Gagné and Furlow (2009), to estimate the models. Maximum likelihood (ML) estimation was used to estimate all model parameters.

When estimating the model parameters, cross-group constraints were imposed on all factor loadings and observed variable intercepts whereas error variances were freely estimated in both groups. When using the RI strategy to scale the factor, the RI's loading was constrained to a value of one in both groups. Two different structured means models were estimated. The traditional structured means model was estimated in which the latent mean of group one was constrained to be equal to zero but the latent mean of group two was estimated freely (the SMM_{κ^*} model) and another model in which the

latent means for both groups were constrained to zero (the SMM_{κ_0} model) was estimated. Also, two factor scaling methods were used to set the scale of the latent variable for each generated data set. When using the RI strategy, the first factor loading was constrained to a value of one across groups, all other factor loadings were constrained to be equal across groups, and factor variances for the two groups were freely estimated. When the factor-variance-based scaling method was implemented, the factor variance was instead constrained to a value of one across groups and all factor loadings were estimated yet constrained to be equal across groups. Thus, for each generated data set, four models (two factor scaling methods $\times$ two latent mean constraints) were estimated. It is important to note that the models using the factor-variance scaling method had one degree of freedom more than the models using the RI strategy.

Data Analysis

The χ^2 statistic associated with each estimated model from each replication was saved to calculate the LRT_{κ} (see Equation 8) between the two estimated models (SMM_{κ^*} and SMM_{κ_0}) when using each of the two factor scaling methods. The performance of the LRT_{κ} was evaluated by summarizing its Type I error rates and power. Type I error rates of the LRT_{κ} , defined as the proportion of incorrect rejections of the null hypothesis ($H_0 : \kappa_1 = \kappa_2$) out of the 1,000 replications in equal latent mean conditions ($\kappa_2 - \kappa_1 = 0$), were evaluated using Bradley's (1978) liberal criterion of $\alpha \pm 1/2\alpha$ (where $\alpha = 0.05$) such that rates less than 2.5% were considered overly conservative and rates greater than 7.5% were considered overly liberal.

The power of the LRT_{κ} is defined as the proportion of correct rejections of the null hypothesis ($H_0 : \kappa_1 = \kappa_2$) out of the 1,000 replications in unequal latent mean conditions ($\kappa_2 - \kappa_1 = 0.5$). A minimum power criterion of 0.8 is traditionally recommended as a reasonable level of power (Cohen, 1988), whereas others

have recommended a minimum power criterion of 0.95 as a more appropriate level of power (Cashen & Geiger 2004; Rossi, 1990). In this study, a minimum power criterion of 0.9 was selected to gauge the adequacy of the power associated with the LRT_{κ} as a compromise between the traditional and more stringent power recommendations.

The latent mean estimate in group two and the factor variance estimates in both groups were saved from the SMM_{κ^*} model, which were used to estimate the standardized latent mean difference effect size, $\hat{\delta}_{\kappa}$ (see Equations 9 and 10). The performance of the $\hat{\delta}_{\kappa}$ was examined through an assessment of its parameter bias and relative parameter bias under specific latent mean difference magnitude conditions. In conditions in which the latent mean difference was equal to zero ($\kappa_2 - \kappa_1 = 0$), the parameter bias of $\hat{\delta}_{\kappa}$ was calculated as follows:

$$B(\hat{\delta}_{\kappa}) = \bar{\hat{\delta}}_{\kappa} - 0, \quad (11)$$

where $\bar{\hat{\delta}}_{\kappa}$ is the mean of the $\hat{\delta}_{\kappa}$ estimates across the 1,000 replications in each relevant condition (Hoogland & Boomsma, 1998). The relative parameter bias of the $\hat{\delta}_{\kappa}$ was calculated with conditions in which the latent mean difference was equal to 0.5 ($\kappa_2 - \kappa_1 = 0.5$) as:

$$RPB(\hat{\delta}_{\kappa}) = \frac{\bar{\hat{\delta}}_{\kappa} - 0.5}{0.5} \quad (12)$$

(Hoogland & Boomsma, 1998). According to Hoogland and Boomsma (1998), conditions in which the $|B(\hat{\delta}_{\kappa})|$ or the $|RPB(\hat{\delta}_{\kappa})|$ is less than 0.05 indicates acceptable levels of bias in the $\hat{\delta}_{\kappa}$.

Results

The results describing the performance of the LRT_{κ} are presented first, including Type I error

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Table 1: Explanations of Abbreviations Used in the Tables of Results

Abbreviation	Explanation
RI	Reference indicator strategy implemented
FV	Factor-variance-based scaling method implemented
Equal Loading	All factor loadings were equal/invariant across groups
1 st Loading Unequal	The first factor loading (RI) was higher in group two than in group one with the condition-specific loading difference
2nd Loading Unequal	The second (non-RI) factor loading was higher in group two than in group one with the condition-specific loading difference
All Lower	Both the first (RI) and second (non-RI) factor loading were higher in group two than in group one with the condition-specific loading difference
Mixed	The first factor loading (RI) was higher in group one than in group two and the second (non-RI) factor loading was higher in group two than in group one with the condition-specific loading difference

rates and power. The results describing the performance of the $\hat{\delta}_\kappa$, including parameter and relative parameter bias, are subsequently presented. Table 1 provides the explanations of abbreviations used in all the Tables illustrating the performance of the LRT_κ and the $\hat{\delta}_\kappa$.

Performance of the LRT_κ : Type I Error Rates

Table 2 presents the observed Type I error rates associated with the LRT_κ under equal latent mean conditions ($\kappa_2 - \kappa_1 = 0$). Values above the dashed line in Table 2 are the Type I error rates in the equal/invariant factor loading conditions and, thus, for scenarios in which the covariance structures are appropriately modeled. Values below the dashed line in Table 2 are the Type I error rates in the unequal/non-invariant factor loading conditions and, thus, for scenarios in which the covariance structures are not modeled appropriately. In each

design cell, Type I error rates when implementing the RI strategy and when implementing the factor-variance (FV) scaling method are both reported. Employing Bradley's (1978) criterion, Table 2 shows overly conservative Type I error rates (i.e., less than or equal to 2.5%) denoted with boldface and italics; overly liberal rates (i.e., greater than or equal to 7.5%) are underlined.

In the equal/invariant factor loading conditions, all observed Type I error rates when using the RI strategy were within the criterion of 0.05 ± 0.025 . Type I error rates did not appear to vary substantially or systematically as a function of group sample size ratio or group factor variance ratio. Upon implementing the factor-variance scaling method, one Type I error rate was found to be overly liberal (0.079) in the condition with the group sample size ratio of 1:4 and the group factor variance ratio of 1.2:0.8.

In the unequal/non-invariant factor loading conditions, the Type I error rates when the RI strategy was implemented were within the

acceptable range of 0.05 ± 0.025 . When the factor-variance scaling method was used, however, twelve observed Type I error rates were beyond the criterion of 0.05 ± 0.025 . These unacceptable Type I error rates all occurred in the unequal sample size conditions such that liberal rates tended to occur in the 4:1 group sample size ratio scenarios and conservative rates tended to occur in the 1:4 group sample size ratio scenarios. Further, the majority (83%) of these unacceptable Type I error rates were found in the large loading difference ($|\lambda_1 - \lambda_2| = 0.4$) magnitude conditions (see Table 2).

Power of the LRT_{κ}

Table 3 presents the observed power rates associated with the LRT_{κ} under conditions in which the latent mean difference was unequal across groups ($\kappa_2 - \kappa_1 = 0.5$). A criterion of 0.90 was used to evaluate the power of the LRT_{κ} ; hence, power rates below 0.90 were deemed too low (see Table 3). In the equal factor loading conditions, three power rates fell below the 0.90 cutoff when the RI strategy was implemented. These occurred in the 1:1 group factor variance ratio with the 4:1 group sample size ratio condition, in the 1.2:0.8 group factor variance ratio with the 1:4 group sample size ratio condition, and in the 0.8:1.2 group factor variance ratio with the 4:1 group sample size ratio condition. Although these values were lower than the cutoff criterion, they were not substantially lower than a value of 0.90, ranging from 0.866 to 0.888. Power tended to be higher in the equal group sample size conditions, but it did not vary substantially or systematically as a function of the group factor variance ratio under the RI strategy.

When the factor-variance scaling method was implemented under equal factor loadings, five out of nine power rates were lower than 0.90. Nonetheless, these values did not deviate substantially from 0.90 (range was from 0.891 to 0.894) and all were found in the unequal sample size conditions. Power rates were higher in the equal sample size conditions than in the unequal sample size conditions. Additionally, power rates when using the factor-variance scaling method did not differ markedly

as a function of the group factor variance ratio (see Table 3).

In the unequal factor loading conditions, five power rates were lower than 0.90 when using the RI strategy which all occurred in conditions in which the loading difference was small ($|\lambda_1 - \lambda_2| = 0.1$) and the group sample sizes were unequal (1:4 or 4:1). Again, these power rates were not substantially lower than the cutoff criterion, ranging from 0.890 to 0.898 (see Table 3). Power tended to be marginally higher when the loading difference was large ($|\lambda_1 - \lambda_2| = 0.4$) than when small ($|\lambda_1 - \lambda_2| = 0.1$). Across the three group sample size ratios, power rates were slightly higher when sample sizes were equal across groups than when they were unequal. Further, power rates under the RI strategy did not vary substantially as a function of the group factor variance ratios or the factor loading patterns.

When the factor-variance scaling method was implemented under unequal factor loadings, two observed power rates were lower than the cutoff criterion, although they did not differ substantially from the 0.90 criterion (0.890 and 0.892). These two low power rates were found in conditions in which the loading difference was small ($|\lambda_1 - \lambda_2| = 0.1$) with the 0.8:1.2 group factor variance ratio and 1:4 group sample size ratio (see Table 3). Power when using the factor-variance scaling method was consistent with the power found when using the RI strategy. Specifically, power rates were marginally higher when the loading difference was large than when it was small and when sample sizes were equal across groups than when unequal. In addition, power rates did not vary considerably as a function of group factor variance ratio or the factor loading pattern when implementing the factor-variance scaling method.

Performance of the $\hat{\delta}_{\kappa}$: Parameter Bias of the $\hat{\delta}_{\kappa}$

Parameter bias of the standardized latent mean difference effect size measure ($\hat{\delta}_{\kappa}$) was calculated in conditions in which the true latent mean difference was equal to zero

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Table 2: Type I Error Rates Associated with the Likelihood Ratio Test as a Function of Manipulated Conditions ($\kappa_2 - \kappa_1 = 0$)

Loading Difference	Loading Pattern	Group Sample Size Ratio	Group Factor Variance Ratio					
			1:1		1.2 :0.8		0.8:1.2	
			RI	FV	RI	FV	RI	FV
0	Equal Loading	250:250	0.056	0.057	0.049	0.051	0.058	0.058
		100:400	0.062	0.052	0.060	<u>0.079</u>	0.059	0.044
		400:100	0.068	0.067	0.051	0.037	0.055	0.070
0.1	1 st Loading Unequal	250:250	0.047	0.045	0.050	0.049	0.057	0.058
		100:400	0.047	0.043	0.046	0.052	0.068	0.046
		400:100	0.043	0.044	0.062	0.054	0.056	0.068
	2 nd Loading Unequal	250:250	0.046	0.046	0.046	0.046	0.050	0.051
		100:400	0.052	0.051	0.047	0.058	0.059	0.047
		400:100	0.038	0.045	0.052	0.040	0.064	<u>0.083</u>
	All Lower	250:250	0.068	0.067	0.057	0.060	0.071	0.071
		100:400	0.056	0.049	0.054	0.064	0.045	0.029
		400:100	0.058	0.070	0.049	0.038	0.051	0.068
	Mixed	250:250	0.048	0.048	0.054	0.055	0.047	0.046
		100:400	0.050	0.049	0.049	0.059	0.052	0.037
		400:100	0.053	0.054	0.056	0.040	0.059	<u>0.081</u>
0.4	1 st Loading Unequal	250:250	0.044	0.043	0.058	0.059	0.044	0.042
		100:400	0.048	0.030	0.053	0.044	0.060	<i>0.019</i>
		400:100	0.058	0.070	0.054	0.054	0.061	<u>0.096</u>
	2 nd Loading Unequal	250:250	0.053	0.050	0.054	0.054	0.055	0.053
		100:400	0.055	0.027	0.053	0.050	0.049	<i>0.025</i>
		400:100	0.050	0.064	0.045	0.043	0.051	<u>0.085</u>
	All Lower	250:250	0.055	0.050	0.048	0.044	0.050	0.040
		100:400	0.044	<i>0.016</i>	0.066	0.046	0.061	<i>0.016</i>
		400:100	0.045	<u>0.082</u>	0.047	0.059	0.051	<u>0.113</u>
	Mixed	250:250	0.055	0.056	0.052	0.052	0.042	0.041
		100:400	0.050	0.041	0.045	0.058	0.040	<i>0.021</i>
		400:100	0.038	0.029	0.045	<i>0.024</i>	0.046	0.052

Note: Type I error rates less than 0.025 are bold and italicized. Type I error rates greater than 0.075 are underlined. Abbreviations used in this table are described in Table 1.

Table 3: Power Associated with the Likelihood Ratio Test as a Function of Manipulated Conditions
($\kappa_2 - \kappa_1 = 0.5$)

Loading Difference	Loading Pattern	Group Sample Size Ratio	Group Factor Variance Ratio					
			1:1		1.2 :0.8		0.8:1.2	
			RI	FV	RI	FV	RI	FV
0	Equal Loading	250:250	0.979	0.979	0.983	0.983	0.982	0.982
		100:400	0.906	0.906	<u>0.866</u>	<u>0.892</u>	0.911	<u>0.893</u>
		400:100	<u>0.888</u>	<u>0.891</u>	0.920	<u>0.894</u>	<u>0.873</u>	<u>0.893</u>
0.1	1 st Loading Unequal	250:250	0.987	0.988	0.983	0.982	0.980	0.981
		100:400	0.924	0.926	0.927	0.937	0.941	0.921
		400:100	<u>0.898</u>	0.905	0.929	0.916	<u>0.897</u>	0.927
	2 nd Loading Unequal	250:250	0.984	0.984	0.988	0.988	0.982	0.982
		100:400	0.925	0.917	<u>0.890</u>	0.911	0.920	<u>0.890</u>
		400:100	0.904	0.912	0.947	0.936	0.912	0.937
	All Lower	250:250	0.991	0.991	0.993	0.993	0.994	0.994
		100:400	0.935	0.928	0.939	0.942	0.953	0.926
		400:100	0.919	0.931	0.938	0.927	0.916	0.929
	Mixed	250:250	0.983	0.984	0.985	0.986	0.986	0.986
		100:400	0.906	0.901	<u>0.890</u>	0.903	0.908	<u>0.892</u>
		400:100	0.911	0.908	0.942	0.924	<u>0.892</u>	0.910
0.4	1 st Loading Unequal	250:250	0.998	0.998	1.000	1.000	0.999	0.999
		100:400	0.971	0.967	0.975	0.978	0.989	0.971
		400:100	0.964	0.973	0.973	0.979	0.940	0.962
	2 nd Loading Unequal	250:250	0.997	0.997	0.999	0.999	0.998	0.998
		100:400	0.984	0.967	0.976	0.979	0.984	0.966
		400:100	0.965	0.974	0.974	0.974	0.944	0.962
	All Lower	250:250	1.000	1.000	0.999	0.999	1.000	1.000
		100:400	0.993	0.980	0.993	0.989	0.995	0.981
		400:100	0.982	0.995	0.993	0.995	0.971	0.990
	Mixed	250:250	0.995	0.996	0.995	0.997	0.998	0.998
		100:400	0.961	0.957	0.953	0.964	0.972	0.959
		400:100	0.925	0.920	0.931	0.906	0.924	0.932

Note: Power rates below 0.90 are underlined. Abbreviations used in this table are described in Table 1.

$(\kappa_2 - \kappa_1 = 0)$. A cutoff value of 0.05 was used to evaluate the acceptability of the parameter bias, meaning that absolute parameter bias values less than 0.05 indicated acceptable bias (Hoogland & Boomsma, 1998). No substantial parameter bias was found across conditions examined with bias values ranging from -0.010 to 0.013 . Although both negative and positive parameter bias was observed, no clear trend was noticed.

Performance of the $\hat{\delta}_\kappa$: Relative Parameter Bias of the $\hat{\delta}_\kappa$

In conditions where the true latent mean difference was equal to 0.5 ($\kappa_2 - \kappa_1 = 0.5$), relative parameter bias of the $\hat{\delta}_\kappa$ was calculated. Table 4 presents the relative parameter bias of the $\hat{\delta}_\kappa$ for each combination of manipulated conditions. Following Hoogland & Boomsma (1998), a minimum cutoff of 0.05 was used to represent a substantial degree of bias (see Table 4).

In the equal factor loading conditions, relative parameter bias was acceptable, regardless of the factor scaling method used. Relative parameter bias when using the RI strategy and the factor-variance scaling method showed consistent trends. Negative relative parameter bias values occurred in conditions in which the group factor variance ratio was 1:1 or 0.8:1.2 and positive relative parameter bias values emerged in conditions in which the group factor variance ratio was 1.2:0.8 (see Table 4). Although the relative parameter bias values were in opposite directions, their absolute values did not differ substantially as a function of group factor variance ratio or group sample size ratio.

Unacceptable relative parameter bias was found when implementing the RI strategy in 33 conditions under the unequal factor loading scenarios. Unacceptable and substantial relative parameter bias was found more often in conditions in which the loading difference was large ($|\lambda_1 - \lambda_2| = 0.4$) than when it was small ($|\lambda_1 - \lambda_2| = 0.1$). Relative parameter bias varied as a function of factor loading pattern as well. For example, relative parameter bias was more

substantial in the all lower factor loading pattern conditions than in the remaining three factor loading scenarios (i.e., 1st loading unequal, 2nd loading unequal and mixed pattern conditions) whereas relative parameter bias was the least substantial in the mixed pattern scenarios (see Table 4). Relative parameter bias values were the smallest in the 1:4 group sample size ratio scenarios whereas they were more substantial in the 4:1 group sample size ratio scenarios. In addition, no clear trend was exhibited across the three group factor variance ratios when using the RI scaling method. When the factor-variance scaling strategy was implemented, relative parameter bias trends closely resembled those found when using the RI scaling strategy as previously described (see Table 4).

Conclusion

The primary question addressed in this study was whether violating the assumptions underlying the RI strategy and/or the factor-variance scaling method (i.e., using a RI with non-invariant factor loadings or constraining unequal factor variances to a value of one across groups) would affect the testing and description of the latent mean difference across groups. When implementing the RI strategy, the Type I error rates associated with the LRT_κ were not adversely affected by factor loading difference magnitude, factor loading pattern, group sample size ratio, or group factor variance ratio. This result indicates that violating the assumption of equivalent reference indicator loadings underlying the RI strategy did not affect Type I error rates associated with the LRT_κ for conditions and models examined here. This is consistent with the findings from the study conducted by Hancock, et al. (2000).

Previous research on SMM has not thoroughly investigated the factor-variance scaling method. The study found that when implementing the factor-variance scaling method, group factor variance ratio, group sample size ratio and loading difference magnitude did affect the Type I error rates associated with the LRT_κ . More specifically, when factor loadings were non-invariant/unequal, all Type I error rates that

Table 4: Relative Parameter Bias of the Standardized Latent Mean Difference Effect Size Measure as a Function of Manipulated Conditions ($\kappa_2 - \kappa_1 = 0.5$)

Loading Difference	Loading Pattern	Group Sample Size Ratio	Group Factor Variance Ratio					
			1:1		1.2 :0.8		0.8:1.2	
			RI	FV	RI	FV	RI	FV
0	Equal Loading	250:250	-0.008	-0.008	0.012	0.012	-0.004	-0.003
		100:400	-0.011	-0.011	0.004	0.005	-0.013	-0.012
		400:100	-0.006	-0.006	0.004	0.004	-0.004	-0.008
0.1	1 st Loading Unequal	250:250	0.017	0.016	0.022	0.024	0.033	0.033
		100:400	0.019	0.019	<u>0.050</u>	<u>0.051</u>	0.013	0.014
		400:100	<u>0.050</u>	<u>0.050</u>	0.049	<u>0.051</u>	0.037	0.037
	2 nd Loading Unequal	250:250	0.013	0.013	0.034	0.035	0.008	0.009
		100:400	0.010	0.010	-0.004	-0.003	-0.014	-0.013
		400:100	0.041	0.041	<u>0.050</u>	<u>0.051</u>	<u>0.057</u>	<u>0.057</u>
	All Lower	250:250	0.046	0.045	<u>0.059</u>	<u>0.061</u>	0.037	0.036
		100:400	0.015	0.014	0.042	0.043	0.010	0.010
		400:100	<u>0.066</u>	<u>0.066</u>	<u>0.074</u>	<u>0.076</u>	<u>0.070</u>	<u>0.068</u>
	Mixed	250:250	0.0004	0.0002	-0.013	-0.011	0.015	0.015
		100:400	-0.002	-0.002	-0.017	-0.017	-0.015	-0.014
		400:100	0.009	0.009	0.016	0.017	0.014	0.011
0.4	1 st Loading Unequal	250:250	<u>0.111</u>	<u>0.103</u>	<u>0.155</u>	<u>0.154</u>	<u>0.097</u>	<u>0.088</u>
		100:400	0.039	0.034	<u>0.052</u>	<u>0.051</u>	0.043	0.037
		400:100	<u>0.215</u>	<u>0.204</u>	<u>0.229</u>	<u>0.229</u>	<u>0.175</u>	<u>0.155</u>
	2 nd Loading Unequal	250:250	<u>0.129</u>	<u>0.121</u>	<u>0.147</u>	<u>0.145</u>	<u>0.092</u>	<u>0.083</u>
		100:400	0.025	0.021	<u>0.077</u>	<u>0.076</u>	0.038	0.032
		400:100	<u>0.198</u>	<u>0.187</u>	<u>0.213</u>	<u>0.214</u>	<u>0.180</u>	<u>0.162</u>
	All Lower	250:250	<u>0.184</u>	<u>0.153</u>	<u>0.230</u>	<u>0.212</u>	<u>0.130</u>	<u>0.091</u>
		100:400	<u>0.060</u>	0.046	<u>0.068</u>	<u>0.059</u>	0.033	0.019
		400:100	<u>0.344</u>	<u>0.313</u>	<u>0.390</u>	<u>0.374</u>	<u>0.299</u>	<u>0.255</u>
	Mixed	250:250	-0.005	-0.006	-0.011	0.008	0.030	0.022
		100:400	0.008	0.006	<u>0.050</u>	<u>0.058</u>	-0.007	-0.012
		400:100	<u>-0.064</u>	<u>-0.058</u>	<u>-0.087</u>	<u>-0.072</u>	-0.015	-0.026

Note: Relative parameter bias values equal to or greater than 0.05 are underlined which represent unacceptable bias. Abbreviations used in this table are described in Table 1.

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were deemed unacceptable occurred when group sample sizes were unequal. Additionally, the majority of unacceptable Type I error rates were found in conditions in which the group factor variance ratio was lower in group one than in group two and the loading difference was large. However, when the sample sizes were equal across groups, violating the equal factor-variance assumption did not have any substantial impact on Type I error rates associated with the LRT_{κ} .

Power associated with the LRT_{κ} was affected by group sample size ratio and loading difference magnitude. For example, when factor loadings were either equal or unequal across groups, power rates below the cutoff criterion of 0.90 were found only in the unequal sample size conditions; this finding is consistent with Kaplan and George (1995). Both group sample size ratio and loading difference magnitude influenced the power of the LRT_{κ} when factor loadings were unequal. That is, power was low only in unequal sample size scenarios and low factor loading difference scenarios. These low power rates, nonetheless, were not considerably lower than 0.90 and would in fact be deemed as acceptable if the traditional, less stringent 0.80 power criterion had been used as the benchmark. High power was particularly observed in the large latent mean difference conditions, as would be expected.

Previous studies have not investigated the performance of the standardized effect size measure, $\hat{\delta}_{\kappa}$, under varying conditions, particularly when the assumptions underlying the RI strategy and the factor-variance scaling method are violated. The findings in this study demonstrate that the $\hat{\delta}_{\kappa}$ is not biased in conditions in which there was no latent mean difference between the two groups. Thus, violating the assumptions associated with the RI strategy and the factor-variance scaling method did not have any substantial or systematic impact on the parameter bias of the $\hat{\delta}_{\kappa}$. Further, the parameter bias of the $\hat{\delta}_{\kappa}$ was not affected by loading difference magnitude, group sample size

ratio, group factor variance ratio, or factor loading pattern.

When there was a latent mean difference between the two groups, the $\hat{\delta}_{\kappa}$ was not biased in the baseline conditions in which factor loadings were equal/invariant. However, substantial relative parameter bias of the $\hat{\delta}_{\kappa}$ was found in the partial metric invariance conditions in which factor loadings were unequal. In addition, the relative parameter bias of the $\hat{\delta}_{\kappa}$ in these partial invariance conditions varied as a function of loading difference magnitude, factor loading pattern, and group sample size ratio, regardless of the factor scaling method used. Overall, the relative parameter bias was more unacceptable when the factor loading difference magnitude was large, when the non-invariant factor loadings were higher in group two, and when sample size in group one was larger than sample size in group two.

Study Limitations

The assumptions underlying the RI strategy and the factor-variance scaling method have not been widely investigated in previous simulation studies. Thus, as a starting point for this line of research, this study included a relatively simple model and investigated latent mean difference comparisons under relatively ideal conditions. Due to the preliminary nature of the research, there are several limitations inherent in this study. For example, only a moderately large latent mean difference was included when investigating the power of the LRT_{κ} .

As a result, power associated with the LRT_{κ} was high in these conditions and did not differ systematically as a function of the factor loading pattern or group factor variance ratio. It was found that violating the assumptions underlying the two factor-scaling methods did not influence the power of the LRT_{κ} . However, it is not clear whether the same findings would be obtained with smaller latent mean differences (e.g., 0.1 and 0.3). In future simulation studies, researchers could include smaller latent mean differences and examine how violating the

assumptions underlying the two factor-scaling methods may affect the power of the LRT_{κ} .

Neither model size nor model complexity was varied in this study. For simplicity, a two-group, one-factor CFA model with six indicator variables was the true generating model. Future researchers could consider more complex models (for example, more observed indicators and/or additional latent variables) to investigate whether varying the model size and/or model complexity would affect the testing and description of the latent mean difference across groups. Future research that includes models with more observed indicators could likewise investigate more severe loading non-invariance conditions. Further, mean comparisons between more than two groups are not uncommon and, hence, the impact of including more than two groups on latent mean comparisons could be examined in future investigations. In addition, multivariate normal data were generated. Future studies could also explore the implications of violating the assumption of normality when using the LRT_{κ} and the $\hat{\delta}_{\kappa}$ to test and describe groups' latent mean differences.

The results of this study suggest that researchers do not necessarily need to be concerned about violating the assumption underlying the RI strategy given that it does not adversely affect the performance of the LRT_{κ} . The results also suggest that researchers do not necessarily need to be concerned about violating the assumptions underlying either of the two factor scaling methods when using the $\hat{\delta}_{\kappa}$ in order to describe the latent mean difference across groups.

The findings concerning the RI factor scaling method are notable because the assumption underlying the RI strategy may be frequently violated given the difficulty of identifying an item with truly invariant factor loadings (Hancock, Stapleton & Arnold-Berkovits, 2009). Nonetheless, more research is necessary in order to assuredly know that violating the RI assumption does not impact latent mean difference testing and that violating either of the factor scaling method assumptions does not impact latent mean difference

descriptions. By contrast, the results clearly indicate that researchers should be aware of the assumption underlying the factor-variance scaling method. In particular, when the sample sizes for the two groups being compared are unequal, constraining unequal factor variances to a value of one across groups is likely to produce overly conservative or liberal Type I error rates associated with the latent mean difference test (LRT_{κ}). Additionally, researchers should cautiously interpret the $\hat{\delta}_{\kappa}$ when factor loadings are non-invariant across groups in combination with unequal group sample sizes, regardless of factor scaling method employed.

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Robust Regression Estimates in the Prediction of Latent Variables in Structural Equation Models

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The incorporation of the robust regression methods Least Median Square (LMS) and Least Trimmed Squares (LTS) is proposed in structural equation modeling. Results show that, in situations of high deviations of symmetry, the evaluated methods would be recommended for applications including smaller sample sizes.

Key words: Accuracy, Monte Carlo simulation, normal asymmetry, precision.

Introduction

Structural equation modeling seeks to reproduce a population covariance matrix through the sample covariance associated with parameter constraints determined by a researcher. The most commonly used estimation methods are based on maximum likelihood, ordinary least squares and partial least squares. These methods, however, show a sensitivity to various factors, for example: violation of the normality assumption (Lei & Lomax, 2005), presence of outliers (Yuan & Bentler, 2001) and samples that show the effects of asymmetry and excess kurtosis compared to the multivariate normal distribution (Gao, et al., 2008).

It is reasonable to assume that the presence of these effects can be explained by observing outliers in the sample and it is also relevant to consider sample size because large data sets are subject to a large number of these observations. Moreover, the violation of the assumption of normality can also be caused by these observations; therefore, a practical (but not

always feasible) alternative is to apply a transformation to the data. Gao, et al. (2008) state that – depending on the transformation to be used – the relationships between variables may be nonlinear. However, applying this statement to structural equation models, where the nature of the relationships between the variables are linear, the application of a transformation may complicate the interpretation of results as well as affect the quality of model fit.

Pilati and Laros (2007) state that, if the assumption of normality is not met, the researcher may choose to use other estimation methods such as the method of partial least squares (PLS) estimators. According to O'Loughlin & Coenders (2004) the disadvantage of this method is that they provide biased estimates. Cassel, et al. (1999) note that the properties of robustness must be further studied due to the fact that the estimates are sensitive to deviations from symmetry in observable variables, multicollinearity among observable variables and incorrect specification of measurement models.

As noted, not all variable distributions are normal and – in the presence of outliers – not all are appropriate to use for robust regression estimators that would be incorporated in structural equation models (SEMs). However, robust regression estimators that have a high breaking point are constructed based on the size of the subsets of data, thus, Hawkins, et al. (1984) state that this size should be minimal,

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that is, the total number of observations belonging to each set should be equal to the number of model parameters. This recommendation is justified due to the fact that the proportion of subsets that will contain at least one observational discrepancy will grow rapidly as a function of the size of the subset. For this reason, by keeping the subsets as small as possible the number of estimates that are not influenced by outliers is maximized.

As a base for this theory, the method of Least Median of Squares (LMS) is cited (Gervini & Yohai, 2002). This method involves minimizing the sum of squares of the ordinary residuals obtained by the method in such a way that the subset formed from the residuals resulting in the lowest median value are considered for the minimization processes. Other robust regression estimators, adequate for incorporation in structural equation modeling (SEM) are defined by the Least Trimmed Squares (LTS) method (Agulló, 2001). This method proposes to minimize the sum of the first h residuals sorted and squared, and h the size of the subset defined by the number of model parameters and sample size (Maronna, et al., 2006).

This article incorporates robust estimators LMS and LTS in structural SEM. For this purpose, the performance of the incorporation of these estimators was evaluated by Monte Carlo simulation considering different degrees of asymmetry in the distributions of the observable variables and errors of the structural and measurement models.

Methodology

Error Distribution of the Structural Equation Model using Monte Carlo Simulation

Following the definition of a structural equation model (SEM), structural error and measurement models were generated following the asymmetric standard normal distribution with probability functions defined respectively as

$$f_{\zeta} = 2\phi(\zeta)\Phi(a\zeta), \zeta \in \mathfrak{R}, a \in \mathfrak{R}; \quad (1)$$

$$f_{\delta} = 2\phi(\delta)\Phi(a\delta), \delta \in \mathfrak{R}, a \in \mathfrak{R}; \quad (2)$$

and

$$f_{\varepsilon} = 2\phi(\varepsilon)\Phi(a\varepsilon), \varepsilon \in \mathfrak{R}, a \in \mathfrak{R}, \quad (3)$$

where $\phi(\cdot)$ and $\Phi(\cdot)$ represent the probability density function and standard normal cumulative distribution $N(0,1)$ and a is the asymmetry parameter. Thus, the notation $\zeta \sim N(0, 1, a)$, $\delta \sim N(0, 1, a)$ and $\varepsilon \sim N(0, 1, a)$ was used. Arbitrarily, the values were set at $a = 20, 0$ and -20 implying the errors presented positive asymmetry, symmetry, and negative asymmetry, respectively; these situations are illustrated in Figures 1-3.

Figure 1: $\zeta, \delta, \varepsilon \sim N(0, 1, 20)$ Error Histogram

Figure 2: $\zeta, \delta, \varepsilon \sim N(0, 1)$ Error Histogram

Figure 3: $\zeta, \delta, \varepsilon \sim N(0, 1, -20)$ Error Histogram

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Structural Equation Models Used in the Monte Carlo Simulation

Keeping the specifications of the error distributions consistent with the proposed objective in the Monte Carlo simulation process, the structural model

$$\eta = \gamma_1 \xi_1 + \gamma_2 \xi_2 + \gamma_3 \xi_3 + \zeta, \quad (4)$$

where γ_i for $i = 1, 2, 3$ represents the regression coefficients and ζ is the structural error with distribution is $N(0,1,a)$ was considered. The observable variables were defined by x_k ($k = 1, \dots, 9$), such that each equation of the measurement model at x was composed by

$$\xi_1 = \pi_1 x_1 + \pi_2 x_2 + \pi_3 x_3 + \delta_1, \quad (5)$$

$$\xi_2 = \pi_4 x_4 + \pi_5 x_5 + \pi_6 x_6 + \delta_2, \quad (6)$$

$$\xi_3 = \pi_7 x_7 + \pi_8 x_8 + \pi_9 x_9 + \delta_3. \quad (7)$$

and where δ_i ($i = 1, 2, 3$) was generated by a normal distribution.

In the case of the measurement model for η , the definition of the equations was given as:

$$y_1 = \lambda_1 \eta + \varepsilon_1, \quad (8)$$

$$y_2 = \lambda_2 \eta + \varepsilon_2, \quad (9)$$

$$y_3 = \lambda_3 \eta + \varepsilon_3, \quad (10)$$

and

$$y_4 = \lambda_4 \eta + \varepsilon_4. \quad (11)$$

Based on these equations, along with assumptions of the structural model in which the expected values of the error vectors and latent variables are equal to zero, ζ and ξ_i , ($i = 1, 2, 3$) are uncorrelated, ε_j ($j = 1, 2, 3, 4$) are uncorrelated with η , ξ_i and δ_i , being δ_i uncorrelated with ξ_i , η and ε_j . With these specifications, the regression coefficient estimators were obtained by robust LMS and

LTS methods and the sample generation was characterized by different degrees of asymmetry for x observable variables distributed as a Beta (α, β) distribution, whose parameters were fixed in accordance with Table 1.

Table 1: Beta (α, β) Distribution Used in the Simulation of the Observable Variables with Different Degrees of Asymmetry

Case	Distribution	Degree of Asymmetry
0	Beta (6, 6)	Perfectly Symmetrical
1	Beta (9, 4)	Moderate Asymmetry to the Right
2	Beta (9, 1)	High Asymmetry to the Right

The illustration of each case is shown in Figures 4-6 and the parametric values used in the simulation of the structural model are shown in Figure 7.

Figure 4: Beta (6, 6)

Figure 5: Beta (9, 4)
Case 1

Figure 6: Beta (9, 1)
Case 2

Robust Regression Estimators Incorporated into the Structural Equation Model

The LMS estimators (Rousseeuw & Leroy, 2003) applied in SEM were incorporated considering structural model (4) and the measurement models related to the independent (models (5)-(7)) and the dependent (models (8)-(11)) variables. For sample sizes fixed at $n = 50$, 200 and 1,000, estimates were obtained by minimizing equations (12)-(14). Thus, with the exception of the structural model, each of the measurement model equations was specified by the index $s = 1, \dots, Q$, where Q is the total number of equations and the parameter estimates of each equation were obtained by the LMS method.

$$\min \left\{ \text{median} \left(\zeta_1^2, \dots, \zeta_n^2 \right) \right\}, \quad (12)$$

$$\min \left\{ \text{median} \left(\varepsilon_{s1}^2, \dots, \varepsilon_{sn}^2 \right) \right\}, s = 1, \dots, (Q=4), \quad (13)$$

and

$$\min \left\{ \text{median} \left(\delta_{s1}^2, \dots, \delta_{sn}^2 \right) \right\} s=1, \dots, (Q=3). \quad (14)$$

In the case of the LTS method (Rousseeuw & Leroy, 2003) the parameter estimates were obtained from expressions:

$$\min \left\{ \sum_{r=1}^h \zeta_r^2, \dots, \zeta_h^2 \right\}; \quad (15)$$

$$\min \left\{ \sum_{r=1}^h \varepsilon_{sr}^2, \dots, \varepsilon_{sh}^2 \right\}; s = 1, \dots, (Q = 4); \quad (16)$$

and

$$\min \left\{ \sum_{r=1}^h \left(\delta_{sr}^2, \dots, \delta_{sh}^2 \right) \right\}; s = 1, \dots, (Q = 3). \quad (17)$$

In all situations, the values of h were recommended by Rousseeuw and Hubert (1994), according to the expression:

$$h = \left\lceil \frac{n+p+1}{2} \right\rceil, \quad (18)$$

where p is the total number of parameters relating to each equation.

Statistical Measurements to Compare the Results

Based on the procedure described, the robust estimators were incorporated into the structural equation model and a program was constructed in software R version 2.11.1 (R Development Core Team, 2010), in which 1,000 Monte Carlo simulations were performed for each sample size for each degree of asymmetry in the errors distributions (see Figures 1-3) and

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Figure 7: Graphical Representation of the Structural Equation Model with the Parametric Values Used in the Monte Carlo Simulation Process

in the observable variables distributions (see Figures 4-6). To evaluate the accuracy for each parameter of structural equation (4), the relative deviations were computed as:

$$B = \frac{\sum_{b=1}^{1000} \left(\frac{\gamma_{ib} - \hat{\gamma}_{ib}}{\gamma_{ib}} \right)}{1000}, \quad i = 1, 2, 3. \quad (19)$$

In terms of the precision of the study, the range given in (20) was used considering the difference between the highest and lowest standard deviation value $S\gamma_i$ obtained by means of the empirical distribution of estimates of each

parameter γ_i ($i = 1, 2, 3$) generated in the simulation process:

$$A_{sd} = \max(S_{\gamma_i}) - \min(S_{\gamma_i}), \quad i = 1, 2, 3. \quad (20)$$

Results

Considering the observable variables generated with perfect symmetry (Case 0; see Table 2), it was observed that, in the situation where errors were symmetrical (Figure 2), the results were similar; the three estimators being considered accurate for all methods evaluated in terms of sample sizes.

Table 2: Estimates of the Relative Bias (B) Considering Different Degrees of Asymmetry of the Distribution of Errors with the Observable Variables Generated by Beta (6, 6)

LS Method									
n	$\zeta; \varepsilon_j; \delta_i \sim N(0, 1)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, 20)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, -20)$		
	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3
50	0.0023	-0.0007	-0.0426	0.1561	0.2666	0.6163	-0.5592	-0.5830	0.1774
200	-0.0017	-0.0015	0.0076	0.1557	0.2684	0.6019	-0.5597	-0.5406	0.2067
1000	-0.0001	-0.0004	0.0081	0.1551	0.2755	0.5831	-0.5625	-0.5335	0.2511
LMS Method									
n	$\zeta; \varepsilon_j; \delta_i \sim N(0, 1)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, 20)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, -20)$		
	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3
50	0.0081	-0.0481	-0.0202	0.0994	0.2009	0.4488	-0.4828	-0.5342	0.0770
200	0.0091	-0.0346	0.0044	0.0927	0.1684	0.3605	-0.4619	-0.3981	0.0890
1000	0.0006	0.0027	0.0087	0.0852	0.1642	0.3227	0.0782	0.1142	0.1043
LTS Method									
n	$\zeta; \varepsilon_j; \delta_i \sim N(0, 1)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, 20)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, -20)$		
	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3
50	0.0245	-0.0596	-0.0452	0.0999	0.1863	0.4770	-0.4754	-0.5223	0.0238
200	-0.0007	-0.0156	-0.0039	0.0834	0.1557	0.3758	-0.4334	-0.3834	0.0548
1000	-0.0018	-0.0033	0.0164	0.0712	0.1479	0.3087	-0.3976	-0.3352	0.1547

This result is consistent with findings by Cassel, et al. (1999) that the parameter estimates resulting from the application of the Partial Least Squares method showed similar results, that is, estimates were not affected by increasing sample size. However, in considering the errors distributed as the normal asymmetric with the parameters of asymmetry $a = 20$ (see Figure 1) and $a = -20$ (see Figure 3), it was observed that the values of the biases in situations where the LMS and LTS methods were used were smaller those when considering the method of Least Squares (LS) estimation. However, it should be emphasized that the robust regression methods in the case of negative asymmetry of the errors

retained results that characterize an inaccuracy and show evidence of a tendency to provide inflated or deflated estimates related to the parameters of the structural equation. This deficiency was corrected by increasing the sample size to $n = 1,000$ with emphasis on the LMS method which provided more accurate results compared to the parametric values imposed on the structural model.

Because results were more accurate for robust methods, in situations where the errors were generated by asymmetric normal distributions precision was evaluated using the statistic given by (20). Thus, the results illustrated in Figure 8 show that the LMS and

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Figure 8: Precision of the Robust Estimates Considering Positive and Negative Asymmetric Errors with Observable Variables Generated by Beta (6, 6)

LTS methods presented similar precision when the errors have a negative asymmetry effect, and the LMS method showed better performance in the case of positive asymmetry.

Considering the distribution of observable variables with a moderate degree of asymmetry (Case 1), the results in Table 3 show that, in the situation where structural errors and measurement were simulated assuming normality without deviations of asymmetry (Figure 2), the LMS and LTS methods continued to provide good accuracy. However, when considering the errors generated by the normal asymmetric distribution, it was observed that the robust estimation methods were less accurate

than those outlined in Table 2, but showed better performance than the least squares estimator. Maintaining the focus on the study of the precision afforded by the robust LMS and LTS methods (see Figure 9) the performance of the two estimators is similar.

Supplementing these findings, in a comparative study of maximum likelihood estimators (MLE) and robust estimation methods applied in the setting of a confirmatory factor analysis, Zhong & Yuan (2011) concluded that, in the case of non-normal distributions, the MLE estimates are biased and inefficient and the use of robust methods provide an improvement on these properties; however, they stressed that the

Table 3: Estimates of Relative Bias (B) Considering Different Degrees of Asymmetry of the Distribution of Errors with the Observable Variables Generated by Beta (9, 4)

LS Method									
n	$\zeta; \varepsilon_j; \delta_i \sim N(0, 1)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, 20)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, -20)$		
	γ_1	γ_2	γ_3		γ_1	γ_2	γ_3		γ_1
50	0.0000	0.0024	-0.0078	50	0.0000	0.0024	-0.0078	50	0.0000
200	-0.0018	0.0047	0.0043	200	-0.0018	0.0047	0.0043	200	-0.0018
1000	-0.0007	0.0051	-0.0064	1000	-0.0007	0.0051	-0.0064	1000	-0.0007
LMS Method									
n	$\zeta; \varepsilon_j; \delta_i \sim N(0, 1)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, 20)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, -20)$		
	γ_1	γ_2	γ_3		γ_1	γ_2	γ_3		γ_1
50	0.0035	-0.0042	-0.0505	50	0.0035	-0.0042	-0.0505	50	0.0035
200	-0.0054	0.0187	0.0039	200	-0.0054	0.0187	0.0039	200	-0.0054
1000	-0.0008	-0.0023	0.0137	1000	-0.0008	-0.0023	0.0137	1000	-0.0008
LTS Method									
n	$\zeta; \varepsilon_j; \delta_i \sim N(0, 1)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, 20)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, -20)$		
	γ_1	γ_2	γ_3		γ_1	γ_2	γ_3		γ_1
50	-0.0134	0.0130	-0.0012	50	-0.0134	0.0130	-0.0012	50	-0.0134
200	-0.0045	0.0082	0.0160	200	-0.0045	0.0082	0.0160	200	-0.0045
1000	-0.0037	-0.0026	0.0385	1000	-0.0037	-0.0026	0.0385	1000	-0.0037

estimates of standard errors must be studied. In this sense, the study of the precision of the estimators is justified, confirming the claims made by Kaplan (1969) referring to the fact that the refinement of precision does not necessarily lead to increased reliability. In addition, in some situations, there could occur a reduction in the reliability of the estimates by a reduction of the accuracy because in practical situations the researcher may encounter systematic errors, for example, errors in the definition of the measurement or recording of the observation and random errors associated with uncontrollable variations.

When a high degree of asymmetry is imposed on the observable variables through

distribution Beta (9, 1) (Case 2; see Table 4), maintaining the structural error and measurement errors distributed according to a normal symmetry (Figure 2), the LMS and LTS methods are accurate and similar results are obtained using the LS method. However, considering the asymmetric error (see Figures 1 and 3), based on the bias, the robust methods were more suitable for use in replacement of the LS method.

In the same situations with different degrees of asymmetry (see Table 1) assuming the measurement errors of the equations ((5)-(7)) and ((8)-(11)) are uniformly distributed, Cassel, et al. (1999) evaluated the biases of the parameter estimates of the structural equation model

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Figure 9: Precision of the Robust Estimates Considering the Positive and Negative Asymmetric Errors with Observable Variables Generated by Beta (9, 4)

resulting from the application of Partial Least Squares method and concluded that the increase in the degree of asymmetry reflected an increase in bias and this is more emphasized in a situation of a high degree of asymmetry (Case 2; see Figure 6). Results obtained in this work are consistent with the Cassel, et al. (1999) findings and there is statistical evidence to argue that robust regression methods are consistent and worthy of being adapted to be used in structural equation modeling.

Relevant to the discussion of the estimates accuracy provided by the LMS and LTS methods it is important to note that, in the violation of the normality assumption, there are numerous works relating other methods that can be used as alternatives. Engel, et al. (2003)

stated that the maximum likelihood method can be applied when the normality deviation is relatively moderate. In this situation the authors recommend $n > 400$. Moreover, Muthén and Muthén (2002) stated that the maximum likelihood estimators can be consistent but not necessarily efficient.

For variables with non-normal distributions, the recommendations are divergent. The minimum sample size for the weighted least squares method to be reliable, should be at least $n = 1,000$ (Hoogland & Boomsma, 1998), and depending on the model and data being analyzed; in some cases even exceeding 4,000 or 5,000 (Boomsma & Hoogland, 2001; Hu, et al., 1992). In general, when considering small sample sizes, Bollen, et

Table 4: Estimates of Relative Biases (B) Considering Different Degrees of Asymmetry of the Distribution of Errors with the Observable Variables Generated by Beta (9, 1)

LS Method									
n	$\zeta; \varepsilon_j; \delta_i \sim N(0, 1)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, 20)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, -20)$		
	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3
50	-0.0030	0.0059	-0.0037	-0.0030	0.0059	-0.0037	-0.0030	0.0059	-0.0037
200	-0.0004	0.0035	-0.0044	-0.0004	0.0035	-0.0044	-0.0004	0.0035	-0.0044
1000	0.0001	0.0007	-0.0009	0.0001	0.0007	-0.0009	0.0001	0.0007	-0.0009
LMS Method									
n	$\zeta; \varepsilon_j; \delta_i \sim N(0, 1)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, 20)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, -20)$		
	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3
50	-0.0022	-0.0019	0.0717	-0.0022	-0.0019	0.0717	-0.0022	-0.0019	0.0717
200	-0.0039	0.0106	-0.0166	-0.0039	0.0106	-0.0166	-0.0039	0.0106	-0.0166
1000	0.0028	-0.0083	-0.0160	0.0028	-0.0083	-0.0160	0.0028	-0.0083	-0.0160
LTS Method									
n	$\zeta; \varepsilon_j; \delta_i \sim N(0, 1)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, 20)$			$\zeta; \varepsilon_j; \delta_i \sim N(0, 1, -20)$		
	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3	γ_1	γ_2	γ_3
50	-0.0160	0.0236	0.0612	-0.0160	0.0236	0.0612	-0.0160	0.0236	0.0612
200	0.0006	0.0046	-0.0094	0.0006	0.0046	-0.0094	0.0006	0.0046	-0.0094
1000	-0.0002	0.0015	-0.0110	-0.0002	0.0015	-0.0110	-0.0002	0.0015	-0.0110

al. (2007) recommended that results should be interpreted with caution. Considering these arguments, it may be stated that the use of the robust estimation methods evaluated in this work are worthy of being considered in SEM, as the results show that the increase in the degree of asymmetry in the distribution of observed variables provided an improvement in the precision of the LMS and LTS estimates.

Conclusion

In situations where the observed variables and errors in a structural equation model show asymmetry deviations, the robust estimation methods LMS and LTS are suitable for application, especially with smaller sample sizes.

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Figure 10: Precision of the Robust Estimates Considering Positive and Negative Asymmetric Errors with Observable Variables Generated by Beta (9, 1)

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Robust Modifications of the Levene and O'Brien Tests for Spread

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Variants of Levene's and O'Brien's procedures not investigated by Keselman, Wilcox & Algina (2008) were examined. Simulations indicate that a new O'Brien variant provides very good Type I error control and is simpler for applied researchers to compute than the method recommended by Keselman, et al.

Key words: Levene test of spread, O'Brien test of spread, Type I error.

Introduction

Keselman, Wilcox, Algina, et al. (2008) compared a number of tests for spread that were based on either least squares or trimmed estimates of central tendency and variability. These estimators were based on either the original data or transformations suggested by Levene (1960) and O'Brien (1981). The adaptive trimming estimators they used were defined by Reed and Stark (1996), estimators which rely on procedures that determine whether data should be trimmed symmetrically, asymmetrically, or not at all. The transformed scores were used in an analysis of variance (ANOVA) F-test, a Welch (1951) test, and a robust ANOVA test due to Lee and Fung (1985). Based on their extensive simulation study, Keselman, et al. recommended a Levene-type

transformation based on empirically determined 20% asymmetric trimmed means, involving a particular adaptive estimator, where the transformed scores are then used with an ANOVA F test.

In their investigation, Keselman, et al. only examined a limited number of variations of the Levene (1960) and O'Brien (1979) methods – variations where, by-in-large, the transformed variables were obtained via the application of asymmetrically trimmed means involving one of the seven hinge estimators defined by Reed and Stark (1996). However, there are many other ways in which the transformed variables may be created. For example, the transformed variables may be based on symmetrically trimmed means and then these transformed variables may be symmetrically/asymmetrically transformed with one of the seven hinge estimators. Thus, the purpose of this study was to examine other variants of the Levene and O'Brien methods not examined by Keselman, et al. (2008).

Background

As Keselman, et al. (2008), and others, have noted, the traditional test for equality of variances, e.g., $F = \frac{s_1^2}{s_2^2}$, where s_j^2 is the usual unbiased sample variance for the j^{th} group, is affected adversely when the data in the groups are not normally distributed (i.e., it is sensitive to kurtosis). That is, the actual level of

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significance can differ substantially from the nominal significance level. In addition, power can be low.

Levene (1960) suggested an alternative test statistic that can be used to assess equality of spread across independent treatment groups. For the one-way layout with model $X_{ij} = \mu_j + \varepsilon_{ij}$ ($i = 1, \dots, n_j; j = 1, \dots, J$), where μ_j is the population mean for the j^{th} group and ε_{ij} is random error, Levene suggested that the scores could be modified with the transformation $z_{ij} = |X_{ij} - \bar{X}_j|$, where $\bar{X}_j$ is the j^{th} sample mean, and then these scores can be used in an ANOVA test. That is, the test suggested by Levene is

$$W_0 = \frac{\sum_{j=1}^J n_j (\bar{z}_j - \bar{z}_{..})^2 / (J-1)}{\sum_{j=1}^J \sum_{i=1}^{n_j} (z_{ij} - \bar{z}_j)^2 / \sum_{j=1}^J (n_j - 1)}, \quad (1)$$

where

$$\bar{z}_j = \sum_{i=1}^{n_j} \frac{z_{ij}}{n_j} \text{ and } \bar{z}_{..} = \frac{\sum_{j=1}^J \sum_{i=1}^{n_j} z_{ij}}{\sum_{j=1}^J n_j}.$$

Critical values for W_0 are obtained from the F -distribution based on $J-1$ and $\sum_{j=1}^J (n_j - 1)$ degrees of freedom. Another statistic relevant to this article is $W_{\bar{X}_i}$. This statistic replaces the group mean in obtaining the transformed Z_{ij} s with the group trimmed mean.

Other methods have also appeared in the literature in addition to Levene's (1960) procedure. Lee and Fung (1985) presented a robust ANOVA F -test based on trimmed means. Keselman, et al. (1979) and others (e.g., O'Brien, 1981) have indicated that a Welch statistic can be adopted instead of the usual ANOVA F -test to assess spread across independent groups. O'Brien (1979) also suggested that a Welch test can be used with his transformation of the data, X_{ij} , namely

$$r_{ij} = \frac{(n_j - 1.5)n_j(X_{ij} - \bar{X}_j)^2 - .5s_j^2(n_j - 1)}{(n_j - 1)(n_j - 2)}. \quad (2)$$

Adaptive Trimming Methods

Keselman, et al. (2008) provided a detailed description of adaptive trimming methods. Reed and Stark (1996) defined seven adaptive location estimators based on measures of tail-length and skewness for a set of n observations based on the work of Hogg (1974, 1982). To define these estimators, measures of tail-length and skewness must first be defined. Using the notation of Hogg (1974, 1982) and Reed and Stark (1996) and based on the ordered values, let L_α = the mean of the smallest $[\alpha n]$ observations, where $[\alpha n]$ denotes the greatest integer less than αn and U_α = the mean of the largest $[\alpha n]$ observations. When $\alpha = .05$, $L_{(.05)}$ is the mean of the smallest $[0.05n]$ observations, B is the mean of the next largest $0.15n$ observations, C is the mean of the next largest $0.30n$ observations, D is the mean of the next largest $0.30n$ observations, E the mean of the next largest $0.15n$ observations, and $U_{(.05)}$ the mean of the largest $0.05n$ observations.

Tail-Length Measures

Hogg (1974) defined two measures of tail-length, Q and Q_1 , where

$$Q = \frac{(U_{(.05)} - L_{(.05)})}{(U_{(.5)} - L_{(.5)})} \quad \text{and} \quad (3)$$

$$Q_1 = \frac{(U_{(.2)} - L_{(.2)})}{(U_{(.5)} - L_{(.5)})}.$$

Q and Q_1 are location free statistics, are uncorrelated with location statistics and can be used to classify symmetric distributions as light-tailed, medium-tailed or heavy-tailed (Reed & Stark, 1996). According to Hogg (1974) and Reed and Stark (1996), values of $Q < 2$ imply a light-tailed distribution, $2.0 \leq Q \leq 2.6$ a medium-tailed distribution, $2.6 \leq Q \leq 3.2$ a heavy-tailed distribution, and $Q > 3.2$ a very

heavy-tailed distribution. The cutoffs for Q_1 are:
 $Q_1 < 1.81$ (light-tailed), $1.81 \leq Q_1 \leq 1.87$
 (medium-tailed) and $Q_1 > 1.87$ (heavy-tailed).

Hogg (1982) introduced yet another measure of tail-length:

$$H_3 = \frac{(U_{(.05)} - L_{(.05)})}{(E - B)}. \quad (4)$$

With this measure, values of $H_3 < 1.26$ suggest that the tails of the distribution are similar to a uniform distribution; values of 1.26 through 1.76 suggest a normal distribution, and values greater than 1.76 suggest the tails are similar to those of a double exponential distribution.

Measures of Skewness

Reed and Stark (1996) defined four measures of skewness as:

$$\begin{aligned} Q_2 &= (U_{(.05)} - T_{(.25)}) / (T_{(.25)} - L_{(.05)}), \\ H_1 &= (U_{(.05)} - D) / (C - L_{(.05)}), \\ SK_2 &= (X_{(1)} - XMD) / (XMD - X_{(n)}) \\ \text{and} \\ SK_5 &= (X_{(1)} - XM) / (XM - X_{(n)}), \end{aligned} \quad (5)$$

where XMD is the median, XM is the arithmetic mean, $T_{(.25)}$ is the 0.25-trimmed mean (T_α) and $X_{(1)}$ and $X_{(n)}$ are the first and last ordered observations, respectively. Reed (1998) defined the α -trimmed mean as:

$$T_\alpha = \frac{1}{n(1-2\alpha)} \left[\sum_{i=k+1}^{n-k} X_i + (k - \alpha n)(X_k + X_{n-k+1}) \right]. \quad (6)$$

In this definition a proportion, α , has been trimmed from each tail and the accompanying Winsorized variance S^2 is defined as:

$$S^2 = \frac{1}{(n-1)(1-2\alpha)^2} \left[\sum_{i=k+1}^{n-k} \left((X_i - T_\alpha)^2 + k(X_k - T_\alpha)^2 \right) \right], \quad (7)$$

where $k = [\alpha n] + 1$.

Based on the definitions of tail-length and skewness, Reed and Stark proposed a set of adaptive linear estimators "that have the capability of asymmetric trimming" (1996, p. 13). They defined a general scheme for their approach as follows:

1. Set the value for the total amount of trimming from the sample, α .
2. Determine the proportion to be trimmed from the lower end of the sample (α_1) by the following proportion:
 $\alpha_1 = \alpha [UW_X / (UW_X + LW_X)]$, where UW_X and LW_X are the numerator and denominator of the defined selector statistics (i.e., tail-length and skewness).
3. The upper trimming proportion is: $\alpha_2 = \alpha - \alpha_1$.

Based on this general schema, Reed and Stark (1996) defined seven hinge estimators, which are trimmed means, as:

1. HQ $\alpha_1 = \alpha [UW_Q / (UW_Q + LW_Q)]$,
2. HQ₁ $\alpha_1 = \alpha [UW_{Q_1} / (UW_{Q_1} + LW_{Q_1})]$,
3. HH₃ $\alpha_1 = \alpha [UW_{H_3} / (UW_{H_3} + LW_{H_3})]$,
4. HQ₂ $\alpha_1 = \alpha [UW_{Q_2} / (UW_{Q_2} + LW_{Q_2})]$,
5. HH₁ $\alpha_1 = \alpha [UW_{H_1} / (UW_{H_1} + LW_{H_1})]$,
6. HSK₂ $\alpha_1 = \alpha [UW_{SK_2} / (UW_{SK_2} + LW_{SK_2})]$,
 and
7. HSK₅ $\alpha_1 = \alpha [UW_{SK_5} / (UW_{SK_5} + LW_{SK_5})]$. (8)

Keselman, et al. (2008), investigating Type I error rates of procedures for testing spread, examined the Reed and Stark (1996) procedure with various values for α because the literature varies on the amount of recommended (symmetric) trimming. Rosenberger and Gasko (1983) recommend 25% when sample sizes are small (although they state that 20% generally suffices), Wilcox (2005) recommends 20% and Mudholkar, Mudholkar and Srivastava (1991) suggest 15%. Ten percent has been considered by Hill and Dixon (1982), Huber (1977), Stigler (1977) and Staudte and Sheather (1990); results reported by Keselman, et al. (2002) also support 10% trimming. In addition, Keselman, et al. (2005) obtained good results with 5% symmetric trimming.

According to Keselman, et al. (2007), Reed and Stark's (1996) tail-length and skewness measures may be modified for the multi-group problem and applied to the modified multi-group measures to the hinge estimators. In particular, they indicated that each of the measures can be modified by taking weighted averages in a manner analogous to the modifications of tail-length and symmetry measures suggested by Babu, Padmanaban and Puri (1999) of each numerator and denominator term. For example, for the multi-group problem, where n_j represents the number of observations in each group, Q_1 and Q_2 can be defined as:

$$Q_1 = \frac{\left[\sum_j n_j (U_{(.2)} - L_{(.2)}) / \sum_j n_j \right]}{\left[\sum_j n_j (U_{(.5)} - L_{(.5)}) / \sum_j n_j \right]},$$

and

$$Q_2 = \frac{\left[\sum_j n_j (U_{(.05)} - T_{(.25)}) / \sum_j n_j \right]}{\left[\sum_j n_j (T_{(.25)} - L_{(.05)}) / \sum_j n_j \right]}.$$
(9)

The other measures would be similarly modified and it is these multi-group measures of tail-length and skewness that are applied to the general scheme proposed by Reed and Stark

(1996), treating the transformed Z_{ij} s as the original variables

One could go a step further than merely applying the transformed Z_{ij} s in a Welch test. It is suggested that the transformed Z_{ij} s be treated as the original random variable in a test statistic that has been found to be generally insensitive to nonnormality, namely a Welch test based on trimmed means, that is, Yuen's (1974) test).

Thus, consider the following. The α trimmed means and Winsorized variances can be defined in a number of different ways (see Hogg, 1974; Reed, 1998; Keselman, et al., 2007; Wilcox, 2003). Let $Z_{(1)j} \leq Z_{(2)j} \leq \dots \leq Z_{(n_j)j}$ represent the ordered observations associated with the j^{th} group. Reed's (1998) approach is based on the work of Hogg (1974). Hogg defined the α -trimmed mean as:

$$m(\alpha) = (1/h) \sum_{i=g+1}^{n_j-g} Z_{(i)j}, \quad (10)$$

where α is selected so that $g = [n_j \alpha]$ and $h = n_j - 2g = n_j - 2[n_j \alpha]$. The standard error of $m(\alpha)$ Hogg suggests is based on the works of Tukey and McLaughlin (1963) and Huber (1970) and is estimated by:

$$S_{m(\alpha)} = \sqrt{\frac{SS(\alpha)}{h(h-1)}}, \quad (11)$$

where $SS(\alpha)$ is the Winsorized sum of squares defined as:

$$\begin{aligned} & (g+1) [Z_{(g+1)} - m(\alpha)]^2 \\ & + [Z_{(g+2)} - m(\alpha)]^2 \\ & + \dots \\ & + [Z_{(n_j-g-1)} - m(\alpha)]^2 \\ & + (g+1) [Z_{(n_j-g)} - m(\alpha)]^2. \end{aligned} \quad (12)$$

When allowing for different amounts of trimming in each tail of the distribution, Hogg (1974) defines the trimmed mean as:

$$m(\alpha_1, \alpha_2) = \left(\frac{1}{h} \right) \sum_{i=g_1+1}^{n_j-g_2} z_{(i)}, \quad (13)$$

where $g_1 = [n_j \alpha_1]$, $g_2 = [n_j \alpha_2]$ and $h_j = n_j - g_1 - g_2$. Hogg suggests that the standard deviation of $m(\alpha_1, \alpha_2)$ can be estimated as:

$$S_{m(\alpha_1, \alpha_2)} = \sqrt{\frac{SS(\alpha_1, \alpha_2)}{h(h-1)}}, \quad (14)$$

where $SS(\alpha_1, \alpha_2)$ can be calculated as

$$SS(\alpha_1, \alpha_2) = \frac{\left(\begin{aligned} &(g_1+1) \left[Z_{(g_1+1)} - m(\alpha_1, \alpha_2) \right]^2 \\ &+ \left[Z_{(g_1+2)} - m(\alpha_1, \alpha_2) \right]^2 \\ &+ \dots \\ &+ \left[Z_{(n_j-g_2-1)} - m(\alpha_1, \alpha_2) \right]^2 \\ &+ (g_2+1) \left[Z_{(n_j-g_2)} - m(\alpha_1, \alpha_2) \right]^2 \\ &- \left\{ (g_1) \left[Z_{(g_1+1)} - m(\alpha_1, \alpha_2) \right] \right. \\ &\quad \left. + (g_2) \left[Z_{(n_j-g_2)} - m(\alpha_1, \alpha_2) \right] \right\}^2 \end{aligned} \right)}{n_j} \quad (15)$$

Test Statistics

$$\text{Let } \hat{\mu}_j = \sum_{i=1}^{n_j} Z_{ij} / n_j \quad \text{and}$$

$s_j^2 = \sum_{i=1}^n (Z_i - \bar{Z}_j)^2 / (n_j - 1)$ where $\hat{\mu}_j$ is the estimate of μ_j and s_j^2 is the unbiased estimate of the variance for population j . A heteroscedastic statistic (Welch, 1951) can be defined as:

$$F_w = \frac{\sum_{j=1}^J w_j (\hat{\mu}_j - \hat{\mu})^2 / (J-1)}{1 + \frac{2(J-2)}{(J^2-1)} \sum_{j=1}^J \frac{(1-w_j/W)^2}{n_j-1}}, \quad (16)$$

where

$$\hat{\mu} = \sum_{j=1}^J w_j \hat{\mu}_j / W,$$

$$W = \sum_{j=1}^J w_j a_j,$$

and

$$w_j = n_j / s_j^2.$$

The test statistic is approximately distributed as an F variate and is referred to the critical value $F[(1-\alpha); (J-1), v_w]$, the $(1-\alpha)$ quantile of the F distribution, where error degrees of freedom are obtained from

$$v_w = \frac{J^2 - 1}{3 \sum_{j=1}^J \frac{(1-w_j/W)^2}{n_j-1}}. \quad (17)$$

A Robust ANOVA F-Test

Lee and Fung (1985) defined an ANOVA F-test based on trimmed means. Because the ANOVA F-test can be more powerful than the Welch F-test, this statistic was chosen for this investigation. The Lee and Fung (1985) statistic is defined as:

$$F_t = \frac{\sum_{j=1}^J h_j (\hat{m}_j - \hat{M}_t)^2 / (J-1)}{\sum_{j=1}^J SS_j(a_1, a_2) / (H-J)} \quad (18)$$

where

$$H = \sum_{j=1}^J h_j,$$

$$\hat{M}_t = \sum_{j=1}^J h_j \hat{m}_j / H,$$

and

$$SS_j(\alpha_1, \alpha_2) = \text{the } (\alpha_1, \alpha_2).$$

The Winsorized sum of squared deviations for the j^{th} group; h_j and $\hat{m}_{ij}$ are defined the same as previously. Note that, when $\alpha_1 = \alpha_2 = 0$, $F_t = F$ (O'Brien, 1979).

O'Brien (1979) indicated that the r_{ij} s can be used in the Welch test. Accordingly, the trimmed mean version is given by:

$$r_{t_{ij}} = \frac{(h_j - 1.5)n_j (X_{ij} - \hat{m}_{ij})^2 - .5s_{mj}^2 (h_j - 1)}{(h_j - 1)(h_j - 2)} \quad (19)$$

where $h_j = n_j - g_1 - g_2$, $\hat{m}_{ij}$ = the (α_1, α_2) trimmed mean of the j^{th} group and $s_{mj}^2 = s_{m(\alpha_1, \alpha_2)}^2$ for group j . The r_{ij} s and $r_{t_{ij}}$ s were also used with the Lee and Fung (1985) test.

Methodology

A total of 170 new Levene (1960) type procedures were created. These procedures were (see Table 2 for a summary of the Levene methods examined):

(A1) Let $Z_{ij} = |X_{ij} - \bar{X}_{.j}|$. The Z_{ij} s were then trimmed symmetrically $\alpha\%$ and the robust F-test, $F_{t\alpha}$ was computed. There are 4 variants with this designation because there are four symmetric trimming percentages: 5%, 10%, 15% and 20%. For example, A_{115} signifies $Z_{ij} = |X_{ij} - \bar{X}_{.j}|$, the Z_{ij} s were trimmed symmetrically 15% and $F_{t\alpha}$ was computed.

(A2) Let $Z_{ij} = |X_{ij} - \bar{X}_{.j}|$, the Z_{ij} s were trimmed asymmetrically $\beta\%$ with a hinge estimator H and the robust F-test, F_{β} computed. A_{210HSK_5} signifies transformation $Z_{ij} = |X_{ij} - \bar{X}_{.j}|$ and these values were subjected to 10% asymmetric trimming with hinge estimator HSK_5 before computing F_{β} .

Because there are four asymmetrical trimming percentages and seven hinge estimators, there are 28 variants with this designation.

(A3) Let $Z_{ij} = |X_{ij} - \bar{X}_{.j}|$. The Z_{ij} s were used with the Welch test, F_W .

(B3) Let $Z_{ij} = |X_{ij} - M_j|$. The Z_{ij} s were used with the Welch test, F_W .

(E1) These variants are designated $E_1\alpha H$, where $Z_{ij} = |X_{ij} - \bar{X}_{t_\alpha}|$, $\bar{X}_{t_\alpha}$ are group $\alpha\%$ symmetric trimmed means. The Z_{ij} s were used with the usual F -test, W , hence variant E_{120} signifies transformed values $Z_{ij} = |X_{ij} - \bar{X}_{t_{20}}|$, where $\bar{X}_{t_{20}}$ are group 20% symmetrically trimmed at tail, computed with W . Because there are four symmetric trimming percentages (5%, 10%, 15% and 20%), there are four variants with this designation.

(E2) In variants $E_2\alpha_1\alpha_2$ let $Z_{ij} = |X_{ij} - \bar{X}_{t_{\alpha_1}}|$. The transformed values were trimmed symmetrically $\alpha_2\%$ and used with $F_{t\alpha_2}$. Therefore, variant E_{21520} signifies transformation $Z_{ij} = |X_{ij} - \bar{X}_{t_{15}}|$, where $\bar{X}_{t_{15}}$ are group 15% symmetric trimmed means and these values were subjected to 20% symmetric trimming before being used with $F_{t\alpha_2}$. Because there are four different $\bar{X}_{t_{\alpha_1}}$'s and four symmetric trimming percentages, there are 16 variants with this designation.

(E3) In variants $E_3\alpha\beta H$, let $Z_{ij} = |X_{ij} - \bar{X}_{t_\alpha}|$. The transformed values were asymmetrically trimmed at $\beta\%$ involving seven hinge estimators (HQ , HQ_1 , HH_3 , HQ_2 , HH_1 , HSK_2 , HSK_3) and used with F_{β} . Hence, $E_{31025HH_3}$

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signifies transformation $Z_{ij} = |X_{ij} - \bar{X}_{t_0}|$, where $\bar{X}_{t_0}$ are group 10% symmetric trimmed means; these values were subjected to 25% asymmetric trimming calculated using the HH_3 hinge estimator before applying $F_{t\beta}$. Because there are four different $\bar{X}_{t_a}$'s and four asymmetric trimming percentages with seven different hinge estimators, there are 112 variants for this designation.

- (E4) Variants $E_4\alpha H$ use $\bar{X}_{t_a}$ in place of $\bar{X}_j$ (A_3) or $M_j(B_3)$, in getting the Z_{ij} values. The Z_{ij} s were then used with the Welch test, F_W . Hence E_410 signifies transformed values $Z_{ij} = |X_{ij} - \bar{X}_{t_0}|$, where $\bar{X}_{t_0}$ are group 10% symmetric trimmed means and used with F_W . Since there are four symmetric trimming percentages, there are four variants with this designation.

A total of 165 O'Brien-type procedures were created (see Table 2 for a summary of the O'Brien methods examined):

- (J) O'Brien transformation based upon group means and variances used with the usual F-test, W (that is, r_{ij} in W).
- (Q1) Variants are designated $Q_1\alpha$. The O'Brien transformation based upon symmetric trimmed means and Winsorized variances of X_{ij} . These trimmed means were calculated at $\alpha = 5\%, 10\%, 15\%$ and 20% . The transformed values, r_{ij} , were used with the usual F-test (that is, r_{ij} in W). Because there are four symmetrical trimming percentages, there are four variants with this designation. Therefore, variants Q_110 signifies transformation of X_{ij} with 10%

symmetric trimmed mean before used with W .

- (Q2) Variants are designated $Q_2\alpha_1\alpha_2$. The O'Brien transformation based upon group symmetric trimmed means and Winsorized variances of X_{ij} . These trimmed means and Winsorized variances were calculated at symmetric trimming percentages ($5\%, 10\%, 15\%$ and 20%). The resultant transformed values, r_{ij} , were symmetrically trimmed based on the same percentages used for X_{ij} and used with the robust ANOVA F_t test (that is, symmetrically trimmed r_{ij} in F_t). Because there are four symmetric trimming percentages used twice, there are 16 variants with this designation. Hence, variant Q_2515 signifies transformation of X_{ij} with 5% symmetric trimmed mean and 15% symmetric trimmed mean for the transform value, r_{ij} , before used with F_t .

- (Q3) Variants are designated $Q_3\alpha\beta H$. The O'Brien transformation based upon symmetric trimmed means and Winsorized variances of X_{ij} . These trimmed means were calculated with the four symmetric trimming percentages ($5\%, 10\%, 15\%$ and 20%). The resultant transformed values, r_{ij} , were then asymmetrically trimmed at $\beta = 10\%, 15\%, 20\%$ and 25% involving seven hinge estimators and used with the robust ANOVA F_t -test (that is, asymmetrically trimmed r_{ij} in F_t). Because there are four symmetric trimming percentages, on X_{ij} , four asymmetric trimming percentages on r_{ij} with seven hinge estimators, there are 112 variants with this designation.

(Q4) Because variants are designated $Q_4\alpha$. The O'Brien transformation based upon symmetric trimmed means Winsorized variances of X_{ij} . These trimmed means were calculated at the four symmetric trimming percentages (5%, 10%, 15% and 20%). The transformed values, r_{ij} , were then used with the Welch test, F_W (that is, r_{ij} in F_W). Because there are four symmetrical trimming percentages, there are four variants with this designation. Hence, variants Q_405 signifies transformation of X_{ij} with 5% symmetric trimmed mean before used with F_W .

Variants are designated $K\beta H$. The O'Brien transformation based upon asymmetric trimmed means Winsorized variances of X_{ij} . These trimmed means were calculated at $\beta = 10\%, 15\%, 20\%$ and 25% involving seven hinge estimators ($HQ, HQ_1, HH_3, HQ_2, HH_1, HSK_2, HSK_5$). The transformed values, r_{ij} , were used with the usual F-test (that is, r_{ij} in W). Because there are four asymmetrical trimming percentages and seven hinge estimators, there are 28 variants with this designation. Hence, variants $K15HSK_2$ signifies transformation of X_{ij} with 15% asymmetric trimmed mean calculated using the HSK_2 hinge estimator before used with W .

Study Conditions

Four variables were employed in the $J = 3$ study: (a) total sample size; (b) degree of sample size inequality; (c) shape of the population distribution; and (d) type and amount of total trimming.

Total Sample Size

The effect of sample size on the performance of the various procedures was evaluated by varying the total sample size (N). The total sample size was manipulated, setting the average group size to $n_j = 20$ and 40 . The

average group-sizes correspond to total sample sizes of $N = 60$ and $N = 120$.

Degree of Sample Size Inequality

Three conditions of sample size equality/inequality were investigated which are referred to as: equal n_j , moderately unequal n_j and extremely unequal n_j (see below for values). These conditions were evaluated because Keselman, et al. (1998) found that unbalanced designs were more common than balanced designs.

Sample Size Values

n_j s
20, 20, 20
15, 20, 25
10, 20, 30
40, 40, 40
35, 40, 45
30, 40, 50

Shape of the Population Distribution

This study investigated distributions ranging from symmetric to skewed and platykurtic to normal-tailed to leptokurtic distributions. In total, seven distributions were employed to compare the procedures. The distributions used were: (i) the Fleishman (1978) transformation of the standard normal distribution into a skewed platykurtic distribution with skewness, $\gamma_1 = 0.5$ and kurtosis, $\gamma_2 = -0.5$; (ii) a second Fleishman transformation of the standard normal distribution into a skewed normal-tailed distribution with $\gamma_1 = 0.75$ and $\gamma_2 = 0$; (iii) the Beta (0.5, 0.5) distribution representing symmetric platykurtic distributions; (iv) a g and h distribution (Hoaglin, 1985) where $g = h = 0$, which is the standard normal distribution with $\gamma_1 = \gamma_2 = 0$; (v) a $g = 0$ and $h = 0.225$ long-tailed distribution with $\gamma_1 = 0$ and $\gamma_2 = 154.84$, representing symmetric leptokurtic distributions; (vi) a $g = 0.76$ and $h = -0.098$ distribution with skew and kurtosis equal to that of an exponential

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Table 1: Description of the Levene (1960) Transformations Used In the Simulations

Designation	Description	Cases
A1	$X_{ij} \rightarrow Z_{ij}$: use group means from X_{ij} . Z_{ij} : symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, apply robust ANOVA F -test.	4
A2	$X_{ij} \rightarrow Z_{ij}$: use group means from X_{ij} . Z_{ij} : asymmetrically trimmed at total proportions: 0.10, 0.15, 0.20, 0.25 and 7 hinge estimators: Q, Q1, H3, Q2, H1, SK2, SK5, apply robust ANOVA F -test.	28
A3	$X_{ij} \rightarrow Z_{ij}$: use group means from X_{ij} . Z_{ij} : apply Welch F -test.	1
B3	$X_{ij} \rightarrow Z_{ij}$: use group medians from X_{ij} . Z_{ij} : apply Welch F -test.	1
E1	$X_{ij} \rightarrow Z_{ij}$: use group symmetric trimmed means from X_{ij} . X_{ij} symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, Z_{ij} : apply usual ANOVA F -test.	4
E2	$X_{ij} \rightarrow Z_{ij}$: use group symmetric trimmed means from X_{ij} . X_{ij} symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, Z_{ij} : symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, apply robust ANOVA F -test.	16
E3	$X_{ij} \rightarrow Z_{ij}$: use group symmetric trimmed means from X_{ij} . X_{ij} symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, Z_{ij} : asymmetrically trimmed at total proportions: 0.10, 0.15, 0.20, 0.25, keeping hinge estimator constant, apply robust ANOVA F -test.	112
E4	$X_{ij} \rightarrow Z_{ij}$: use group symmetric trimmed means from X_{ij} . X_{ij} symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, Z_{ij} : apply Welch F -test.	4
Total		170

Table 2: Description of the O'Brien (1979) Designations Used In the Simulations

Designation	Description	Cases
J	$X_{ij} \rightarrow R_{ij}$: use group means and variances from X_{ij} . R_{ij} : apply usual ANOVA F -test.	1
Q1	$X_{ij} \rightarrow R_{ij}$: use group symmetric trimmed means and Winsorized variances from X_{ij} . X_{ij} symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, R_{ij} : apply usual F -test.	4
Q2	$X_{ij} \rightarrow R_{ij}$: use group symmetric trimmed means and Winsorized variances from X_{ij} . X_{ij} symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, R_{ij} : symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, apply robust ANOVA F -test.	16
Q3	$X_{ij} \rightarrow R_{ij}$: use group symmetric trimmed means and Winsorized variances from X_{ij} . X_{ij} symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, R_{ij} : asymmetrically trimmed at total proportions: 0.10, 0.15, 0.20, 0.25 and 7 hinge estimators: Q, Q1, H3, Q2, H1, SK2, SK5. Apply robust ANOVA F -test.	112
Q4	$X_{ij} \rightarrow R_{ij}$: use group symmetric trimmed means and Winsorized variances from X_{ij} . X_{ij} symmetrically trimmed at tail proportions: 0.05, 0.10, 0.15, 0.20, R_{ij} : apply Welch F -test.	4
K	$X_{ij} \rightarrow R_{ij}$: use group asymmetric trimmed means and Winsorized variances from X_{ij} . X_{ij} asymmetrically trimmed at total proportions: 0.10, 0.15, 0.20, 0.25 and 7 hinge estimators: Q, Q1, H3, Q2, H1, SK2, SK5. R_{ij} : apply usual F -test.	28
Total:		165

distribution ($\gamma_1 = 2, \gamma_2 = 6$); and (vii) a $g = 0.225$ and $h = 0.225$ distribution, which is also a long-tailed skewed distribution ($\gamma_1 = 4.90, \gamma_2 = 4673.80$). The last two distributions represent skewed leptokurtic distributions, with (vii) more severe than (vi). These distribution conditions were selected in order to evaluate the operating characteristics of the procedures across a variety of distributions and because they have been examined in other studies (e.g., Algina, Keselman & Penfield, 2007).

The Fleishman (1978) power transformation is of the form $Y = a + bZ + cZ^2 + dZ^3$, where Z are standard normal variates. Fleishman provided a table of values for the coefficients, b, c , and d that enables the standard normal distribution to be transformed into a nonnormal distribution, also having mean zero and variance one, but with different degrees of skewness and kurtosis. The extra coefficient a is obtained through the relation $a = -c$ as a direct result of constraining $E(Y) = 0$. Two sets of coefficients (b, c, d) were selected from Fleishman (1978) and used in the preceding equation to generate Z_{ij} s from the RANDGEN function (SAS, 2006) with the normal distribution option to produce distributions (i) and (ii). This RANDGEN SAS subroutine allows a user to generate 20 known distributions, both discrete and continuous. Data from the third distribution was also generated using the RANDGEN function but with the beta distribution option. Beta (0.5, 0.5) is a symmetric u-shaped distribution, hence the negative kurtosis.

To generate data from a g and h distribution, standard unit normal variables (Z_{ij}) were converted to g and h distributed random variables via

$$Y_{ij} = \frac{\exp(g Z_{ij}) - 1}{g} \exp\left(\frac{h Z_{ij}^2}{2}\right), \quad (20)$$

where both g and h are non-zero. When g is zero

$$Y_{ij} = Z_{ij} \exp\left(\frac{h Z_{ij}^2}{2}\right). \quad (21)$$

The Z_{ij} scores were generated using the generator RANDGEN with the normal distribution option.

Observations generated for distributions (iii), (v), (vi) and (vii), where the variances were not equal to one, were standardized so that they were one, to reflect the null hypothesis, $H_0: \sigma_1^2 = \sigma_2^2 = \sigma_3^2$; that is, in the simulations, $\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = 1$.

Percentages of Total Trimming

Four values of total trimming, namely 10%, 15%, 20% and 25% were examined when data were asymmetrically trimmed, whether to obtain the values used in the transformation of the X_{ij} data or when trimming was carried out on the Levene transformed values Z_{ij} or O'Brien's transformed values, r_{ij} and r_{tj} . Symmetric trimming values of 5%, 10%, 15% and 20% were also investigated. As noted, the literature varies on the amount of recommended (symmetric) trimming and thus these values were chosen to cover the range of values recommended. For each condition 5,000 replications were conducted and the nominal levels of significance for all tests were 0.05 and 0.10.

Results

Tables 4 and 5 summarize the ten best results for the modified Levene (1960) tests for spread. Table 4 shows the average rates of Type I error, the absolute values of the difference between the average rates and 0.05, and the percent of cases falling in three intervals – (0.025, 0.050), (0.045, 0.055), and (0.045, 0.050). The last column indicates total percentage of cases falling in (0.025, 0.055); using simple set theory algebra, this is just percent of cases in (0.025, 0.050) and in (0.045, 0.055) minus percent of cases in (0.045, 0.050). Based on these findings the following are noted:

1. All ten methods examined provided very good Type I error control. Indeed, the

empirical rates ranged from 0.046 to 0.0579; and

2. In order to identify the best method(s) the percentages reported in the last column were relied upon. From this information, B_3 was identified as the best of the Levene (1960) modifications defined and examined.

Table 5 presents Type I error rates for each characteristic of the distributions investigated, as well as the overall rate, indicates that the method that selected as best, contains average Type I errors of 0.048.

The same information is presented in Tables 6 and 7 for the ten best modified O'Brien (1981) tests for spread. Based on these findings, the ten best O'Brien variants provided tight Type I error control ranging from 0.490 to 0.0508. The last column of Table 6 identifies two of the modified procedures, $Q_31025HQ_1$ and $K20HH_3$, as the best of the O'Brien (1981) modifications. Table 7 presents Type I error rates for each characteristic of the distributions investigated, as well as the overall rate, and indicates that the both methods that selected as best contain Type I errors averaging 0.050.

Conclusion

This study examined the Type I error rate (for $\alpha = 0.05$) of various modifications of Levene's (1960) and O'Brien's (1981) procedures that could be used to compare variability across groups in independent groups designs, specifically variations not examined by Keselman, et al. (2008). The procedures examined used Levene (1960) or O'Brien (1981) type transformations of the original scores or transformed scores, except as opposed to using the measures of central tendency and variability suggested by Levene and O'Brien, robust measures of central tendency and/or variability were adopted.

The robust values of central tendency and variability (i.e., the trimmed means and Winsorized variances) were based on symmetric or asymmetric trimming rules, that is, rules that either set *a priori* the amount of total trimming or determined empirically the amount to be trimmed from the tails (if at all) based on varied

recommendations for total trimming. These approaches were also applied to various test statistics: the ANOVA F-test, a robust F-test (Lee & Fung, 1985), the Welch (1951) test, and bootstrapped versions of these statistics. The procedures were compared under seven distributions when group sizes were equal, moderately, or very unequal. The skewness and kurtosis of the distributions examined varied from the normal distribution ($\gamma_1 = 0$, $\gamma_2 = 0$ respectively) to distributions that were nonnormal, $\gamma_1 = 4.9$ and $\gamma_2 = 4673.80$, respectively).

The procedures were compared on four measures: the average rate of Type I error across the 42 conditions examined, the percentage of empirical Type I errors that fell within the intervals (0.025, 0.05), (0.045, 0.055) and (0.045, 0.05), and the absolute value of the difference between the mean Type I error rate and 0.05. Finally, it should be noted that though it was intended to examine bootstrapped versions of these procedures, this was not pursued because very good Type I error control was achieved without resorting to bootstrapping. Results indicated that the results reported by Keselman, et al. (2008) could not be improved upon with respect to the Levene (1960) test. That is, though the new Levene modifications all worked very well in controlling Type I error rates, they did not result in as many cases falling into the three intervals defined for good Type I error control as reported by Keselman, et al. (2008).

Conversely, two of the O'Brien (1960) modifications did perform well, at least as well as the variants examined by Keselman, et al. (2008) and their recommended Levene variant. These were $Q_31025HQ_1$ and $K20HH_3$ with tighter Type I error control and a decent number of cases falling into the three intervals defined for good Type I error control by Keselman, et al. (2008).

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Table 4: Type I Error Rates for the 10 Best Performing New Levene's Variants and Percentages of Type I Error Rates within Various Intervals

No.	Variant	Average p-Values	Mean-0.05	Percent Within 2.5,5.0	Percent Within 4.5,5.5	Percent Within 4.5,5.0	Total %
1	B ₃	.0476	.0024	54.76	30.95	14.29	71
2	E ₁ 20	.0531	.0031	47.62	40.48	23.81	64
3	E ₃ 0525HH ₁	.0555	.0055	33.33	28.57	14.29	48
4	E ₃ 1025HH ₁	.0564	.0064	26.19	21.43	4.76	43
5	E ₃ 0525HH ₃	.0566	.0066	38.10	23.81	16.67	45
6	E ₃ 0525HHQ ₂	.0566	.0066	28.57	26.19	9.52	45
7	E ₃ 0525HHQ	.0568	.0068	33.33	23.81	9.52	48
8	E ₃ 1025HHQ ₂	.0577	.0077	28.57	19.05	7.14	41
9	E ₁ 15	.0579	.0079	35.71	47.62	28.57	55
10	E ₃ 1025HHQ	.0579	.0079	26.19	40.48	21.43	45

Table 5: Type I Error Rates for the 10 Best Performing Variants of Levene's Procedure

No.	Variant	Overall	Skewed	Symmetric	Leptokurtic	Normal Tailed	Platykurtic
1	B ₃	.048	.053	.042	.055	.048	.038
2	E ₁ 20	.053	.057	.048	.052	.055	.052
3	E ₃ 0525HH ₁	.056	.060	.050	.052	.058	.058
4	E ₃ 1025HH ₁	.056	.059	.053	.052	.058	.062
5	E ₃ 0525HH ₃	.057	.061	.051	.055	.058	.058
6	E ₃ 0525HHQ ₂	.057	.061	.051	.053	.059	.059
7	E ₃ 0525HHQ	.057	.062	.050	.054	.060	.058
8	E ₃ 1025HHQ ₂	.058	.061	.053	.053	.059	.063
9	E ₁ 15	.058	.064	.050	.058	.059	.057
10	E ₃ 1025HHQ	.058	.063	.051	.058	.058	.058

Table 6: Type I Error Rates for the 10 Best Performing O'Brien (1979) Variants and Percentages of Type I Error Rates within Various Intervals

No.	Variant	Average p-Values	Mean-0.05	Percent Within 2.5, 5.0	Percent Within 4.5, 5.5	Percent Within 4.5, 5.0	Total %
1	Q ₃ 2015HH ₃	.0499	.0001	35.71	11.90	9.52	38
2	Q ₃ 1515HH ₃	.0498	.0002	35.71	19.05	9.52	45
3	K10HQ ₁	.0503	.0003	54.76	23.81	16.67	62
4	Q ₃ 1025HQ ₁	.0503	.0003	57.14	26.19	11.90	71
5	Q ₂ 0515	.0504	.0004	52.38	19.05	9.52	62
6	K20HH ₃	.0496	.0004	54.76	28.57	14.29	69
7	K10HH ₃	.0506	.0006	54.76	23.81	16.67	62
8	Q ₃ 1010HQ	.0507	.0007	42.86	28.57	16.67	55
9	Q ₃ 2015HQ	.0508	.0008	33.33	16.67	9.52	40
10	K25HQ ₁	.0490	.0010	54.76	9.52	9.52	55

Table 7: Type I Error Rates for the 10 Best Performing Variants of O'Brien's (1979) Procedure

No.	Variant	Overall	Skewed	Symmetric	Leptokurtic	Normal Tailed	Platykurtic
1	Q ₃ 2015HH ₃	.050	.051	.049	.035	.056	.066
2	Q ₃ 1515HH ₃	.050	.051	.049	.036	.058	.063
3	K10HQ ₁	.050	.056	.043	.045	.056	.053
4	Q ₃ 1025HQ ₁	.050	.052	.048	.045	.059	.051
5	Q ₂ 0515	.050	.054	.046	.043	.059	.053
6	K20HH ₃	.050	.055	.042	.043	.058	.052
7	K10HH ₃	.051	.057	.043	.046	.056	.053
8	Q ₃ 1010HQ	.051	.052	.049	.040	.058	.059
9	Q ₃ 2015HQ	.051	.053	.048	.038	.059	.062
10	K25HQ ₁	.049	.058	.038	.042	.058	.052

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An Extension of the Seasonal KPSS Test

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The limit theory of the seasonal KPSS test is established under the null hypothesis using seasonal dummy variables. Taking these variables into account can result in improved finite sample performance of the test. The seasonal KPSS test can be interpreted as a test of deterministic seasonality and it may be used in addition to seasonal unit root tests to analyze the dynamic properties of time series. The seasonal indicator variables provide the test with an explicit model-based regression that in itself constitutes a support for its limit theory.

Key words: KPSS test, deterministic seasonality, Brownian motion, C32 time series models.

Introduction

The use of seasonally unadjusted data has become increasingly popular in empirical studies; there are several possible reasons for this. One key reason is the argument that seasonal adjustment distorts inference in dynamic models, for example, seasonal unit roots can be seriously affected when working with seasonally adjusted data. In this respect, Ghysels and Perron (1993) showed that seasonal adjustment filters affect finite sample distributions of unit root test statistics under the null hypothesis. Further, the seasonal component is an unobserved part of a time series, thus it must be taken into consideration because its elimination can lead to detrimental information loss. It was found in several cases that the seasonal component and other systematic components, such as trend and cycle, are in fact non-separable. From a statistical viewpoint this could be attributed to the fact that economic propagation mechanisms transmitting seasonal

fluctuations from exogenous to endogenous variables are systematically related to business cycle fluctuations. Beaulieu, MacKie-Mason and Miron (1992) and Miron (1996) showed this in their studies of international economic aggregates such as output, labor input, interest rates, and prices. Canova and Ghysels (1994) also found that seasonality tends to differ across business cycle stages of recessions and expansions referring to an empirical study of U. S. macroeconomic time series. Consequently, a forced seasonal adjustment may lead to inaccurate predictions, which in turn may result in wrong decisions.

The literature presents several different models of seasonality. As highlighted by Canova and Hansen (1995), the first approach is to model seasonality as a deterministic component. This approach is generally adopted by macroeconomists, as shown by Barsky and Miron (1989). The second approach is to consider seasonality as a deterministic process along with its stationary stochastic pattern as illustrated by Canova (1992). The third approach is to consider seasonality as a stochastic component by allowing for seasonal unit roots.

A famous testing framework proposed by Hylleberg, et al. (1990) used the null hypothesis of seasonal non-stationarity induced by the presence of seasonal unit root(s) to make the distinction between unit roots at different seasonal frequencies. The subsequent rejection of their null hypothesis implies a strong result

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that the series exhibits a stationary seasonal pattern but their test was found to suffer from the problem of low power with moderate sample sizes. Because testing for seasonal unit roots is an important step in time series analysis these tests are often used as a pre-test for seasonal co-integration (Johansen & Schaumberg, 1999), several authors have contributed to the development of these types of tests (Canova & Hansen, 1995; Caner, 1998). In the testing approach the rejection of the null hypothesis would show evidence that the data are non-stationary. Another reason why this testing method is interesting to practitioners could be explained by the necessity to take into account the cost of spurious inference when testing the dummy variables model as argued in Franses, Hylleberg and Lee (1995).

Canova and Hansen (1995) and Taylor (2003) generalized the KPSS testing framework to seasonal data to test the stationarity hypothesis against (seasonal) unit roots. After specifying a general regression for their tests, the authors examined specific cases related to testing stationarity against (seasonal) unit root or some unit roots among a well-defined set. Lyhagen (2006) proposed another version of the KPSS test in the seasonal context which results in a frequency-based test and tested the hypothesis of level stationarity against a single seasonal unit root. In this study, seasonal indicator variables are included in the seasonal KPSS suggested by Lyhagen (2006). This approach may several have advantages over existing methods: It provides a model-based regression to the test, which is different from Lyhagen's method, where the limit theory based on an explicit form of the model was not established. The novelty of results from this study is the development of an asymptotic theory of the test in the presence of seasonal dummies which leads to a natural extension of the SKPSS to include deterministic seasonality.

Preliminaries on the Seasonal KPSS Test

Let y_t be a time series observed quarterly. This frequency was chosen because it provides a simple and clear analysis, however it should be noted that results of this study are valid for all seasonal frequencies (e.g., monthly

or daily data) by simply defining seasonal unit roots according to their corresponding seasonal frequencies. Because the goal of this research is to test for the presence of negative unit root, it would be suitable to use the appropriate filter in order to isolate the effects of other unit roots in the series. Therefore, the test will be applied to the transformed series:

$$y_t^{(1)} = (1 - L + L^2 - L^3)y_t,$$

where L is the lag operator.

Next, test the unit root of -1 in the series

$$y_t^{(1)} = x_t' \beta + r_t + u_t, \quad (1)$$

$$t = 1, \dots, T,$$

where $T = 4N$, $\beta' x_t = \sum_{i=1}^4 a_i D_{it}$, the shorthand notation $D_{it} = \delta(i, t - 4[(t-1)/4])$, $[\cdot]$ denotes the largest integer function and $\delta(i, j)$ is the Kronecker's δ function. The term u_t is zero mean weakly dependent process with autocovariogram $\gamma_h = E(u_t u_{t+h})$ and a strictly positive long run variance ω_u^2 .

The component r_t is drawn from the following process:

$$r_t = -r_{t-1} + v_t, \quad (2)$$

where v_t is zero mean weakly process with variance σ_v^2 and long run variance $\omega_v^2 > 0$. The transformation required to carry out the seasonal KPSS test for complex unit roots $\pm i$ is given by the variable, $y_t^{(2)} = (1 - L^2)y_t$. The test of such complex unit roots is based on the regression,

$$y_t^{(2)} = x_t' \lambda + c_t + e_t, \quad (3)$$

where e_t is zero mean weakly dependent process with long run variance $\omega_e^2 > 0$ and $\lambda'x_t = \sum_{i=1}^4 b_i D_{it}$. The component c_t is given by

$$c_t = -c_{t-2} + \varepsilon_t, \quad (4)$$

where ε_t is another zero mean weakly dependent process with variance σ_ε^2 and strictly positive long run variance ω_ε^2 .

Adding the deterministic terms in (1) and (3) is very important because it enables the seasonal KPSS test to be extended to include deterministic seasonality. The testing procedure follows in two steps: First, test for the existence of unit root -1 , and second, test for the complex roots where the null hypothesis will be specified thereafter.

The seasonal KPSS test is a Lagrange Multiplier-based test, hence, the null hypothesis of a root equal to -1 is $H_0 : \sigma_v^2 = 0$. Under this null hypothesis

$$y_t^{(1)} = x_t' \beta + u_t, \quad (5)$$

where the series is trend stationary after seasonal mean correction. Under the alternative hypothesis $H_1 : \sigma_v^2 > 0$, $y_t^{(1)}$ has a unit root corresponding to Nyquist frequency.

Let $\tilde{u}_t$ be the residual series obtained from least squares regression applied to equation (5), $t = 1, 2, \dots, T$. Following Breitung and Franses (1998, Eq. (18), p. 209), Busetti and Harvey (2003, Eq. (8), p. 422) and Taylor (2003, Eq. (38), p. 605), replace the long-run variance ω_u^2 by an estimate of (2π) times the spectrum at the observed frequency in order to deal with unconditional heteroscedasticity and serial correlation. This nonparametric estimation of the long-run variance is a useful solution to the nuisance parameter problem (Taylor, 2003). Thus, the Nyquist frequency is

$$\begin{aligned} \tilde{\omega}_u^2(l) = \\ T^{-1} \sum_{t=1}^T \tilde{u}_t^2 + 2T^{-1} \sum_{k=1}^l w(k, l) \left(\sum_{t=k+1}^T \tilde{u}_t \tilde{u}_{t-k} \right) \cos(\pi k), \end{aligned} \quad (6)$$

where the weight function $w(k, l) = 1 - \frac{k}{l+1}$

and l is a lag truncation parameter such that $l \rightarrow \infty$ as $T \rightarrow \infty$ and $l = o(n^{1/2})$. From equation (6), a Bartlett kernel following Newey and West (1987) can now be chosen. It should be noted that Andrews (1991) and Kwaikowski, et al. (1992) showed that such a truncation lag can produce good results in practice. Similarly, the null hypothesis of the test regarding complex unit roots is given by $H_0 : \sigma_\varepsilon^2 = 0$; under this null hypothesis

$$y_t^{(2)} = x_t' \lambda + e_t \quad (7)$$

Using the residuals $\tilde{e}_t$ obtained from the least squares regression of equation (7), the Bartlett kernel estimator ω_e^2 is computed as:

$$\begin{aligned} \tilde{\omega}_e^2(l) = \\ T^{-1} \sum_{t=1}^T \tilde{e}_t^2 + 2T^{-1} \sum_{k=1}^l w(k, l) \left(\sum_{t=k+1}^T \tilde{e}_t \tilde{e}_{t-k} \right) \cos\left(\frac{\pi}{2} k\right), \end{aligned} \quad (8)$$

with the partial sums defined as $\tilde{S}_t = \sum_{j=1}^t e^{i\pi j} \tilde{u}_j$

and $\tilde{P}_t = \sum_{j=1}^t e^{i\frac{\pi}{2} j} \tilde{e}_j$.

It follows that the test statistics for unit root of -1 is given by:

$$\eta^{(-1)} = \frac{1}{T^2} \frac{\sum_{t=1}^T \tilde{S}_t \tilde{S}_t'}{\tilde{\omega}_u^2(l)}. \quad (9)$$

This statistic may be written for the complex unit roots, as

$$\eta^{(\pm i)} = \frac{1}{T^2} \frac{\sum_{t=1}^T \tilde{P}_t \tilde{\bar{P}}_t}{\tilde{\omega}_e^2(l)}, \quad (10)$$

where $\tilde{S}_t$ and $\tilde{\bar{P}}_t$ are the conjugate numbers of $\tilde{S}_t$ and $\tilde{P}_t$, respectively.

Asymptotic Results

Next, the asymptotic distribution of $\eta^{(1)}$ and $\eta^{(\pm i)}$ is shown.

Theorem

a) Under

$$H_0 : \sigma_v^2 = 0, \eta^{(-1)} \rightarrow_d \int_0^1 V(r)^2 dr$$

where $V(r)$ is a standard Brownian bridge, and $\rightarrow_d$ denotes weak convergence in probability and $r \in [0,1]$.

b) Under

$$H_0 : \sigma_\varepsilon^2 = 0,$$

$$\eta^{(\pm i)} \rightarrow_d \frac{1}{2} \int_0^1 [V_R^c(\tau)^2 + V_I^c(\tau)^2] d\tau$$

where $V_R^c(\tau)$ and $V_I^c(\tau)$ are two independent standard Brownian bridges and $\tau \in [0,1]$.

Proof

Starting with the first part of the theorem and referring to Jin and Phillips (2002) whose results showed that seasonal dummies maintain the asymptotic properties of the KPSS test unchanged. Also, given the mirror image of negative unit roots,

$$\frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} (-1)^j u_j \rightarrow_d B(r)$$

where $B(r)$ is a Brownian motion. The standardized partial sum process can be written as follows:

$$\begin{aligned} \frac{\tilde{S}_{[Tr]}}{\sqrt{T}} &= \frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} e^{i(\pi j)} \tilde{u}_j \\ &= \frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} (-1)^j \tilde{u}_j \\ &= \frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} (-1)^j [u_j - x_j'(\tilde{\beta} - \beta)] \\ &= \frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} (-1)^j u_j - \\ &\quad \frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} (-1)^j x_j' (X'X)^{-1} (X'u), \end{aligned}$$

where $r \in [0,1]$. Thus the following is obtained,

$$\begin{aligned} \frac{\tilde{S}_{[Tr]}}{\sqrt{T}} &= \frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} (-1)^j u_j - \\ &\quad \left(\frac{\sum_{j=1}^{[Tr]} (-1)^j x_j'}{T} \right) \left(\frac{X'X}{T} \right)^{-1} \left(\frac{X'u}{\sqrt{T}} \right). \end{aligned} \quad (11)$$

In addition,

$$\frac{1}{T} \sum_{j=1}^{[Tr]} (-1)^j x_j' \rightarrow \left(-\frac{r}{4}, \frac{r}{4}, -\frac{r}{4}, \frac{r}{4} \right),$$

$$T^{-1} X'X \rightarrow (1/4)I_4,$$

and

$$\frac{1}{\sqrt{T}} X' u = \frac{1}{2} \frac{1}{\sqrt{\frac{T}{4}}} \begin{pmatrix} \sum_{j=1}^{\frac{T}{4}} u_{4j-3} \\ \sum_{j=1}^{\frac{T}{4}} u_{4j-2} \\ \sum_{j=1}^{\frac{T}{4}} u_{4j-1} \\ \sum_{j=1}^{\frac{T}{4}} u_{4j} \end{pmatrix} \rightarrow \frac{1}{2} \begin{pmatrix} B_{u,1} \\ B_{u,2} \\ B_{u,3} \\ B_{u,4} \end{pmatrix}$$

$$\equiv \frac{1}{2} N \left(0, \begin{pmatrix} \omega_0 & \omega_1 & \omega_2 & \omega_3 \\ \omega_1 & \omega_0 & \omega_1 & \omega_2 \\ \omega_2 & \omega_1 & \omega_0 & \omega_1 \\ \omega_3 & \omega_2 & \omega_1 & \omega_0 \end{pmatrix} \right), \quad (12)$$

where $B_{u,i}(1) = {}_d N(0, \omega_0)$, $i = 1, \dots, 4$,

$$\omega_0 = \gamma_0 + 2 \sum_{h=1}^{\infty} \gamma_{4h}, \omega_1 = \sum_{h=1}^{\infty} \gamma_{2h-1} = \omega_3, \quad \text{and}$$

$$\omega_2 = 2 \sum_{h=1}^{\infty} \gamma_{4h-2}. \text{ It follows that}$$

$$\left(\frac{\sum_{j=1}^{[Tr]} (-1)^j x'_j}{T} \right) \left(\frac{X' X}{T} \right)^{-1} \left(\frac{X' u}{\sqrt{T}} \right) \rightarrow$$

$${}_d \left(-\frac{r}{4}, \frac{r}{4}, -\frac{r}{4}, \frac{r}{4} \right) \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{pmatrix} \frac{1}{2} \begin{pmatrix} B_{u,1}(1) \\ B_{u,2}(1) \\ B_{u,3}(1) \\ B_{u,4}(1) \end{pmatrix}$$

$$\rightarrow {}_d \frac{1}{2} r [-B_{u,1}(1) + B_{u,2}(1) - B_{u,3}(1) + B_{u,4}(1)]$$

$$\rightarrow {}_d \frac{1}{2} r [-B_1(1) + B_2(1) - B_3(1) + B_4(1)] = r B(1)$$

and

$$\frac{1}{\sqrt{T}} \tilde{S}_{[Tr]} \rightarrow {}_d B(r) - r B(1),$$

which results in the following:

$$T^{-2} \sum_{t=1}^T \tilde{S}_t^2 \rightarrow {}_d \omega_u^2 \int_0^1 V(r)^2 dr, \quad (13)$$

where $V(r)$ is a standard Brownian bridge process. Further, because $\tilde{\omega}_u^2(l)$ is a consistent estimate of ω_u^2 , it can be shown that $\eta^{(-1)} \rightarrow {}_d \int_0^1 V(r)^2 dr$.

Next it is necessary to prove the second part of the theorem. Because complex-valued roots come in conjugate pairs, it is only necessary to consider the complex root i

associated with frequency $\frac{\pi}{2}$. In this case the

standardized partial sum process can be written as follows:

$$\begin{aligned} \frac{\tilde{P}_{[Tr]}}{\sqrt{T}} &= \frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} e^{i(j\frac{\pi}{2})} \tilde{e}_j \\ &= \frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} e^{i(j\frac{\pi}{2})} \tilde{e}_j \\ &= \frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} e^{i(j\frac{\pi}{2})} [e_j - x'_j(\tilde{\lambda} - \lambda)] \end{aligned}$$

where

$$\frac{\tilde{S}_{[Tr]}}{\sqrt{T}} =$$

$$\frac{1}{\sqrt{T}} \sum_{j=1}^{[Tr]} e^{i(j\frac{\pi}{2})} e_j - \left(\frac{\sum_{j=1}^{[Tr]} e^{i(j\frac{\pi}{2})} x'_j}{T} \right) \left(\frac{X' X}{T} \right)^{-1} \left(\frac{X' e}{\sqrt{T}} \right)$$

Chan and Wei (1988) showed that

$$\frac{1}{\sqrt{T}} \sum_{j=1}^{[T\tau]} e^{i(j\frac{\pi}{2})} e_j \rightarrow_d B^*(\tau),$$

where $B^*(\tau) = B_R^*(\tau) + iB_I^*(\tau)$ and $B_R^*(\tau)$ and $B_I^*(\tau)$ are two independent real Brownian motions and

$$\frac{1}{T} \sum_{j=1}^{[T\tau]} e^{i(j\frac{\pi}{2})} x_j' \rightarrow \left(0, -\frac{r}{4}, 0, \frac{r}{4}\right) + i\left(\frac{r}{4}, 0, -\frac{r}{4}, 0\right).$$

Therefore,

$$\left(\frac{\sum_{j=1}^{[T\tau]} e^{i(j\frac{\pi}{2})} x_j'}{T} \right) \left(\frac{X'X}{T} \right)^{-1} \left(\frac{X'e}{\sqrt{T}} \right) \rightarrow \left[\begin{array}{l} 4 \times \left(0, -\frac{r}{4}, 0, \frac{r}{4}\right) I_4 \times \frac{1}{2} \begin{pmatrix} B_{e.1} \\ B_{e.2} \\ B_{e.3} \\ B_{e.4} \end{pmatrix} \\ + i \left[4 \times \left(\frac{r}{4}, 0, -\frac{r}{4}, 0\right) I_4 \times \frac{1}{2} \begin{pmatrix} B_{e.1} \\ B_{e.2} \\ B_{e.3} \\ B_{e.4} \end{pmatrix} \right] \end{array} \right],$$

where $B_{e.i}$ are defined similarly to $B_{u.i}$ in equation (12), $i = 1, \dots, 4$. It follows that

$$\begin{aligned} & \left(\frac{\sum_{j=1}^{[T\tau]} e^{i(j\frac{\pi}{2})} x_j'}{T} \right) \left(\frac{X'X}{T} \right)^{-1} \left(\frac{X'e}{\sqrt{T}} \right) \rightarrow \\ & \left(\begin{array}{l} \frac{1}{\sqrt{2}} \frac{\sqrt{2}}{2} \tau (-B^{(2)}(1) + B^{(4)}(1)) \\ + i \frac{1}{\sqrt{2}} \frac{\sqrt{2}}{2} \tau (B^{(1)}(1) - B^{(3)}(1)) \end{array} \right) \\ & = \frac{1}{\sqrt{2}} \tau (B_R^*(1) + i B_I^*(1)) = \frac{1}{\sqrt{2}} \tau B^*(1), \end{aligned}$$

where $B^{(i)}(\tau)$, $i = 1, \dots, 4$, $B_R^*(\tau)$ and $B_I^*(\tau)$ are all real Brownian motions and the last two processes are independent.

It is evident that $\frac{\tilde{P}_{[T\tau]}}{\sqrt{T}} \rightarrow_d \sqrt{\frac{\omega_e^2}{2}} V^c(\tau)$, where $V^c(\tau)$ is a complex Brownian bridge that can be written as $V^c(\tau) = V_R^c(\tau) + iV_I^c(\tau)$ $V_R^c(\tau)$ and $V_I^c(\tau)$ are two independent real standard Brownian bridges. As a result,

$$\frac{1}{T^2} \sum_{t=1}^T \tilde{P}_t \tilde{P}_t' \rightarrow_d \frac{\omega_e^2}{2} \int_0^1 [(V_R^c)^2(\tau) + (V_I^c)^2(\tau)] d\tau \quad (14)$$

because $\tilde{\omega}_e^2(I)$ is a convergent estimate of ω_e^2 , it may be concluded that

$$\eta^{(\pm i)} \rightarrow_d \frac{1}{2} \int_0^1 [(V_R^c)^2(\tau) + (V_I^c)^2(\tau)] d\tau, \quad (15)$$

as claimed.

It should be noted that asymptotically $\eta^{(-1)}$ has the Cramer-von Mises distribution (CvM) under the null hypothesis, although the limit theory of $\eta^{(\pm i)}$ was shown as a function of a generalized CvM with two degrees, specifically, $\eta^{(\pm i)} \rightarrow_d \frac{1}{2} \text{CvM}(2)$. The critical values of the seasonal KPSS test with seasonal

dummies can be computed from Nyblom (1989) or from Canova and Hansen (1995). These critical values are shown in Table 1.

Table 1: Critical Values of the Seasonal KPSS Test

	1%	5%	10%
Root -1	0.743	0.461	0.347
Roots $\pm i$	0.537	0.374	0.3035

Monte Carlo Analysis

To evaluate the size performance of the seasonal KPSS statistic, Monte Carlo simulation experiments were conducted using seasonal roots of a quarterly process. The data generating process (DGP) for the negative unit root is

$$\begin{aligned} y_t &= x_t' \beta + r_t, \\ t &= 1, \dots, T, \end{aligned} \quad (16a)$$

where $x_t' \beta$ is defined as in (1) and the autoregressive process r_t is given by:

$$r_t = \alpha r_{t-1} + v_t, \quad (16b)$$

The error terms v_t are normally distributed with zero mean and unit variance. The DGP for complex unit roots is given by:

$$\begin{aligned} y_t &= x_t' \lambda + c_t, \\ t &= 1, \dots, T, \end{aligned} \quad (17a)$$

where $x_t' \lambda$ is defined in (3) and the process c_t is given by:

$$c_t = \alpha c_{t-2} + \varepsilon_t, \quad (17b)$$

and ε_t are normally distributed with zero mean and unit variance.

Alternative values of $\alpha \in \{-1, -0.8, -0.2, 0, 0.2, 0.8\}$ were chosen and only the 5% nominal size was considered. The bandwidth values chosen in these experiments are given by: $l_0 = 0$, $l_4 = \text{integer } [4(T/100)^{1/4}]$ and $l_{12} = \text{integer } [12(T/100)^{1/4}]$. Twenty-thousand (20,000) replications were conducted and all the simulation experiments were carried out with Matlab programs.

Results in Table 2 show that the test size increases as values of α decrease. Also note that larger data samples do not significantly affect the test size. These simulations raised another point, which was observed by Lyhagen (2006) for similar testing but without deterministic components: they show that, as opposed to the original KPSS testing framework, l_4 and l_{12} do not have better size performance than l_0 . In fact, in the seasonal KPSS framework, the test size deterioration induces substantial power. Results of the simulation experiments performed in this study (see Table 1) suggest an overall good power performance of the seasonal KPSS test, particularly against near seasonal unit root alternatives.

Conclusion

The joint use of unit root and stationarity tests is recommended in empirical studies. Such a joint use can lead to a more in-depth analysis of the dynamic properties of the time series. This article established asymptotic theory of the seasonal KPSS test in the presence of seasonal dummies and extended SKPSS to include deterministic seasonality. Given that seasonal unit root tests have low power in moderate samples, the test represents an adequate solution as illustrated by the simulation results. Lyhagen (2006) also showed good power properties of the test when there is no deterministic term in the model, however, it would be interesting to study both power and size performance of the test when factors affecting the time series such as measurement errors and additive outliers are present. Khedhiri and El Montasser (2010) used

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Monte Carlo methods to show that the seasonal KPSS test is robust to the magnitude and the number of additive outliers. Furthermore, the statistical results obtained demonstrate overall good performance on the finite-sample properties of the test.

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Table 2: Rejection Frequencies for the Seasonal KPSS Test with Seasonal Dummies for Seasonal Quarterly Unit Roots

$\eta^{(-1)}$				$\eta^{(\pm i)}$			
α	T	l0	l4	l12	l0	l4	l12
-1	80	0.99	0.8192	0.5314	0.9969	0.9708	0.7755
	200	0.9997	0.9469	0.7268	1	0.9970	0.9264
-0.9	80	0.9229	0.4780	0.1409	0.9736	0.8436	0.3735
	200	0.9700	0.4960	0.1727	0.9973	0.9014	0.4613
-0.2	80	0.1359	0.0558	0.0279	0.1598	0.0851	0.0423
	200	0.1262	0.0575	0.0425	0.1645	0.0861	0.0515
0	80	0.0543	0.0418	0.0240	0.0505	0.0420	0.0325
	200	0.0526	0.0449	0.0389	0.0508	0.0467	0.0413
0.2	80	0.0183	0.0308	0.0205	0.0112	0.0223	0.0246
	200	0.0144	0.0360	0.0351	0.0086	0.0251	0.0326
0.9	80	0.00	0.0066	0.0038	0.00	0.0055	0.0050
	200	0.00	0.0002	0.0066	0.00	0.0001	0.0012

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Gamma-Pareto Distribution and Its Applications

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A new distribution, the gamma-Pareto, is defined and studied and various properties of the distribution are obtained. Results for moments, limiting behavior and entropies are provided. The method of maximum likelihood is proposed for estimating the parameters and the distribution is applied to fit three real data sets.

Key words: Estimation, moments, T-X family, unimodality.

Introduction

The Pareto distribution was named after Swiss economist Vilfredo Pareto (1848-1923) who discovered it while studying distributions for modeling income in Switzerland. Since that time, the Pareto distribution has been widely used in modeling heavy-tailed distributions, such as income distribution. Many applications of the Pareto distribution in economics, biology and physics can be found throughout the literature. Burroughs and Tebbens (2001) discussed applications of the Pareto distribution in modeling earthquakes, forest fire areas and oil and gas field sizes, and Schroeder, et al. (2010) presented an application of the Pareto distribution in modeling disk drive sector errors. To add flexibility to the Pareto distribution, various generalizations of the distribution have been derived, including: the generalized Pareto distribution (Pickands, 1975), the beta-Pareto distribution (Akinsete, et al., 2008), and the beta generalized Pareto distribution (Mahmoudi, 2011).

Let $F(x)$ be the cumulative distribution function (CDF) of any random variable X and $r(t)$ be the probability density function (PDF) of a random variable, T , defined on $[0, \infty)$. The CDF of the T - X family of distributions defined by Alzaatreh, et al. (2012) is given by

$$G(x) = \int_0^{-\log(1-F(x))} r(t) dt. \quad (1.1)$$

Alzaatreh, et al. (2012) named this family of distributions the Transformed-Transformer family (or T - X family). When X is a continuous random variable, the probability density function of the T - X family is

$$\begin{aligned} g(x) &= \frac{f(x)}{1-F(x)} r(-\log(1-F(x))) \\ &= h(x) r(H(x)). \end{aligned} \quad (1.2)$$

If a random variable T follows the gamma distribution with parameters α and β , then

$$r(t) = \left(\beta^\alpha \Gamma(\alpha) \right)^{-1} t^{\alpha-1} e^{-t/\beta}, \quad t \geq 0,$$

and the definition in (1.2) leads to the gamma- X family with PDF

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$$g(x) = \frac{f(x)(-\log(1-F(x)))^{\alpha-1}(1-F(x))^{\frac{1}{\beta}-1}}{\Gamma(\alpha)\beta^\alpha}. \quad (1.3)$$

When $\beta=1$, the gamma- X family in (1.3) reduces to

$$g(x) = \frac{1}{\Gamma(\alpha)} f(x)(-\log(1-F(x)))^{\alpha-1}. \quad (1.4)$$

Alzaatreh, et al. (2012) noted that, when $\alpha=n$ where n is a positive integer, the distribution in (1.4) can be written as

$$g(x) = \frac{1}{(n-1)!} f(x)(-\log(1-F(x)))^{n-1},$$

which is the density function of the upper record values, $X_{U(n)}$, arising from a sequence $\{X_i\}_{i=1}^n$ of identically independent random variables with PDF $f(x)$ and CDF $F(x)$ (Johnson, et al., 1994).

The Gamma-Pareto Distribution

If X is a Pareto random variable with density function $f(x) = k\theta^k / x^{k+1}$, $x > \theta$, then (1.3) results in

$$g(x) = \frac{k^\alpha}{x\Gamma(\alpha)\beta^\alpha} \left(\frac{\theta}{x}\right)^{k/\beta} \left(\log\left(\frac{x}{\theta}\right)\right)^{\alpha-1}, \quad x > \theta. \quad (2.1)$$

Setting $\beta/k = c$, (2.1) reduces to

$$g(x) = \frac{1}{x\Gamma(\alpha)c^\alpha} \left(\frac{\theta}{x}\right)^{1/c} \left(\log\left(\frac{x}{\theta}\right)\right)^{\alpha-1}, \quad \alpha, c, \theta > 0; x > \theta. \quad (2.2)$$

A random variable X with the PDF $g(x)$ in (2.2) is said to follow the gamma-Pareto distribution. When $\alpha=1$ the gamma-Pareto distribution reduces to the Pareto distribution with parameters $1/c$ and θ , and when $\alpha=n+1$, it reduces to the upper record value distribution arising from Pareto identically independent random variables (Ahsanullah & Houchens, 1989). From (2.2), the CDF of the gamma-Pareto distribution is obtained as

$$G(x) = \gamma\{\alpha, c^{-1} \log(x/\theta)\} / \Gamma(\alpha), \quad (2.3)$$

where $\gamma(\alpha, t) = \int_0^t u^{\alpha-1} e^{-u} du$ is the incomplete gamma function.

Johnson, et al. (1994) discussed different types of Pareto distributions and their CDFs. These are

$$\text{Pareto II: } F(x) = 1 - \frac{\theta^a}{(x+\theta)^a}, \quad x > 0.$$

$$\text{Pareto III: } F(x) = 1 - \frac{\theta e^{-bx}}{(x+\theta)^a}, \quad x > 0.$$

$$\text{Pareto IV: } F(x) = 1 - \left[1 + \left(\frac{x-\mu}{\sigma}\right)^{1/\gamma}\right]^{-a}, \quad x > \mu.$$

Using equation (1.3), the corresponding PDF of gamma-Pareto II, gamma-Pareto III, and gamma-Pareto IV can be written as shown in Table 1.

Some relationships among these distributions are:

- If Y follows the gamma-Pareto distribution in (2.2), then the translation $X = Y - \theta$ follows the gamma-Pareto II distribution.
- When $a = 1$ and $b = 0$, the gamma-Pareto III distribution reduces to the gamma-Pareto II distribution.

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Table 1: Corresponding PDFs of gamma-Pareto Distributions

gamma-Pareto II:	$g(x) = \frac{\theta^{1/c}}{c^\alpha \Gamma(\alpha)} (x + \theta)^{-1-1/c} [\log(1 + x / \theta)]^{\alpha-1}, \quad x > 0, \text{ where } c = \frac{\beta}{a}. \quad (2.4)$
gamma-Pareto III:	$g(x) = \frac{1}{\beta^\alpha \Gamma(\alpha)} \left(b + \frac{a}{x + \theta} \right) \left[\frac{\theta e^{-bx}}{(x + \theta)^a} \right]^{1/\beta} \left[-\log \left(\frac{\theta e^{-bx}}{(x + \theta)^a} \right) \right]^{\alpha-1}, \quad x > 0. \quad (2.5)$
gamma-Pareto IV:	$g(x) = \frac{1}{\gamma \sigma c^\alpha \Gamma(\alpha)} \left(\frac{x - \mu}{\sigma} \right)^{-1+1/\gamma} \left(1 + \left(\frac{x - \mu}{\sigma} \right)^{1/\gamma} \right)^{-1-1/c} \left[\log \left(1 + \left(\frac{x - \mu}{\sigma} \right)^{1/\gamma} \right) \right]^{\alpha-1}, \quad (2.6)$ $x > \mu, \text{ where } c = \beta / a.$

- When $\gamma=1$ and $\mu = \sigma = \theta$, the gamma-Pareto IV distribution reduces to the gamma-Pareto distribution in (2.2) with parameters α , c and θ .
- When $\gamma=1$ and $\mu = 0$, the gamma-Pareto IV distribution reduces to the gamma-Pareto II distribution.

Properties of the gamma-Pareto distribution

The following Lemma shows the relationship between the gamma-Pareto distribution and the gamma distribution.

Lemma 1

If a random variable Y follows the gamma distribution with parameters α and c , then the random variable $X = \theta e^Y$ follows the gamma-Pareto distribution with parameters α , c and θ .

Lemma 1 Proof

The result follows by using the transformation technique.

The hazard function associated with the gamma-Pareto distribution is

$$\begin{aligned} h(x) &= \frac{g(x)}{1 - G(x)} \\ &= \frac{\theta^{1/c} (\log(x / \theta))^{\alpha-1}}{x^{1+1/c} c^\alpha (\Gamma(\alpha) - \gamma \{ \alpha, c^{-1} \log(x / \theta) \})}, \\ & \quad x > \theta, \end{aligned} \quad (3.1)$$

and the limiting behaviors of the gamma-Pareto PDF and the hazard function are given in the following theorem.

Theorem 1

The limit of the gamma-Pareto density function and the gamma-Pareto hazard function

as $x \rightarrow \infty$ is 0 and the limit as $x \rightarrow \theta^+$ is given by

$$\lim_{x \rightarrow \theta^+} g(x) = \lim_{x \rightarrow \theta^+} h(x) = \begin{cases} 0, & \alpha > 1 \\ 1/(c\theta), & \alpha = 1 \\ \infty, & \alpha < 1. \end{cases} \quad (3.2)$$

Theorem 1 Proof

First it can be shown that $\lim_{x \rightarrow \infty} g(x) = 0$. If $\alpha \leq 1$, then from definition (2.2) $\lim_{x \rightarrow \infty} g(x) = 0$, and if $\alpha > 1$, then

$$\begin{aligned} \lim_{x \rightarrow \infty} g(x) &= \lim_{x \rightarrow \infty} \frac{(\theta/x)^{1/c}}{\Gamma(\alpha)c^\alpha} \times \lim_{x \rightarrow \infty} \left(\log\left(\frac{x}{\theta}\right) \right)^{\alpha-1} \frac{1}{x} \\ &= 0 \times \lim_{x \rightarrow \infty} \left(\log\left(\frac{x}{\theta}\right) / x^{1/(\alpha-1)} \right)^{\alpha-1}. \end{aligned}$$

Using L'Hôpital's rule, it can be shown that

$$\lim_{x \rightarrow \infty} \left(\log(x/\theta) / x^{1/(\alpha-1)} \right)^{\alpha-1} = 0.$$

To show that $\lim_{x \rightarrow \infty} h(x) = 0$, we have

$$\begin{aligned} \lim_{x \rightarrow \infty} h(x) &= \lim_{x \rightarrow \infty} g(x) / (1 - G(x)). \quad \text{Because} \\ \lim_{x \rightarrow \infty} g(x) &= 0, \text{ L'Hôpital's rule can be applied} \\ &\text{and implies that} \end{aligned}$$

$$\begin{aligned} \lim_{x \rightarrow \infty} h(x) &= \lim_{x \rightarrow \infty} g'(x) / g(x) \\ &= \lim_{x \rightarrow \infty} \left\{ \frac{\alpha-1}{x \log(x/\theta)} - \frac{c+1}{cx} \right\} \\ &= 0. \end{aligned}$$

The result in (3.2) follows directly from the definition of (2.2) and $h(x) = g(x) / (1 - G(x))$. The following theorem shows that the gamma-Pareto distribution is unimodal.

Theorem 2

The gamma-Pareto distribution has a unique mode at $x = x_0$. When $\alpha \leq 1$ the mode is $x_0 = \theta$ and when $\alpha > 1$ the mode is $x_0 = \theta e^{c(\alpha-1)/(c+1)}$.

Theorem 2 Proof

The derivative with respect to x of equation (2.2) is given by

$$\begin{aligned} g'(x) &= \theta^{1/c} x^{2-1/c} \Gamma(\alpha) \\ &\times \left(\log\left(\frac{x}{\theta}\right) \right)^{\alpha-2} \left\{ c(\alpha-1) - (c+1) \log\left(\frac{x}{\theta}\right) \right\}. \end{aligned} \quad (3.3)$$

From (3.3) the critical points of $g(x)$ are $x = \theta$ and $x = \theta e^{c(\alpha-1)/(c+1)}$. For $\alpha \leq 1$, it may be observed from (3.3) that $g'(x) < 0$, therefore $g(x)$ is strictly decreasing. Also, from Theorem 1, $\lim_{x \rightarrow \theta^+} g(x) = 1/(c\theta)$ when $\alpha = 1$ and $\lim_{x \rightarrow \theta^+} g(x) = \infty$ when $\alpha < 1$. Thus, $g(x)$ has a unique mode at $x = \theta$. Using Theorem 1, for $\alpha > 1$, $\lim_{x \rightarrow \theta^+} g(x) = 0$ implies that $x = \theta$ cannot be a modal point, hence the mode is $x_0 = \theta e^{c(\alpha-1)/(c+1)}$.

Graphs of $g(x)$ and $h(x)$ are displayed in Figures 1-3. The plots show that the gamma-Pareto PDF has a very long right tail and also that when parameters c and θ increase, the peak of the distribution decreases. In addition, the graphs of the gamma-Pareto PDF indicate that $g(x)$ is a right skewed distribution. The plots in Figure 3 illustrate that the gamma-Pareto hazard function is either monotone decreasing or upside-down bathtub.

The entropy of a random variable X is a measure of variation of uncertainty (Rényi, 1961). Shannon entropy (Shannon, 1948) for a random variable X with PDF $g(x)$ is defined as $E\{-\log(g(X))\}$. Shannon showed important applications of this entropy in communication theory and many applications have been used in

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Figure 1: The gamma-Pareto PDF for Various Values of α , c and θ

Figure 2: The gamma-Pareto PDF for Various Values of α , c and θ

Figure 3: The gamma-Pareto Hazard Function for Various Values of α , c and θ

different areas such as engineering, physics, biology and economics.

Lemma 2

The Shannon entropy of the gamma- X family of distributions is given by

$$\eta_X = -E\left\{\log f\left(F^{-1}\left(1-e^{-T}\right)\right)\right\} + \alpha(1-\beta) + \log \beta + \log \Gamma(\alpha) + (1-\alpha)\psi(\alpha),$$

where ψ is the digamma function and T is the gamma random variable with parameters α and β .

Lemma 2 Proof

See Alzaatreh, et al. (2012) for proof details.

Theorem 3

The Shannon entropy for the gamma-Pareto distribution is given by

$$\begin{aligned} \eta_X &= \log c + \log \theta + \log \Gamma(\alpha) \\ &\quad + \alpha(c+1) + (1-\alpha)\psi(\alpha). \end{aligned} \quad (3.4)$$

Theorem 3 Proof

First it is necessary to find $-E\left\{\log f\left(F^{-1}\left(1-e^{-T}\right)\right)\right\}$, where $f(x) = k\theta^k / x^{k+1}$. It can be shown that $F^{-1}(x) = \theta(1-x)^{-1/k}$, thus

$$\begin{aligned} -E\left\{\log f\left(F^{-1}\left(1-e^{-T}\right)\right)\right\} &= \\ \log \theta - \log k + (1+1/k)E(T) \end{aligned}$$

The result follows from Lemma 2 by noting that $E(T) = \alpha\beta$ and $c = \beta/k$ (see equation 2.1).

The Rényi (1961) entropy for the random variable X with PDF $g(x)$ is defined as

$$I_R(s) = \frac{1}{1-s} \log \left\{ \int g^s(x) dx \right\}, \quad s > 0, \quad s \neq 1. \quad (3.5)$$

By using the gamma-Pareto PDF in (2.2), we have

$$\begin{aligned} \int_{\theta}^{\infty} g^s(x) dx &= c^{-s\alpha} \Gamma^{-s}(\alpha) \\ &\times \int_{\theta}^{\infty} x^{-s} \left(\frac{\theta}{x} \right)^{s/c} \left[\log \left(\frac{x}{\theta} \right) \right]^{s(\alpha-1)} dx. \end{aligned} \quad (3.6)$$

Substituting $u = \log(x/\theta)$, (3.6) can be re-written as

$$\int_{\theta}^{\infty} g^s(x) dx = \frac{\theta^{1-s} \Gamma(s(\alpha-1)+1)}{c^{s\alpha} \Gamma^s(\alpha) [s(1+1/c)-1]^{s(\alpha-1)+1}}. \quad (3.7)$$

Using equation (3.7), the Rényi entropy in (3.5) can be written as

$$I_R(s) = \log \theta - \frac{1}{1-s} \left\{ s\alpha \log c + s \log \Gamma(\alpha) - \log \Gamma(\xi) + \xi \log(s(1+c^{-1})) \right\} \quad (3.8)$$

where $\xi = s(\alpha-1)+1$. Shannon entropy is a special case of Rényi entropy obtained by taking the limit of Rényi entropy as $s \rightarrow 1$. The result in (3.4) follows by using the L'Hôpital's rule for evaluating the limit of equation (3.8) as $s \rightarrow 1$.

Moments and Mean Deviations

The non-central moments for the gamma-Pareto distribution in (2.2) can be written as

$$\begin{aligned} E(X^r) &= c^{-\alpha} \Gamma^{-1}(\alpha) \\ &\times \int_{\theta}^{\infty} x^{r-1} \left(\frac{\theta}{x} \right)^{1/c} \left[\log \left(\frac{x}{\theta} \right) \right]^{\alpha-1} dx. \end{aligned} \quad (4.1)$$

Substituting $u = \log(x/\theta)$ reduces (4.1) to

$$E(X^r) = \theta^r (1-rc)^{-\alpha}, \quad c < 1/r. \quad (4.2)$$

Hence, the mean for the gamma-Pareto distribution is

$$\mu = \theta(1-c)^{-\alpha}, \quad c < 1.$$

Note that when $\alpha=1$ in equation (4.2), $E(X^r) = \theta^r (1-rc)^{-1}$ which represents the non-central moments for the Pareto distribution with parameters $1/c$ and θ .

Using the binomial expansion for $(X-\mu)^r$, the central moments $E(X-\mu)^r$ for any random variable X can be written as

$$E(X-\mu)^r = \sum_{k=0}^r \binom{r}{k} (-1)^{r-k} \mu^{r-k} E(X^k). \quad (4.3)$$

Using equations (4.2) and (4.3), the central moments for the gamma-Pareto random variable X can be simplified to

$$\begin{aligned} E(X-\mu)^r &= \\ &\theta^r \sum_{k=0}^r \binom{r}{k} (-1)^{r-k} (1-c)^{(k-r)\alpha} (1-kc)^{-\alpha}. \end{aligned} \quad (4.4)$$

Note that equation (4.4) indicates that the central moments of the gamma-Pareto distribution is an increasing function of θ . Using (4.4), the variance, the skewness and the kurtosis for the gamma-Pareto distribution are respectively expressed as

$$\sigma^2 = \theta^2 [(1-2c)^{-\alpha} - (1-c)^{-2\alpha}], \quad c < 0.5 \quad (4.5)$$

$$\gamma_1 = \frac{(1-3c)^{-\alpha} + 2(1-c)^{-3\alpha} - 3(1-2c)^{-\alpha} (1-c)^{-\alpha}}{((1-2c)^{-\alpha} - (1-c)^{-2\alpha})^{3/2}} \quad (4.6)$$

$$\gamma_2 = [(1-2c)^{-\alpha} - (1-c)^{-2\alpha}]^{-2} \left\{ (1-4c)^{-\alpha} - 3(1-c)^{-4\alpha} + 6(1-2c)^{-\alpha} (1-c)^{-2\alpha} - 4(1-3c)^{-\alpha} (1-c)^{-\alpha} \right\}. \quad (4.7)$$

Equations (4.6) and (4.7) show that the skewness and the kurtosis are free of θ . Theorem 4 shows that when $\alpha \geq 1$ (or $\alpha < 1$), the non-central moments of gamma-Pareto distribution is bounded below (or above) by the non-central moments of the Pareto distribution.

Theorem 4

Let X be a random variable that follows the gamma-Pareto distribution. If $\alpha \geq 1$, then $E(X^s) \geq \theta^r / (1-rc)$ and if $\alpha < 1$, then $E(X^s) < \theta^r / (1-rc)$.

Theorem 4 Proof

Because $0 < rc < 1$ or $0 < 1-rc < 1$ this implies that for $\alpha \geq 1$, $(1-rc)^\alpha \leq 1-rc$ and for $\alpha < 1$, $(1-rc)^\alpha > 1-rc$. Thus, if $\alpha \geq 1$, then $\theta^r (1-rc)^{-\alpha} \geq \theta^r (1-rc)^{-1}$ and if $\alpha < 1$, then $\theta^r (1-rc)^{-\alpha} < \theta^r (1-rc)^{-1}$.

Table 2 provides the mode, mean, variance, skewness and kurtosis of the gamma-Pareto distribution for various values of α and c when $\theta = 1$. For fixed α and θ , the mean, variance, skewness and kurtosis are increasing functions of c . For fixed c and θ , the mean, median and variance are increasing functions of α . When $\alpha > 1$, the following trends for the mode are observed: (1) it increases as c increases with fixed α and θ , and (2) it increases as α increases with fixed c and θ . Table 2 also shows that the skewness is always positive and for fixed α and it increases rapidly as c increases.

Table 2: Mode, Mean, Variance, Skewness and Kurtosis for Some Values of α and c with $\theta = 1$ (*: Undefined)

α	c	Mode	Mean	Variance	Skewness	Kurtosis
0.5	0.1	1	1.0541	0.0069	3.6850	27.6334
	0.2	1	1.1180	0.0410	5.5537	95.1825
	0.3	1	1.1952	0.1526	15.2326	*
	0.4	1	1.2910	0.5694	*	*
1	0.1	1	1.1111	0.0154	2.8111	17.8286
	0.2	1	1.2500	0.1042	4.6476	73.8000
	0.3	1	1.4286	0.4592	16.4438	*
	0.4	1	1.6667	2.2222	*	*
2	0.1	1.0952	1.2346	0.0383	2.2819	13.2512
	0.2	1.1814	1.5625	0.3364	4.4009	77.3004
	0.3	1.2596	2.0408	2.0851	26.1507	*
	0.4	1.3307	2.7778	17.2840	*	*
3	0.1	1.1994	1.3717	0.0714	2.1075	12.0304
	0.2	1.3956	1.9531	0.8149	4.6209	98.2327
	0.3	1.5865	2.9155	7.1251	47.9991	*
	0.4	1.7708	4.6296	103.5670	*	*

The deviation from the mean and the median are used to measure the dispersion and spread in a population from the center. If the median is denoted by M , then the mean deviation from the mean, $D(\mu)$, and the mean deviation from the median, $D(M)$, can be written as

$$\begin{aligned} D(\mu) &= \int_{\theta}^{\mu} (\mu - x)g(x)dx + \int_{\mu}^{\infty} (x - \mu)g(x)dx \\ &= 2 \int_{\theta}^{\mu} (\mu - x)g(x)dx \\ &= 2\mu G(\mu) - 2 \int_{\theta}^{\mu} xg(x)dx. \end{aligned} \quad (4.6)$$

$$\begin{aligned} D(M) &= \int_{\theta}^M (M - x)g(x)dx + \int_M^{\infty} (x - M)g(x)dx \\ &= 2 \int_{\theta}^M (M - x)g(x)dx + E(X) - M \\ &= 2MG(M) + \mu - M - 2 \int_{\theta}^M xg(x)dx \\ &= \mu - 2 \int_{\theta}^M xg(x)dx. \end{aligned} \quad (4.7)$$

Consider the integral

$$\begin{aligned} \int_{\theta}^m xg(x)dx &= \\ &= \frac{1}{c^{\alpha}\Gamma(\alpha)} \int_{\theta}^m (\theta/x)^{1/c} (\log(x/\theta))^{\alpha-1} dx. \end{aligned} \quad (4.8)$$

Using the substitution $u = \log(x/\theta)$, the equation (4.8) can be written as

$$\int_{\theta}^m xg(x)dx = \frac{\mu}{\Gamma(\alpha)} \gamma[\alpha, (c^{-1} - 1) \log(m/\theta)], \quad (4.9)$$

and by using equations (2.3) and (4.9), the mean deviation from the mean is

$$D(\mu) = \frac{2\mu \left\{ \gamma[\alpha, c^{-1} \log(\mu/\theta)] - \gamma[\alpha, (c^{-1} - 1) \log(\mu/\theta)] \right\}}{\Gamma(\alpha)}, \quad c < 1,$$

and the mean deviation from the median is

$$D(M) = \mu \left\{ 1 - \frac{2}{\Gamma(\alpha)} \gamma \left[\alpha, \left(\frac{1}{c} - 1 \right) \log \left(\frac{M}{\theta} \right) \right] \right\}, \quad c < 1.$$

Parameter Estimation

When $\alpha < 1$, the likelihood function for the gamma-Pareto distribution goes to infinity as θ approaches the sample minimum $x_{(1)}$; thus, when $\alpha < 1$ and θ is estimated by $x_{(1)}$, no MLE for α and c exists. A similar problem was studied by Smith (1985) who proposed an alternative approach for estimating the parameters as follows: If sample data $x_1, x_2, \dots, x_n$ are observed, estimate the parameter θ by the sample minimum $x_{(1)}$ and then use the MLE method to estimate α and c by excluding the sample minimum.

Applying Smith's method to obtain the MLE for the gamma-Pareto parameters, the log-likelihood function for the gamma-Pareto distribution is given by

$$\begin{aligned} \log L(\alpha, c) &= \sum_{x_i \neq x_{(1)}} \log g(x_i; x_{(1)}, \alpha, c) \\ &= \sum_{x_i \neq x_{(1)}} \left\{ -\alpha \log c - \log \Gamma(\alpha) - \log x_{(1)} - (1 + c^{-1}) \right. \\ &\quad \left. \times \log(x_i / x_{(1)}) + (\alpha - 1) \log(\log(x_i / x_{(1)})) \right\}. \end{aligned} \quad (5.1)$$

The derivatives of (5.1) with respect to α and c are given by

$$\frac{\partial \log L}{\partial \alpha} = \sum_{x_i \neq x_{(1)}} \left\{ -\log c - \psi(\alpha) - \log \left(\log \left(\frac{x_i}{x_{(1)}} \right) \right) \right\} \quad (5.2)$$

$$\frac{\partial \log L}{\partial c} = \sum_{x_i \neq x_{(1)}} \left\{ \frac{-\alpha}{c} + \frac{1}{c^2} \log \left(\frac{x_i}{x_{(1)}} \right) \right\}. \quad (5.3)$$

Setting (5.3) to zero and simplifying results in

$$c = \frac{1}{(n-n')\alpha} \sum_{x_i \neq x_{(1)}} \log(x_i / x_{(1)}), \quad (5.4)$$

where n' is the frequency of $x_{(1)}$. Equation (5.4) can be written as

$$c = \frac{1}{\alpha} m_1^*, \quad (5.5)$$

where $m_1^* = \sum_{x_i \neq x_{(1)}} \log(x_i / x_{(1)}) / (n-n')$ is the sample mean for $\log(x_i / x_{(1)})$ after excluding $x_{(1)}$.

Setting (5.2) to zero and using equation (5.5) results in

$$\psi(\alpha) - \log(\alpha) + \log(m_1^*) - m_2^* = 0, \quad (5.6)$$

where $m_2^* = \sum_{x_i \neq x_{(1)}} \log(\log(x_i / x_{(1)})) / (n-n')$ is

the sample mean for $\log(\log(x_i / x_{(1)}))$ after excluding $x_{(1)}$. The MLE $\hat{\alpha}$ of α is the solution of equation (5.6) and the MLE $\hat{c}$ of c can be determined by substituting the estimate $\hat{\alpha}$ in equation (5.5).

The initial values for the parameters α and c can be obtained by assuming the random sample $Y_i = \log(X_i / x_{(1)})$, $i = 1, \dots, n$ are taken from the gamma distribution with parameters α and c . By equating the population mean and the population variance of gamma distribution (with parameters α and c) to the corresponding sample mean and sample variance of y_i , $i = 1, \dots, n$ and then solving for α and c , the initial values are $c_0 = s_y^2 / \bar{y}$ and

$\alpha_0 = \bar{y}^2 / s_y^2$, where s_y^2 and $\bar{y}$ are the sample variance and the sample mean for $y_1, y_2, \dots, y_n$.

Lemma 3

The Fisher information matrix for the gamma-Pareto distribution when θ is known is given by

$$I = n \begin{bmatrix} \psi'(\alpha) & 1/c \\ 1/c & \alpha/c^2 \end{bmatrix}. \quad (5.7)$$

Lemma 3 Proof

The Fisher information matrix is defined by $I = [I_{ij}]$ with

$$I_{ij} = E \left\{ \frac{-\partial^2}{\partial \tau_i \partial \tau_j} \log(L(x_i, \bar{\tau})) \right\}, \text{ where } \tau_1 = \alpha$$

and $\tau_2 = c$. To find I , the second derivatives of $\log L(\alpha, c) = \sum_{i=1}^n \log g(x_i; \theta, \alpha, c)$, are needed. These can be obtained from the derivatives of (5.2) and (5.3), where $x_{(1)}$ is replaced by θ and the sums are taken from $i=1$ to n . The second derivatives of $\log L(\alpha, c)$ can be written as

$$\partial^2 \log L / \partial \alpha^2 = -n\psi'(\alpha),$$

$$\partial^2 \log L / \partial \alpha \partial c = -n/c,$$

and

$$\partial^2 \log L / \partial c^2 = n\alpha c^{-2} - 2c^{-3} \sum_{i=1}^n \log(x_i / \theta).$$

From Lemma 1, it may be concluded that $E(\log(X / \theta)) = \alpha c$. The results of (5.7) follow from taking the negative expected values of the second derivatives.

Theorem 5

The variance-covariance matrix for the gamma-Pareto distribution when θ is known is given by

$$\Sigma = \frac{1}{n(\alpha\psi'(\alpha)-1)} \begin{bmatrix} \alpha & -c \\ -c & c^2\psi'(\alpha) \end{bmatrix}. \quad (5.8)$$

Theorem 5 Proof

The result follows by taking the inverse of the Fisher information matrix in (5.7). From (5.8), the variance of the ML estimates $\hat{\alpha}$ and $\hat{c}$ are respectively given by

$$\begin{aligned} \text{var}(\hat{\alpha}) &= \frac{\alpha}{n(\alpha\psi'(\alpha)-1)} \\ \text{and} \\ \text{var}(\hat{c}) &= \frac{c^2\psi'(\alpha)}{n(\alpha\psi'(\alpha)-1)}. \end{aligned} \quad (5.9)$$

From (5.9), the variance of $\hat{\alpha}$ does not depend on the parameter c . Also, as c increases the variance of $\hat{c}$ increases. Using the approximation $\psi'(\alpha) \approx \alpha^{-1} + \frac{1}{2}\alpha^{-2} + \frac{1}{6}\alpha^{-3}$ (Johnson, et al., 1994, page 357), equations (5.9) can be approximated as

$$\begin{aligned} \text{var}(\hat{\alpha}) &\approx \frac{6\alpha^3}{n(3\alpha+1)} \\ \text{and} \\ \text{var}(\hat{c}) &\approx \frac{c^2(6\alpha^2+3\alpha+1)}{n\alpha(3\alpha+1)}. \end{aligned} \quad (5.10)$$

Based on the Central Limit Theorem, $(\hat{\alpha} - \alpha) / se(\hat{\alpha}) \xrightarrow{d} N(0, 1)$ and $(\hat{c} - c) / se(\hat{c}) \xrightarrow{d} N(0, 1)$ where $se(\hat{\alpha})$ and $se(\hat{c})$ are the standard errors of $\hat{\alpha}$ and $\hat{c}$ respectively.

In the following, the uniformly minimum variance unbiased estimator (UMVUE) is derived for the parameter c assuming that the parameters α and θ are known. The following theorem by Lehmann & Scheffé (1950) is needed in order to find the UMVUE for the parameter c .

Theorem 6

Let $X_1, X_2, \dots, X_n$ be a random sample from PDF $g(x, \beta)$, $\beta \in \Omega$. Let T be a sufficient statistic for β and let the family $\{g(T, \beta), \beta \in \Omega\}$ of probability density functions be complete. If there is a function of T that is an unbiased estimator of β , then this function of T is the UMVUE of β .

Lemma 4

If α and θ are known for the gamma-Pareto distribution, then $T = \sum_{i=1}^n \log(x_i / \theta)$ is a sufficient statistic for the parameter c .

Lemma 4 Proof

Let $X_1, X_2, \dots, X_n$ be a random sample from the gamma-Pareto distribution, the joint density function is then given by

$$\begin{aligned} g(x_1, x_2, \dots, x_n | c) &= \prod_{i=1}^n \frac{(\theta / x_i)^{1/c} (\log(x_i / \theta))^{\alpha-1}}{x_i c^\alpha \Gamma(\alpha)} \\ &= k(c, T) h(x_1, x_2, \dots, x_n) \end{aligned}$$

where $k(c, T) = \exp\{-n\alpha \log c + (1 + c^{-1})T\}$,
 $h(x_1, x_2, \dots, x_n) = \exp\{-\log(\theta \Gamma(\alpha)) + (\alpha - 1) \log(\log(x_i / \theta))\}$

and $T = \sum_{i=1}^n \log(x_i / \theta)$. Thus, by using the factorization theorem, the statistic T is sufficient for the parameter c because the parameters α and θ are known.

Theorem 7

If α and θ are known for the gamma-Pareto distribution, then $m_1 = (n\alpha)^{-1} \sum_{i=1}^n \log(x_i / \theta)$ is the UMVU estimator for the parameter c .

Theorem 7 Proof

By using Lemma 4, $T = \sum_{i=1}^n \log(x_i / \theta)$ is a sufficient statistic for c . It follows from Lemma 1 that

$T = \sum_{i=1}^n \log(x_i / \theta)$ has a gamma distribution with parameters $n\alpha$ and c . Because gamma density belongs to the exponential family, this implies that $\{g(T, c), c > 0\}$ is a complete family where $g(x)$ is the gamma-Pareto density. Also from Lemma 1, $E(m_1) = c$, hence m_1 is an unbiased estimator for parameter c . By applying Theorem 6, the statistic m_1 is the UMVUE of c . From equation (5.5), it is interesting to note that when $\theta (= x_{(1)})$ and α are known, the MLE of c is the UMVUE of parameter c .

Applications

The gamma-Pareto is applied to three data sets: The first data set (see Table 3) was analyzed by Akinsete, et al. (2008) and represents Floyd River flood rates for the years 1935-1973 in Iowa, USA. The second data set (see Table 5) is from Mahmoudi (2011) and it represents the fatigue life of 6061-T6 aluminum coupons cut parallel with the direction of rolling and oscillated at 18 cycles per second. The third data set (see Table 7) was analyzed by Eugene (2001) and represents the observed frequencies for Tribolium Confusum Strain #3. The maximum likelihood estimates, the log-likelihood value and the AIC (Akaike Information Criterion) values for the fitted distributions are reported in Tables 4, 6 and 8.

Akinsete (2008) fitted the data in Table 3 to the beta-Pareto distribution and compared the result with the Pareto and the generalized

Pareto distribution (Pickands, 1975). Results are shown in Table 4, along with the result obtained by fitting the gamma-Pareto distribution to the data. The results show that both beta-Pareto and gamma-Pareto distributions provide adequate fit to the data. Because the gamma-Pareto distribution has only three parameters, this is an advantage for using it over the four-parameter beta-Pareto distribution. In examining the distribution of this data, observe that the data has a reversed J-shape distribution; this suggests that the gamma-Pareto distribution performs well in modeling reversed J-shape distribution. Figure 4 displays the empirical and the fitted cumulative distribution functions and supports the results shown in Table 4.

Mahmoudi (2011) proposed a five-parameter beta generalized Pareto distribution. He fitted the data (shown in Table 5) and compared the result with beta-Pareto, three-parameter generalized Pareto, Weibull and Pareto distributions. To conserve space, only the results of fitting beta generalized Pareto and beta-Pareto from Mahmoudi (2011) are reported in Table 6 along with the result of fitting the gamma-Pareto distribution to the data. The results in Table 6 indicate that the gamma-Pareto distribution provides the best fit among the distributions. The distribution of this data indicates that the data is approximately symmetric. This example suggests that the gamma-Pareto distribution does very well in fitting the distribution of data which is approximately symmetric. Figure 5 displays the empirical and the fitted cumulative distribution functions and supports the results shown in Table 6.

Table 3: Annual Flood Discharge Rates of the Floyd River Data

Years	Flood Discharge (ft3/s)									
1935-1944	1460	4050	3570	2060	1300	1390	1720	6280	1360	7440
1945-1954	5320	1400	3240	2710	4520	4840	8320	13900	71500	6250
1955-1964	2260	318	1330	970	1920	15100	2870	20600	3810	726
1965-1973	7500	7170	2000	829	17300	4740	13400	2940	5660	

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Table 4: Parameter Estimates for the Floyd River Flood Data

Distribution	Parameter Estimates	Log Likelihood	AIC
Pareto	$\hat{k} = 0.4125$ $\hat{\theta} = 318$	-392.81	789.62
Generalized Pareto	$\hat{k} = -0.3071$ $\hat{\theta} = 4520$	-379.55	763.09
Beta-Pareto	$\hat{\alpha} = 6.1550$ $\hat{\beta} = 24.2434$ $\hat{k} = 0.0926$ $\hat{\theta} = 318$	-365.45	738.9
Gamma-Pareto	$\hat{\alpha} = 5.1454$ $\hat{c} = 0.4712$ $\hat{\theta} = 318$	-365.81	734.9

Figure 4: CDF for Fitted Distributions for Floyd River Flood Data

Table 5: Fatigue Life of 6061-T6 Aluminum Coupons Data

70	90	96	97	99	100	103	104	104	105
107	108	108	108	109	109	112	112	113	114
114	114	116	119	120	120	120	121	121	123
124	124	124	124	124	128	128	129	129	130
130	130	131	131	131	131	131	132	132	132
133	134	134	134	134	134	136	136	137	138
138	138	139	139	141	141	142	142	142	142
142	142	144	144	145	146	148	148	149	151
151	152	155	156	157	157	157	157	158	159
162	163	163	164	166	166	168	170	174	196
212									

Table 6: Parameter Estimates for the Fatigue Life of 6061-T6 Aluminum Coupons Data

Distribution	Parameter Estimates	Log Likelihood	AIC
Pareto	$\hat{\alpha} = 1.579$ $\hat{\theta} = 70$	-548	1100
Beta Pareto	$\hat{\alpha} = 485.47$ $\hat{\beta} = 162.06$ $\hat{k} = 0.3943$ $\hat{\theta} = 3.91$	-458.65	925.3
Beta- Generalized Pareto	$\hat{\alpha} = 12.112$ $\hat{\beta} = 1.702$ $\hat{\mu} = 40.564$ $\hat{k} = 0.273$ $\hat{\theta} = 54.837$	-457.85	925.7
Gamma-Pareto	$\hat{\alpha} = 15.0209$ $\hat{c} = 0.04258$ $\hat{\theta} = 70$	-448.53	900.6

Eugene (2001) proposed the beta-normal distribution and termed it the generalized normal distribution. Eugene (2001) fitted the data in Table 7 and compared the result with gamma distribution and Lagrange-gamma distribution proposed by Famoye and Govindarajulu (1998). These results are reported in Table 8 along with the result of fitting the data to the gamma-Pareto distribution. The results from the log-likelihood and AIC values indicate that the gamma-Pareto and the generalized normal distributions fit the data best. Figure 6 displays the empirical and the fitted cumulative distribution functions. Figure 6 shows that the generalized normal distribution does not fit the left tail very well, however, the gamma-Pareto distribution does provide a good fit. The distribution shows that the data has a long right tail. This example suggests that the gamma-Pareto distribution does very well in fitting the distributions of data with a long right tail characteristic.

Conclusion

This article defined the gamma- X family and studied a special case of the gamma- X family, the gamma-Pareto distribution. Various properties of the gamma-Pareto distribution were investigated, including moments, deviations from the mean and median, hazard function, unimodality, entropies and Fisher information matrix. Results of the uniformly minimum variance unbiased estimator was obtained for one of the shape parameters of the gamma-Pareto distribution. Three real data sets were fitted to the gamma-Pareto distribution and compared with other known distributions. Results show that the gamma-Pareto distribution provides a good fit to each data set and suggests that the gamma-Pareto distribution can be a good model to fit data with a reversed J-shape, approximately symmetric and long right tail characteristics.

Figure 5: CDF for Fitted Distributions for Fatigue Life of 6061-T6 Aluminum Data

Table 7: Observed frequencies for Tribolium Confusum Strain # 3

x-Values	Frequency	x-Values	Frequency	x-Values	Frequency
55	3	125	51	195	1
65	20	135	20	205	2
75	53	145	11	215	0
85	78	155	6	225	1
95	86	165	4	235	1
105	86	175	7	245	1
115	68	185	5		

Table 8: Parameter Estimates for the Tribolium Confusum Strain # 3 Data

Distribution	Parameter Estimates	Log Likelihood	AIC
Gamma	$\hat{\alpha} = 15.15$ $\hat{\beta} = 6.92$	-2335.31	4674.62
Lagrange-gamma	$\hat{r} = 31$ $\hat{\lambda} = 0.36842$ $\hat{\theta} = 0.02913$	-2314.2	4640.41
Generalized Normal	$\hat{\alpha} = 28.68$ $\hat{\beta} = 0.20$ $\hat{\mu} = 30.65$ $\hat{\sigma} = 22.04$	-2290.85	4597.71
Gamma-Pareto	$\hat{\alpha} = 6.3513$ $\hat{c} = 0.09743$ $\hat{\theta} = 55$	-2297.7	4599.4

Figure 6: CDF for Fitted Distributions for Tribolium Confusum Strain # 3 Data

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Comparison of Re-sampling Methods to Generalized Linear Models and Transformations in Factorial and Fractional Factorial Designs

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Experimental situations in which observations are not normally distributed frequently occur in practice. A common situation occurs when responses are discrete in nature, for example counts. One way to analyze such experimental data is to use a transformation for the responses; another is to use a link function based on a generalized linear model (GLM) approach. Re-sampling is employed as an alternative method to analyze non-normal, discrete data. Results are compared to those obtained by the previous two methods.

Key words: Factorial experiments, fractional factorial experiments, effect estimation, confidence intervals.

Introduction

Transformation, generalized linear model (GLM) and bootstrap (re-sampling) are methods employed to examine data when systematic and error assumptions may not hold; this suggests a need for inference procedures which are not based on ordinary least squares. Montgomery and Myers (1997) used a GLM approach to analyze data from research conducted by Bisgaard and Fuller (1994) where the response variable was a count of the number of defects in car grille opening panels; they concluded that using GLMs will provide shorter confidence intervals for the mean predicted response compared to those obtained using transformations. This study shows that this is not necessarily true: it depends on the type of data at hand.

Benski (1994) compared nine different techniques to determine active factors. Qumsiyeh and Shaughnessy (2008) showed that

the bootstrap (re-sampling) could be used to determine the active factors (factors that have an effect on the response) without any requirements on the type of data provided. This study shows that this method of determining active factors agrees with other methods, such as the half-normal plots, in addition this study shows how this method can be used to obtain confidence intervals for responses after determining active factors.

The bootstrap has been shown to provide better than normal estimates of distribution functions of studentized statistics (see Singh, 1981; Bickle & Freedman, 1980; Babu & Singh 1983; Babu and Singh 1984). Qumsiyeh (1994) demonstrated that bootstrap approximation for the distribution of the studentized least square estimate is asymptotically better, not only than the normal approximation, but also than the two-term Edgeworth expansion. Lahiri (1992) showed the superiority of the bootstrap for approximating the distribution of M-estimators. Bhattacharya and Qumsiyeh (1989) conducted an L^p -comparison between the bootstrap and Edgeworth expansions. Finally, Qumsiyeh and Shaughnessy (2010) showed that the bootstrap can be used to determine the active factors in two level designs with missing responses.

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The Data

The data consist of three examples taken from the literature, the first two are fractional factorial and the third is full factorial. The third example presents data that can be analyzed using ordinary least squares. Results obtained were compared with results obtained using ordinary least squares.

Box, Hunter and Hunter

Box, Hunter and Hunter (1978) presented an example where the response Y_1 is the glossiness of car paint measured as counts on a scale of 1 to 100; this measure depended on the setting of 8 factors and sixteen readings were taken, thus, it is part of a 2^{8-4} fractional factorial design. The first four factors are listed in standard order, other factors have the alias structure: $E=ABC$, $F=ABD$, $G=ACD$, $H=BCD$. Using normal plots, factors A and B appear to be the active factors. Using the transformation

$$Y = \left(\sqrt{Y_1} + \sqrt{Y_1 + 1} \right) / 2,$$

the final model for the transformed responses is:

$$\hat{Y} = 8.04 + 0.5173*A + 0.3916*B. \quad (1)$$

Bisgaard and Fuller

Bisgaard and Fuller (1994) presented an example of a 2^{9-5} fractional factorial. The response Y_2 is the number of defects in the finish of sheet molded grille opening panels. The first four factors are listed in the standard order. Other factors have the alias structure: $E=BD$, $F=BCD$, $G=AC$, $H=ACD$, $J=AB$. Using the transformation

$$Y = \left(\sqrt{Y_2} + \sqrt{Y_2 + 1} \right) / 2,$$

as well as normal plots, Bisgaard and Fuller determined that the final model for the transformed responses is:

$$\hat{Y} = 2.513 - 0.996*D - 1.21*F - 0.772*BG, \quad (2)$$

where D , $F=BCD$ and $BG=ABC$ are the active factors.

Walpole and Myers

In this third example, the data are from a study to determine factors that influence the shrinkage of molded parts. The response variable Y_3 is the deviation from nominal shrinkage in $\text{cm} \times 10^4$ and it is part of a 2^4 full factorial design. This example is from Walpole and Myers (1993) and differs from the other two examples, because ordinary least squares can be applied to this data without the need for transformation. Using the half-normal plot, it was determined that factors A, B and the AB interaction are the active factors and the final model is:

$$\hat{Y}_3 = 80 + 5.28*A + 6.22*B + 5.70*AB. \quad (3)$$

The experimental grid for the three examples is shown in Table 1 and the half-normal plots for the three examples are shown in Table 2. In Table 2, based on the normal plots, it is clear that factors A and B are the active factors for the first data set, factors A, B and the AB interaction are the active factors for the third data set and for the second data set D and F and the two factor interaction GH are active.

Bootstrap Method to Determine Active Factors

The bootstrap method can be used, without need for transformation, to determine the active factors (that is, factors that have an effect on the response) and provide models similar to equations (1), (2) and (3). The bootstrap can also be used to provide confidence intervals for the size of the effect. The procedure is as follows: Assume a data set has N total responses (16 in the examples provided). In order to test whether some factor, for example Z, is active (Z could be the interaction of other factors):

- 1) Sample N/2 responses with replacement from the data at the (+1) level of the factor Z.

Table 1: Experimental Grid for Examples

	A	B	C	D	Y_1	Y_2	Y_3
(-)	-1	-1	-1	-1	53	56	72.68
A	1	-1	-1	-1	60	17	71.74
B	-1	1	-1	-1	68	2	76.09
AB	1	1	-1	-1	78	4	93.19
C	-1	-1	1	-1	48	3	71.25
AC	1	-1	1	-1	67	4	70.59
BC	-1	1	1	-1	55	50	70.92
ABC	1	1	1	-1	78	2	104.96
D	-1	-1	-1	1	49	1	73.52
AD	1	-1	-1	1	68	0	75.97
BD	-1	1	-1	1	61	3	74.28
ABD	1	1	-1	1	81	12	92.87
CD	-1	-1	1	1	52	3	79.34
ACD	1	-1	1	1	70	4	75.12
BCD	-1	1	1	1	65	0	79.67
ABCD	1	1	1	1	82	0	97.8

- 2) Sample $N/2$ responses with replacement at the (-1) level of the factor Z .
- 3) Estimate the effect of that factor using the difference between the average at the $(+1)$ level and (-1) levels.
- 4) Repeat the sampling procedure a large number of times, for example, 500.
- 5) Take the average of the differences of the averages at the $+1$ level and -1 levels across the 500 samples: this is the effect size estimate.
- 6) Determine the upper $(1-\alpha/2)$ and lower $\alpha/2$ percentile points of the re-sampled effect values.
- 7) Use these values to construct the $(1-\alpha) \times 100\%$ confidence interval for the effect size.

- 8) If the confidence interval does not contain zero then the factor is identified as an active factor.

The mean effect size and confidence intervals for the different effect sizes for the three different examples were determined using this procedure (see Table 3).

Table 3 shows the LCL (2.5 percentile lower confidence limit) and UCL (97.5 percentile upper confidence limit). The only confidence intervals that do not contain zero in the first example are those of A and B, this matches the results of the normal plots and Box, Hunter and Hunter. In addition, the only confidence intervals that do not contain zero in the third example are those of A, B and the AB interaction, this matches the results of the half-normal plots and of Walpole and Myers. With respect to the second example, the only confidence intervals that do not contain zero are those of D and F. The two-factor interaction BG

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Table 2: Half-Normal Plots for the Three Examples

may also be considered active, because the upper confidence limit is very close to zero; this agrees with the results of Bisgaard and Fuller and the half-normal plots. The half-normal plots do not clearly show that BG is active.

Bootstrap Method to Determine Confidence Intervals

Confidence intervals for the mean predicted responses can be obtained as follows: For each effect size determined in step (3) of the

bootstrap method, find the predicted value of Y_1 for the first example, (Y_2 for the second example and Y_3 for the third), using the two active factors found for the first example, A and B, and use as coefficients the effect size divided by two. (Note that there are 3 active factors for the second and the third examples). Because the data consists of counts for the first two examples, if the predicted value is negative, zero was substituted for its value. This was necessary for the Bisgaard and Fuller example, however it was not

necessary for the first and third examples because none of the responses were zero and responses were large positive values. Re-sampling was repeated 1,000 times, and one thousand predicted values were produced at each setting of the active factors. These 1,000 values were used to construct 95% confidence intervals for the mean predicted responses. Results are summarized and shown Tables 4-8. Note that, for the first two examples, after finding the confidence intervals for the transformed mean and for the lower and upper confidence limit, the results are un-transformed using a software package that can solve for x , when y is known in the equation: $y = (\sqrt{x} + \sqrt{x+1})/2$. For the third example, because no transformation was used, the confidence interval provided by the ordinary least squares method is reported.

Table 7 gives the mean predicted values and confidence intervals for the mean predicted values, these results were obtained using the SQL procedure in the statistical software SAS. Re-sampling was repeated 1,000 times. A slight

difference occurred between re-sampling 500 and 1,000 times; the length of the confidence interval was slightly smaller when re-sampling 1,000 times. Very little difference was observed between re-sampling 1,000 times and re-sampling more than 1,000 times.

Table 8 shows the length of the confidence intervals using the different methods for the three different examples. For the Box, Hunter and Hunter example the Bootstrap gave shorter confidence intervals than those of the Generalized Linear Model (GLM). For the Bisgaard and Fuller example, the bootstrap results are not inferior to the untransformed or GLM procedures. For data with count responses where some of the responses are zeros using a transformation is questionable, therefore the bootstrap provides a good alternative. For data such as the third example taken from Walpole and Myers, ordinary least squares (OLS) can be applied and this method results in confidence intervals that are shorter than both the Bootstrap and GLM approaches.

Table 3: Mean Effect Size and Confidence Intervals for the Different Effect Sizes for the Three Different Examples

Factors	Box Hunter and Hunter			Bisgaard and Fuller			Walpole and Myers		
	Mean	LCL	UCL	Mean	LCL	UCL	Mean	LCL	UCL
A	16.82	10.75	22.50	-9.16	-24.63	4.38	16.82	10.75	22.50
B	13.12	6.00	20.75	-1.97	-17.13	15.00	13.12	6.00	20.75
C	0.07	-10.75	10.75	-4.04	-20.50	11.75	0.07	-10.75	10.75
D	2.59	-6.75	12.50	-14.97	-32.50	-1.13	2.59	-6.75	12.50
AB	1.19	-10.63	13.38	0.06	-16.88	16.00	11.43	2.45	20.14
AC	3.03	-6.00	13.38	-2.17	-17.25	13.75	1.30	-8.33	11.90
AD	1.69	-9.00	12.25	11.58	-2.38	27.50	-1.67	-12.09	7.86
BC	-2.27	-11.63	7.75	10.77	-2.63	26.25	2.01	-8.28	12.02
BD	0.18	-9.88	10.75	3.87	-13.88	19.75	-2.20	-13.31	7.88
CD	2.75	-7.00	13.00	0.55	-15.75	16.25	1.45	-9.30	11.11
ABC	-0.04	-9.75	9.25	-11.84	-28.38	0.68	2.58	-5.36	12.15
ABD	-0.60	-11.50	10.38	2.28	-14.50	18.25	-1.94	-11.70	7.38
ACD	-3.64	-13.13	6.13	0.88	-14.88	17.00	-2.99	-13.07	5.32
BCD	2.11	-10.00	12.63	-16.95	-32.25	-3.38	-0.29	-10.19	9.22
ABCD	-0.32	-10.75	10.00	10.24	-5.13	29.00	-1.59	-10.82	7.97

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Table 4: Results of the Box, Hunter and Hunter (1978) Example

Obs.	Least Squares				GLM Poisson	
	Transformed		Untransformed			
	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval
1	7.14	(6.92, 7.36)	50.42	(47.32, 53.63)	51.26	(42.45, 61.9)
2	8.17	(7.95, 8.39)	66.26	(62.7, 69.92)	11.74	(8.14, 16.94)
3	7.92	(7.7, 8.14)	62.22	(58.76, 65.76)	1.12	(0.6, 2.08)
4	8.95	(8.73, 9.17)	79.67	(75.76, 83.68)	4.88	(2.87, 8.32)
5	7.14	(6.92, 7.36)	50.42	(47.32, 53.63)	1.12	(0.6, 2.08)
6	8.17	(7.95, 8.39)	66.26	(62.7, 69.92)	4.88	(2.87, 8.32)
7	7.92	(7.7, 8.14)	62.22	(58.76, 65.76)	51.26	(42.45, 61.9)
8	8.95	(8.73, 9.17)	79.67	(75.76, 83.68)	11.74	(8.14, 16.94)
9	7.14	(6.92, 7.36)	50.42	(47.32, 53.63)	0.81	(0.42, 1.56)
10	8.17	(7.95, 8.39)	66.26	(62.7, 69.92)	0.19	(0.09, 0.38)
11	7.92	(7.7, 8.14)	62.22	(58.76, 65.76)	1.96	(1.16, 3.3)
12	8.95	(8.73, 9.17)	79.67	(75.76, 83.68)	8.54	(5.62, 12.98)
13	7.14	(6.92, 7.36)	50.42	(47.32, 53.63)	1.96	(1.16, 3.3)
14	8.17	(7.95, 8.39)	66.26	(62.7, 69.92)	8.54	(5.62, 12.98)
15	7.92	(7.7, 8.14)	62.22	(58.76, 65.76)	0.81	(0.42, 1.56)
16	8.95	(8.73, 9.17)	79.67	(75.76, 83.68)	0.19	(0.09, 0.38)

Table 5: Results of Montgomery and Myers (1997) for the Bisgaard and Fuller Example

Obs.	Least Squares				GLM Poisson	
	Transformed		Untransformed			
	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval
1	5.50	(4.13, 6.84)	29.75	(16.65, 46.41)	51.26	(42.45, 61.9)
2	3.95	(2.6, 5.3)	15.11	(6.25, 27.65)	11.74	(8.14, 16.94)
3	1.53	(0.17, 2.88)	1.86	(**, 7.78)	1.12	(0.6, 2.08)
4	3.07	(1.71, 4.42)	8.9	(2.45, 19.04)	4.88	(2.87, 8.32)
5	1.53	(0.17, 2.88)	1.86	(**, 7.78)	1.12	(0.6, 2.08)
6	3.07	(1.71, 4.42)	8.9	(2.45, 19.04)	4.88	(2.87, 8.32)
7	5.49	(4.13, 6.84)	29.61	(16.65, 46.41)	51.26	(42.45, 61.9)
8	3.95	(2.6, 5.3)	15.11	(6.25, 27.65)	11.74	(8.14, 16.94)
9	1.07	(-0.28, 2.42)	0.7	(*, 5.41)	0.81	(0.42, 1.56)
10	-0.47	(-1.82, 0.89)	*	(*, 0.36)	0.19	(0.09, 0.38)
11	1.96	(0.6, 3.31)	3.34	(0.04, 10.49)	1.96	(1.16, 3.3)
12	3.49	(2.14, 4.85)	11.7	(4.13, 23.1)	8.54	(5.62, 12.98)
13	1.96	(0.6, 3.31)	3.34	(0.04, 10.49)	1.96	(1.16, 3.3)
14	3.49	(2.14, 4.85)	11.7	(4.13, 23.1)	8.54	(5.62, 12.98)
15	1.07	(-0.28, 2.42)	0.7	(*, 5.41)	0.81	(0.42, 1.56)
16	-0.47	(-1.82, 0.89)	*	(*, 0.36)	0.19	(0.09, 0.38)

*values that can't be calculated using the transformation because of the negative predicted value;

**values that appear to be incorrectly calculated in Montgomery and Myers (1997) work.

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Table 6: Results of the Walpole and Myers (1993) Example

Obs.	Least Squares		GLM Poisson	
	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval
1	74.20	(69.82, 78.57)	74.2	(66.22, 83.14)
2	73.36	(68.98, 77.73)	73.36	(65.42, 82.25)
3	75.24	(70.87, 79.61)	75.24	(67.2, 84.24)
4	97.21	(92.83, 101.58)	97.21	(88.01, 107.36)
5	74.20	(69.82, 78.57)	74.2	(66.22, 83.14)
6	73.36	(68.98, 77.73)	73.36	(65.42, 82.25)
7	75.24	(70.87, 79.61)	75.24	(67.2, 84.24)
8	97.21	(92.83, 101.58)	97.21	(88.01, 107.36)
9	74.20	(69.82, 78.57)	74.2	(66.22, 83.14)
10	73.36	(68.98, 77.73)	73.36	(65.42, 82.25)
11	75.24	(70.87, 79.61)	75.24	(67.2, 84.24)
12	97.21	(92.83, 101.58)	97.21	(88.01, 107.36)
13	74.20	(69.82, 78.57)	74.2	(66.22, 83.14)
14	73.36	(68.98, 77.73)	73.36	(65.42, 82.25)
15	75.24	(70.87, 79.61)	75.24	(67.2, 84.24)
16	97.21	(92.83, 101.58)	97.21	(88.01, 107.36)

Table 7: Bootstrap Mean and Confidence Interval for the Predicted Values for the Three Examples

Obs.	Bootstrap (Re-sampling)					
	Box, Hunter and Hunter		Bisgaard and Fuller		Walpole and Myers	
	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval	Predicted Value	95% Confidence Interval
1	50.87	(45.39, 57.03)	31.86	(19.22, 45.56)	73.95	(66.32, 82.06)
2	65.88	(59.29, 73.19)	19.19	(5.06, 33.72)	73.65	(66.08, 81.29)
3	61.88	(55.57, 68.9)	10.26	(0, 26.78)	75.18	(68.45, 81.64)
4	80.12	(72.63, 88.38)	15.05	(3.44, 27.34)	97.22	(89.44, 105.26)
5	50.87	(45.39, 57.03)	10.26	(0, 26.78)	73.95	(66.32, 82.06)
6	65.88	(59.29, 73.19)	15.05	(3.44, 27.34)	73.65	(66.08, 81.29)
7	61.88	(55.57, 68.9)	31.86	(19.22, 45.56)	75.18	(68.45, 81.64)
8	80.12	(72.63, 88.38)	19.19	(5.06, 33.72)	97.22	(89.44, 105.26)
9	50.87	(45.39, 57.03)	3.41	(0, 15.06)	73.95	(66.32, 82.06)
10	65.88	(59.29, 73.19)	0.07	(0, 0.91)	73.65	(66.08, 81.29)
11	61.88	(55.57, 68.9)	5.72	(0, 16.69)	75.18	(68.45, 81.64)
12	80.12	(72.63, 88.38)	17.76	(5.44, 30.38)	97.22	(89.44, 105.26)
13	50.87	(45.39, 57.03)	5.72	(0, 16.69)	73.95	(66.32, 82.06)
14	65.88	(59.29, 73.19)	17.76	(5.44, 30.38)	73.65	(66.08, 81.29)
15	61.88	(55.57, 68.9)	3.41	(0, 15.06)	75.18	(68.45, 81.64)
16	80.12	(72.63, 88.38)	0.07	(0, 0.91)	97.22	(89.44, 105.26)

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Table 8: Length of Confidence Intervals for the Three Examples Using the Different Methods

Confidence Interval Length								
Box, Hunter and Hunter			Bisgaard and Fuller			Walpole and Myers		
Untrans.	GLM	Bootstrap	Untrans.	GLM	Bootstrap	OLS	GLM	Bootstrap
6.31	11.64	9.44	29.76	19.45	26.34	8.75	16.92	15.75
7.22	13.90	11.16	21.40	8.80	27.84	8.75	16.83	15.21
7.00	13.34	11.16	**	1.47	26.78	8.75	17.04	13.20
7.92	15.75	9.44	16.59	5.45	23.91	8.75	19.35	15.82
6.31	11.64	9.44	**	1.47	26.78	8.75	16.92	15.75
7.22	13.90	11.16	16.59	5.45	23.91	8.75	16.83	15.21
7.00	13.34	11.16	29.76	19.45	26.34	8.75	17.04	13.20
7.92	15.75	9.44	21.40	8.80	27.84	8.75	19.35	15.82
6.31	11.64	9.44	*	1.13	14.25	8.75	16.92	15.75
7.22	13.90	11.16	*	0.29	0.91	8.75	16.83	15.21
7.00	13.34	11.16	10.45	2.14	16.69	8.75	17.04	13.20
7.92	15.75	9.44	18.97	7.35	24.22	8.75	19.35	15.82
6.31	11.64	9.44	10.45	2.14	16.69	8.75	16.92	15.75
7.22	13.90	11.16	18.97	7.35	24.22	8.75	16.83	15.21
7.00	13.34	11.16	*	1.13	14.25	8.75	17.04	13.20
7.92	15.75	9.44	*	0.29	0.91	8.75	19.35	15.82

*values that can't be calculated using the transformation because of the negative predicted value; **values that appear to be incorrectly calculated in Montgomery and Myers (1997) work.

Conclusion

The bootstrap method can be used to determine active factors and to construct confidence intervals for effect size and for a predicted mean response. The results are not inferior to those obtained using transformations or generalized linear models procedures and are actually better in some situations. The availability of computers and statistical software makes using re-sampling (bootstrap) easy and fast and provides good predictions.

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Estimation of Multinomial Proportions using Higher Order Moments of Scrambling Variables in Randomized Response Sampling

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An extension to estimating multinomial proportions of potentially sensitive attributes in survey sampling is proposed using higher order moments of scrambling variables at the estimation stage to produce unbiased estimators. The variance and covariance expressions are derived and the relative efficiency of the proposed estimators based on scrambling variables is investigated.

Key words: Estimation of sensitive multinomial proportions, randomized response sampling, respondents protection.

Introduction

The problem of estimating the proportion of potentially sensitive attributes in survey sampling has been very well addressed in the literature following the pioneering work of Warner (1965), and the use of randomized response sampling in social, medical and environmental sciences has been well documented (Waltz, et al., 2004; Blank, 2008). Singh and Chen (2009) introduced the use of higher order moments of scrambling variables to improve single proportion estimates without affecting respondent cooperation in survey research.

The problem of estimating trinomial proportions has been very useful, especially during election periods in the United States of America. Voters in the US can be divided into three mutually exclusive groups: Democrat, Republican and Other. At this time, expressing preference for one of these three groups does not

pose a threat to an individual's privacy; however, the competition for the presidential position is becoming more difficult and there may be a time when voters will not feel safe disclosing their preferences to vote in the US. A new method is developed here that could be useful in such circumstances to organizations that conduct surveys about the prediction of future president for the US in the forthcoming elections. It is assumed that the partition of voters will remain trinomial because it may not be easy to establish a new competitive party as strong as those that are currently functioning; however, the proposed model can be extended to the case of a multinomial distribution if required.

This same argument can be extended to other applications if a population can be captured completely within three mutually exclusive groups. As noted by Singh, Kim and Grewal (2008), a sensitive question in one survey could be non-sensitive in another survey depending on the situation, particularly when there are three categories that are feasible when an answer is: exactly known, exactly unknown and not sure; hence leading to the problem of trinomial proportions estimation.

In a careful examination of the literature in randomized response sampling (Tracy & Mangat, 1996), not much attention has been paid to estimate sensitive multinomial proportions. Abul-Ela, et al. (1967) extended Warner's (1965) design to the multichotomous case when

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a population can be considered to be divided into t disjoint classes C_j with unknown proportions π_j ($j=1,2,\dots,t$, $0 < \pi_j < 1$, $\sum \pi_j = 1$). It is assumed that at least one of the classes carries a stigma and at least one carries no stigma. They suggested drawing s ($=t-1$) independent simple random with replacement samples sized n_i ($i=1,2,\dots,s$, $\sum n_i = n$), and then employing a randomized response device to each of the samples. Abul-Ela, et al. (1967) examined the extent of bias and the mean square error of estimators for $t=3$.

Bourke and Dalenius (1973, 1974) proposed a Latin square measurement design to extend Warner's model to the multinomial case; their design uses t different possible responses and requires only one sample. A respondent is asked to select one of a t -type cards using a random device. Each of the t -mutually exclusive classes is described on each card, except that the order of the description is permuted from card to card and the permutation for t -cards forms a Latin square.

The respondent reads the cards selected and reports only the position of the card (i.e., $t=1, 2, \dots, (t-1)$ or t) of the statement describing the class to which he/she belongs. The unrelated question design was also extended by Bourke (1974) to estimate the proportion of a population in each of t mutually exclusive classes of which $(t-1)$ are sensitive. One sample is needed if the distribution of the unrelated character is known. The design uses a deck of cards, each of which contains a number of statements. The arrangement of the statements is a part of the design.

Hochberg (1975) outlined an alternative scheme for estimating the t group proportions of which, at most, $(t-2)$ are stigmatizing. The realizations for any sampled individuals constitute a two-stage scheme. The second stage is conditional on the random individual's response in the first stage. Drane (1976) used a forced yes stochastic model to estimate the proportion of more than one sensitive character. The use of supplemented block, balanced incomplete block and spring balance weighing designs were introduced by Raghavarao and

Federer (1979); their models allow the surveyor to obtain answers to several sensitive questions. Mukhopadhyay (1980), Mukherjee (1981), Tamhane (1981), Bourke (1981, 1982, 1990), Silva (1983) and Christofides (2003) have also considered the estimation of multi-attribute parameters.

Guerriero and Sandri (2007) pointed out that the family of models proposed by Kuk (1990) is better than the Simmons' family (refer to Greenberg *et al.* (1969)) in terms of efficiency and privacy protection. From an empirical standpoint, van der Heijden, et al. (2000) showed that Kuk's procedure performs slightly better than the forced-response procedure and markedly better than face-to-face direct questioning and computer assisted self-interviewing.

They also noted that the recommendations and successful applications of Kuk's procedure have been reported in van den Hout and van der Heijden (2002), and these results should be even more marked for the model proposed by Christofides (2003). In addition, an adequate analysis of the efficiency and the respondents' protection is always necessary when proposing new randomized response models. Thus, following Guerriero and Sandri (2007), it is worthwhile to extend the Kuk (1990) and Franklin (1989) type models. Note that the the Mangat (1994), Mangat and Singh (1990), Gjestvang and Singh (2006) and Kuk (1990) models are special cases of the Franklin (1989) model. Additional work on randomized response sampling is available in Singh and Kim (2011), Diana and Perri (2009), Tan, et al. (2009) and Esponda and Guerrero (2009).

Proposed Randomized Response Technique

In the proposed randomized response device, if a person selected in the sample belongs to the first sensitive group A_1 then that person is requested to draw a random number S_1 from a density function $f_1(s)$ and report to the interviewer; if that person belongs to second sensitive group A_2 then that person is requested to draw a random number S_2 from a density function $f_2(s)$ and report to the interviewer; and if that person belongs to the third sensitive

group A_3 , then that person is requested to draw a random number S_3 from a density function $f_3(s)$ and report to the interviewer. The respondent is further requested not to disclose the mode of response.

Let Ω be the population under study; $\Omega = \bigcup_{k=1}^3 A_k$ and the groups A_k are mutually exclusive. The choice of the three densities $f_1(s)$, $f_2(s)$ and $f_3(s)$ are comprised such that respondents should feel safe in reporting the random number drawn. In other words, to maintain the privacy of respondents from all the three groups, the mean values and the variances of the three densities should not deviate too greatly from each other. In particular, the densities $f_1(s)$, $f_2(s)$ and $f_3(s)$ could be normal, beta, gamma or some other distribution.

Let π_1 , π_2 and π_3 represent the true proportions of persons belonging to groups A_1 , A_2 and A_3 respectively such that $\pi_1 + \pi_2 + \pi_3 = 1$. Assume that E denotes the expected value over the proposed randomization response device, and let $\theta_1 = E(S_1)$, $\theta_2 = E(S_2)$, $\theta_3 = E(S_3)$, and

$\gamma_{abc} = E[(S_1 - \theta_1)^a (S_2 - \theta_2)^b (S_3 - \theta_3)^c]$, where a , b and c are non-negative integers and are known moments of the three scrambling variables used in the proposed randomization device. Consider a simple random with replacement sample (SRSWR) of n respondents. Interestingly, it can be shown that, based on only single sample information, three unbiased estimates of the three different parameters can be proposed. The distribution of the responses will be as follows:

$$Z_i = \begin{cases} S_1 & \text{with probability } \pi_1 \\ S_2 & \text{with probability } \pi_2 \\ S_3 & \text{with probability } \pi_3 \end{cases} \quad (2.1)$$

If

$$E(Z_i) = \pi_1 \theta_1 + \pi_2 \theta_2 + (1 - \pi_1 - \pi_2) \theta_3 \quad (2.2)$$

then, following Singh and Chen (2009),

$$Z_i^2 = \begin{cases} S_1^2 & \text{with probability } \pi_1 \\ S_2^2 & \text{with probability } \pi_2 \\ S_3^2 & \text{with probability } \pi_3 \end{cases} \quad (2.3)$$

where $E(S_1^2) = \gamma_{200} + \theta_1^2$, $E(S_2^2) = \gamma_{020} + \theta_2^2$ and $E(S_3^2) = \gamma_{002} + \theta_3^2$.

If

$$E(Z_i^2) = \pi_1 (\gamma_{200} + \theta_1^2) + \pi_2 (\gamma_{020} + \theta_2^2) + (1 - \pi_1 - \pi_2) (\gamma_{002} + \theta_3^2) \quad (2.4)$$

and defining

$$\Delta = (\theta_1 - \theta_3) \{ (\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \} - (\theta_2 - \theta_3) \{ (\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \}, \quad (2.5)$$

several theorems and lemmas may be put forth (see Appendix A).

Empirical Comparisons

It is possible to use the Warner (1965) model three times to estimate the three non-overlapping parameters π_k , $k=1,2,3$. Each respondent selected in the sample could be provided with three randomization devices, for example, R_k , $k=1,2,3$. The randomization R_k bears two types of statements, are you a member of group A_k ?, and are you a member of group A_k^c ? with probabilities P_k and $(1 - P_k)$, respectively. Based on a sample of n respondents, if n_k reports yes related to the k^{th} group, then the unbiased estimator of π_k is

$$\hat{\pi}_{k(w)} = \frac{n_k / n - (1 - P_k)}{2P_k - 1}, \quad (3.1)$$

$$P_k \neq 0.5$$

with variance

$$V(\hat{\pi}_{k(w)}) = \frac{\pi_k(1-\pi_k)}{n} + \frac{P_k(1-P_k)}{n(2P_k-1)^2}. \quad (3.2)$$

The relative efficiency of the proposed estimator $\hat{\pi}_k$ (as defined in the Appendix) with respect to the corresponding estimator $\hat{\pi}_{k(w)}$ (Warner, 1965) is:

$$RE(k) = \frac{V(\hat{\pi}_{k(w)})}{V(\hat{\pi}_k)} \times 100\%, \quad (3.3)$$

$k = 1, 2, 3.$

Results

Choosing $P_k = 0.7$, $k = 1, 2, 3$, based on Warner (1965) is a reasonable and practical choice for the model, considering the problem of estimation of π_k with their respective estimators $\hat{\pi}_{k(w)}$ for $k = 1, 2, 3$. A privacy protection criterion is suggested, that is:

$$\lambda_{Z_{k,i}} = \frac{f(Z_k | k \in A_i)}{f(Z_k | k \notin A_i)} \quad (3.4)$$

and refers to the privacy protection with respect to response Z_k for a respondent k being a member of A_i . For these measures $0 \leq \lambda_{Z_{k,i}} < \infty$ applies with $\lambda_{Z_{k,1}} = 1$ indicating data privacy protection for unit k being a member of group A_i . This means that the value Z_k contains absolutely no information on the variable of interest; the more the λ -measure differs from unity the more information on the variable under study is contained in the response, meaning the less the privacy protection. The maximum $\lambda_{Z_{k,i}} = \infty$ (or 0) describes a situation where membership or the non-membership of A_i may be concluded based on the answer Z_k directly. A respondent would answer untruthfully or not answer at all in such a case.

Bearing in mind the proposed privacy protection criterion in (3.4), choice of the known parameters of the scrambling variables was: $\theta_1 = 57$, $\theta_2 = 62$, $\theta_3 = 60$, $\gamma_{200} = 0.5$,

$\gamma_{020} = 3.5$, and $\gamma_{002} = 4.5$ in the proposed model with three scrambling variables. Based on the three sigma empirical rule, most of the values of the scrambling variables S_1 , S_2 and S_3 could be any real numbers in the ranges: (54.87, 59.12); (56.38, 67.61), and (53.63, 66.36) respectively, but those values are not 100% bounded to these intervals. Due to an overlap between the three intervals, it is difficult to guess the status of the respondents based on their reported responses. Using the four sigma rule the scrambling variables S_1 , S_2 and S_3 could, respectively, be any real numbers in the ranges: (54.17, 59.82); (54.51, 69.48), and (51.51, 68.48), and the six sigma empirical rule can be considered in a similar manner.

To study the effect of known higher order moments, such as skewness and kurtosis, of the scrambling variables on the relative efficiencies $RE(k)$ of the proposed estimators we studied different values of $\gamma_3 = \gamma_{300} = \gamma_{030} = \gamma_{003}$ as $-2, 0, 3, 5, 10$ and 20 ; and the values of the $\gamma_4 = \gamma_{400} = \gamma_{040} = \gamma_{004}$ as $2, 3, 5$ and 10 . The minimum relative efficiency of 103% was retained by assuming that a minimum 3% gain is enough if one methodology could gain over the other without affecting the respondents' cooperation (see Table 1).

Note that, while estimating rare attributes in two groups such as $\pi_1 = 0.1$, and $\pi_2 = 0.1$, then $\pi_3 = 0.8$ and based on 3 observations, the relative efficiencies $RE(1)$, $RE(2)$ and $RE(3)$ remain as 615.3%, 451.1%, 713.4% for $\gamma_{300} = \gamma_{030} = \gamma_{003} = -2$ and $\gamma_{400} = \gamma_{040} = \gamma_{004} = 10$. Keeping the same value of $\gamma_{400} = \gamma_{040} = \gamma_{004} = 10$, for $\gamma_{300} = \gamma_{030} = \gamma_{003} = 0$, the $RE(1)$, and $RE(3)$ values become 919.0%, 306.8% and 562.5%. Thus, changing the value of $\gamma_{300} = \gamma_{030} = \gamma_{003}$ from -2 to 0 , the $RE(1)$ increases from 615.3% to 919.0%, but the value of $RE(2)$ decreases from 451.1% to 306.8%, and the value of $RE(3)$ decreases from 713.4% to 562.5%. As the values of $\gamma_{300} = \gamma_{030} = \gamma_{003}$ increase to 3 , there is huge increase in the value of $RE(1)$ to 3543.1%, whereas a decrease in the values of $RE(2)$ and

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Table 1: Relative efficiencies, $RE(k)$, $k = 1, 2, 3$, of Proposed Estimators for Difference Choices of Known Higher Order Moments of the Three Scrambling Variables

π_1	π_2	π_3	γ_{300}	γ_{030}	γ_{003}	γ_{400}	γ_{040}	γ_{004}	$RE(1)$	$RE(2)$	$RE(3)$
0.1	0.1	0.8	-2	-2	-2	10	10	10	615.3	451.1	713.4
			0	0	0	10	10	10	919.0	306.8	562.5
			3	3	3	10	10	10	3543.1	207.3	426.9
	0.2	0.7	-2	-2	-2	2	2	2	977.6	358.7	1368.6
			-2	-2	-2	3	3	3	907.5	338.1	843.5
			-2	-2	-2	5	5	5	793.7	303.4	477.3
			-2	-2	-2	10	10	10	604.3	241.4	228.9
			0	0	0	2	2	2	1633.8	246.8	548.7
			0	0	0	3	3	3	1447.0	236.9	439.1
			0	0	0	5	5	5	1177.7	219.3	313.8
			0	0	0	10	10	10	803.8	185.0	183.1
			3	3	3	3	3	3	13358.9	163.5	255.4
			3	3	3	5	5	5	4294.3	154.9	207.3
			3	3	3	10	10	10	1592.6	136.9	140.9
			5	5	5	10	10	10	4606.9	116.7	122.1
	0.3	0.6	-2	-2	-2	2	2	2	950.1	220.8	282.2
			-2	-2	-2	3	3	3	883.8	213.1	250.7
			-2	-2	-2	5	5	5	775.5	199.2	204.9
			-2	-2	-2	10	10	10	593.6	171.2	140.6
			0	0	0	2	2	2	1301.9	166.3	187.7
			0	0	0	3	3	3	1180.5	161.9	173.2
			0	0	0	5	5	5	994.9	153.7	150.0
			0	0	0	10	10	10	714.2	136.5	112.4
			3	3	3	2	2	2	2928.3	121.3	124.9
			3	3	3	3	3	3	2378.1	119.0	118.3
			3	3	3	5	5	5	1728.6	114.5	107.0
	0.4	0.5	-2	-2	-2	2	2	2	924.1	163.6	161.3
			-2	-2	-2	3	3	3	861.2	159.5	150.5
			-2	-2	-2	5	5	5	758.1	151.7	132.8
			0	0	0	2	2	2	1082.1	127.8	115.2
			0	0	0	3	3	3	996.9	125.2	109.6
	0.5	0.4	-2	-2	-2	2	2	2	899.5	131.5	113.5
			-2	-2	-2	3	3	3	839.8	128.8	108.0

Table 1 (continued): Relative efficiencies, $RE(k)$, $k = 1, 2, 3$, of Proposed Estimators for Difference Choices of Known Higher Order Moments of the Three Scrambling Variables

π_1	π_2	π_3	γ_{300}	γ_{030}	γ_{003}	γ_{400}	γ_{040}	γ_{004}	$RE(1)$	$RE(2)$	$RE(3)$
0.2	0.1	0.7	-2	-2	-2	2	2	2	529.7	657.2	1375.4
			-2	-2	-2	3	3	3	509.4	588.5	846.1
			-2	-2	-2	5	5	5	473.1	486.6	478.1
			-2	-2	-2	10	10	10	401.6	339.7	229.0
			0	0	0	3	3	3	786.8	431.9	2202.0
			0	0	0	5	5	5	703.5	374.4	733.2
			0	0	0	10	10	10	556.3	280.9	274.9
			3	3	3	5	5	5	2610.9	278.1	3673.9
			3	3	3	10	10	10	1317.1	223.0	392.7
			5	5	5	10	10	10	14931.8	196.1	549.8
	0.2	0.6	-2	-2	-2	2	2	2	521.9	287.3	282.5
			-2	-2	-2	3	3	3	502.1	274.0	250.9
			-2	-2	-2	5	5	5	466.9	250.7	205.0
			-2	-2	-2	10	10	10	397.1	206.8	140.7
			0	0	0	2	2	2	743.9	230.5	282.5
			0	0	0	3	3	3	704.4	221.8	250.9
			0	0	0	5	5	5	636.9	206.3	205.0
			0	0	0	10	10	10	513.8	175.7	140.7
			3	3	3	2	2	2	2055.6	177.8	282.5
			3	3	3	3	3	3	1780.2	172.6	250.9
			3	3	3	5	5	5	1404.0	163.1	205.0
			3	3	3	10	10	10	918.7	143.3	140.7
			5	5	5	5	5	5	7125.6	143.0	205.0
			5	5	5	10	10	10	1935.8	127.6	140.7
	0.3	0.5	-2	-2	-2	2	2	2	514.3	192.3	161.3
			-2	-2	-2	3	3	3	495.1	186.5	150.6
			-2	-2	-2	5	5	5	460.8	175.7	132.8
			0	0	0	2	2	2	669.8	159.0	144.8
			0	0	0	3	3	3	637.7	154.9	136.0
			0	0	0	5	5	5	581.8	147.4	121.4
			3	3	3	2	2	2	1226.0	126.1	125.5
			3	3	3	3	3	3	1122.4	123.6	118.9
			3	3	3	5	5	5	960.2	118.8	107.5
			5	5	5	2	2	2	2745.7	110.9	115.2
			5	5	5	3	3	3	2275.6	108.9	109.6
	0.4	0.4	-2	-2	-2	2	2	2	506.9	147.8	113.5
			-2	-2	-2	3	3	3	488.3	144.3	108.1

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Table 1 (continued): Relative efficiencies, $RE(k)$, $k = 1, 2, 3$, of Proposed Estimators for Difference Choices of Known Higher Order Moments of the Three Scrambling Variables

π_1	π_2	π_3	γ_{300}	γ_{030}	γ_{003}	γ_{400}	γ_{040}	γ_{004}	$RE(1)$	$RE(2)$	$RE(3)$
0.3	0.1	0.6	-2	-2	-2	2	2	2	383.8	444.7	282.8
			-2	-2	-2	3	3	3	373.4	412.2	251.1
			-2	-2	-2	5	5	5	354.1	359.5	205.2
			-2	-2	-2	10	10	10	313.7	272.4	140.8
			0	0	0	2	2	2	567.7	410.2	570.8
			0	0	0	3	3	3	545.2	382.3	454.9
			0	0	0	5	5	5	505.1	336.5	323.6
			0	0	0	10	10	10	426.7	259.1	188.0
			3	3	3	5	5	5	1401.7	307.1	2416.8
			3	3	3	10	10	10	928.3	241.3	378.2
			5	5	5	10	10	10	4290.6	230.7	1163.0
	0.2	0.5	-2	-2	-2	2	2	2	379.8	239.7	161.4
			-2	-2	-2	3	3	3	369.6	230.3	150.7
			-2	-2	-2	5	5	5	350.7	213.6	132.9
			0	0	0	2	2	2	524.9	216.3	194.9
			0	0	0	3	3	3	505.6	208.6	179.4
			0	0	0	5	5	5	470.9	194.9	154.8
			0	0	0	10	10	10	402.0	167.3	115.3
			3	3	3	2	2	2	1229.3	188.6	282.9
			3	3	3	3	3	3	1128.4	182.8	251.4
			3	3	3	5	5	5	969.2	172.1	205.6
			3	3	3	10	10	10	716.5	150.2	141.2
			5	5	5	2	2	2	11669.3	173.8	404.6
			5	5	5	3	3	3	6310.2	168.9	343.1
			5	5	5	5	5	5	3289.2	159.7	263.1
			5	5	5	10	10	10	1497.2	140.7	166.2
	0.3	0.4	-2	-2	-2	2	2	2	375.9	170.4	113.6
			-2	-2	-2	3	3	3	365.9	165.8	108.1
			0	0	0	2	2	2	488.1	152.3	118.4
			0	0	0	3	3	3	471.3	148.6	112.5
			3	3	3	2	2	2	883.5	131.3	126.4
			3	3	3	3	3	3	830.1	128.5	119.7
			3	3	3	5	5	5	740.6	123.4	108.1
			5	5	5	2	2	2	1921.1	120.3	132.4
			5	5	5	3	3	3	1685.4	118.0	125.0
			5	5	5	5	5	5	1353.4	113.6	112.5

Table 1 (continued): Relative efficiencies, $RE(k)$, $k = 1, 2, 3$, of Proposed Estimators for Difference Choices of Known Higher Order Moments of the Three Scrambling Variables

π_1	π_2	π_3	γ_{300}	γ_{030}	γ_{003}	γ_{400}	γ_{040}	γ_{004}	$RE(1)$	$RE(2)$	$RE(3)$
0.4	0.1	0.5	-2	-2	-2	2	2	2	313.4	336.1	161.5
			-2	-2	-2	3	3	3	306.5	317.2	150.7
			-2	-2	-2	5	5	5	293.7	285.0	133.0
			0	0	0	2	2	2	456.2	365.2	298.1
			0	0	0	3	3	3	441.9	342.9	263.3
			0	0	0	5	5	5	415.6	305.7	213.5
			0	0	0	10	10	10	362.0	240.4	144.9
			3	3	3	5	5	5	1102.4	342.9	2330.8
			3	3	3	10	10	10	791.2	262.8	378.1
	0.2	0.4	-2	-2	-2	2	2	2	310.8	205.5	113.6
			-2	-2	-2	3	3	3	304.0	198.6	108.2
			0	0	0	2	2	2	428.7	203.7	150.2
			0	0	0	3	3	3	416.0	196.9	140.8
			0	0	0	5	5	5	392.6	184.6	125.0
			3	3	3	2	2	2	994.8	200.9	290.1
			3	3	3	3	3	3	928.8	194.3	256.9
			3	3	3	5	5	5	820.1	182.3	209.0
			3	3	3	10	10	10	634.4	157.9	142.5
			5	5	5	2	2	2	8315.3	199.1	765.8
			5	5	5	3	3	3	5218.4	192.6	570.8
			5	5	5	5	5	5	2990.7	180.8	378.2
			5	5	5	10	10	10	1446.7	156.8	205.2
	0.3	0.3	3	3	3	2	2	2	759.0	136.9	127.8
			3	3	3	3	3	3	720.0	133.9	120.8
			3	3	3	5	5	5	652.9	128.3	108.8
			5	5	5	2	2	2	1829.2	131.4	157.1
			5	5	5	3	3	3	1617.9	128.7	146.6
			5	5	5	5	5	5	1314.4	123.5	129.3

MULTINOMIAL PROPORTION ESTIMATION USING HIGHER ORDER MOMENTS

Table 1 (continued): Relative efficiencies, $RE(k)$, $k=1,2,3$, of Proposed Estimators for Difference Choices of Known Higher Order Moments of the Three Scrambling Variables

π_1	π_2	π_3	γ_{300}	γ_{030}	γ_{003}	γ_{400}	γ_{040}	γ_{004}	$RE(1)$	$RE(2)$	$RE(3)$
0.5	0.1	0.4	-2	-2	-2	2	2	2	272.2	270.1	113.7
			-2	-2	-2	3	3	3	267.0	257.7	108.2
			0	0	0	2	2	2	398.2	329.1	205.3
			0	0	0	3	3	3	387.3	310.9	188.1
			0	0	0	5	5	5	367.1	280.0	161.1
			0	0	0	10	10	10	324.8	224.2	118.5
			3	3	3	5	5	5	1020.9	388.1	3115.4
			3	3	3	10	10	10	749.6	288.6	392.0
	0.2	0.3	0	0	0	2	2	2	377.2	192.5	122.2
			0	0	0	3	3	3	367.3	186.4	115.8
			0	0	0	5	5	5	349.2	175.3	104.7
			3	3	3	2	2	2	928.5	214.9	305.8
			3	3	3	3	3	3	871.1	207.3	268.4
			3	3	3	5	5	5	775.3	193.7	215.7
			3	3	3	10	10	10	608.2	166.4	144.7
			5	5	5	3	3	3	10163.3	224.1	2219.8
			5	5	5	5	5	5	4162.8	208.3	735.2
			5	5	5	10	10	10	1681.3	177.1	275.1
	0.3	0.2	3	3	3	2	2	2	720.8	143.1	129.9
			3	3	3	3	3	3	685.8	139.8	122.4
			3	3	3	5	5	5	625.0	133.7	109.8
			5	5	5	2	2	2	2216.4	144.9	197.4
			5	5	5	3	3	3	1915.3	141.5	180.6
			5	5	5	5	5	5	1506.2	135.3	154.4
			5	5	5	10	10	10	981.8	121.8	113.3

Table 1 (continued): Relative efficiencies, $RE(k)$, $k = 1, 2, 3$, of Proposed Estimators for Difference Choices of Known Higher Order Moments of the Three Scrambling Variables

π_1	π_2	π_3	γ_{300}	γ_{030}	γ_{003}	γ_{400}	γ_{040}	γ_{004}	$RE(1)$	$RE(2)$	$RE(3)$
0.6	0.1	0.3	0	0	0	2	2	2	365.7	299.5	157.2
			0	0	0	3	3	3	356.4	284.4	146.7
			0	0	0	5	5	5	339.2	258.3	129.5
			3	3	3	5	5	5	1068.8	447.1	12053.1
			3	3	3	10	10	10	773.7	320.0	424.2
	0.2	0.2	3	3	3	2	2	2	967.3	230.9	334.1
			3	3	3	3	3	3	904.8	222.2	288.7
			3	3	3	5	5	5	801.3	206.7	227.1
			3	3	3	10	10	10	623.1	175.9	148.0
			5	5	5	10	10	10	2651.1	203.3	446.3
	0.3	0.1	3	3	3	2	2	2	742.9	149.8	132.7
			3	3	3	3	3	3	705.5	146.2	124.6
			3	3	3	5	5	5	641.0	139.5	110.9
			5	5	5	2	2	2	4297.9	161.4	279.0
			5	5	5	3	3	3	3289.0	157.2	245.3
			5	5	5	5	5	5	2238.2	149.5	197.4
			5	5	5	10	10	10	1244.3	133.2	132.7
0.7	0.1	0.2	0	0	0	2	2	2	348.7	274.8	126.9
			0	0	0	3	3	3	340.1	262.0	119.7
			0	0	0	5	5	5	324.1	239.7	107.6
			3	3	3	10	10	10	880.7	359.0	488.1
	0.2	0.1	3	3	3	2	2	2	1147.2	249.6	385.8
			3	3	3	3	3	3	1058.8	239.4	324.1
			3	3	3	5	5	5	917.4	221.5	245.5
			3	3	3	10	10	10	687.8	186.5	152.9
			5	5	5	10	10	10	36398.8	238.8	1620.7
0.8	0.1	0.1	0	0	0	2	2	2	343.5	253.9	105.3
			3	3	3	10	10	10	1177.1	408.8	624.8

$RE(3)$ is 207.3% and 426.9%. Thus, for this case the minimum values of the relative efficiencies $RE(1)$, $RE(2)$ and $RE(3)$ are 615.3%, 207.3% and 426.9%, while the maximum values are 3543.1%, 451.1% and 713.4% respectively.

Consider another situation: If one of the attributes is rare, $\pi_1 = 0.1$, and the second attribute is moderate, $\pi_2 = 0.3$, then $\pi_3 = 0.6$ and based on 11 observations, the average relative efficiencies $RE(1)$, $RE(2)$ and $RE(3)$ remain as 1311.77%, 161.59%, 168.35% with standard deviations 742.70%, 37.46% and 58.19% respectively as the values different parameters of the scrambling variables changes. The medians of the relative efficiencies $RE(1)$, $RE(2)$ and $RE(3)$ remain 994.9%, 161.9% and 150.0%. The minimum values of the relative efficiencies $RE(1)$, $RE(2)$ and $RE(3)$ are 593.6%, 114.5% and 107.0% while the maximum values are 2928.3%, 220.8% and 282.2% respectively.

By contrast, when all three variables have moderate prevalence over the population as $\pi_1 = 0.3$, $\pi_2 = 0.3$ and $\pi_3 = 0.4$ then, based on 10 observations, the average relative efficiencies $RE(1)$, $RE(2)$ and $RE(3)$ remain as 911.53%, 137.22%, 117.67% with standard deviations 558.53%, 20.52% and 8.19% respectively as the values different parameters of the scrambling variables changes. The medians of the relative efficiencies $RE(1)$, $RE(2)$ and $RE(3)$ remain 785.35%, 129.90% and 166.00%. The minimum values of the relative efficiencies $RE(1)$, $RE(2)$ and $RE(3)$ are 365.90%, 113.60% and 108.1% while the maximum values are 1921.10%, 170.40% and 132.40% respectively (see Table 1).

Note that in Table 1 the $RE(1)$, $RE(2)$ and $RE(3)$ for $\pi_1 = 0.1$, $\pi_2 = 0.1$ and $\pi_3 = 0.8$ are not the same as for $\pi_1 = 0.8$, $\pi_2 = 0.1$ and $\pi_3 = 0.1$ because of different choices of mean and variances of the scrambling variables for the three categories. Further note that the choice of parameters considered herein, shows in majority when π_1 remains close to zero, for example $\pi_1 = 0.1$ and $\pi_2 = 0.1$ there are three situations where the proposed method remains efficient

and as soon as π_1 becomes 0.8 the proposed method shows efficiency only in two situations.

Thus, the proposed randomization device should be considered for a situation when the first attribute is rare, the second attribute is moderate and the third attribute is widespread. It may be concluded that the proposed randomized response technique based on higher order moments of the scrambling variables can be used to estimate multinomial proportions. The choice of the scrambling variables for a particular study may require an expert to decide based on simulation studies or past experience. The FORTRAN codes used in the simulation study are provided in Appendix A.

Generalization to the Case of a Multinomial Distribution

Consider a population Ω consisting of m mutually exclusive groups such that $\Omega = \bigcup_{k=1}^m A_k$. Let π_k be the proportion of a sensitive attribute is the k^{th} group. Then extending the proposed randomized response model from Section 2, that a respondent belonging to the k^{th} group is requested to report a random number from the k^{th} scrambling variable S_k for $k = 1, 2, \dots, m$, then $(m-1)$ unbiased estimates of the population proportion π_k for $k = 1, 2, \dots, (m-1)$ are given by

$$\hat{\Pi}_{(m-1) \times 1} = (A^{-1})_{(m-1) \times (m-1)} Z_{(m-1) \times 1} \quad (4.1)$$

where

$$\hat{\Pi} = \begin{bmatrix} \hat{\pi}_1 \\ \hat{\pi}_2 \\ \vdots \\ \hat{\pi}_{m-1} \end{bmatrix},$$

$$Z = \begin{bmatrix} \frac{1}{n} \sum_{i=1}^n Z_i - E(S_m) \\ \frac{1}{n} \sum_{i=1}^n Z_i^2 - E(S_m^2) \\ \vdots \\ \frac{1}{n} \sum_{i=1}^n Z_i^{m-1} - E(S_m^{m-1}) \end{bmatrix}$$

and

$A =$

$$\begin{bmatrix} E(S_1) - E(S_m), E(S_2) - E(S_m), \dots, E(S_{m-1}) - E(S_m) \\ E(S_1^2) - E(S_m^2), E(S_2^2) - E(S_m^2), \dots, E(S_{m-1}^2) - E(S_m^2) \\ E(S_1^{m-1}) - E(S_m^{m-1}), E(S_2^{m-1}) - E(S_m^{m-1}), \dots, E(S_{m-1}^{m-1}) - E(S_m^{m-1}) \end{bmatrix}$$

and, the unbiased estimate of the proportion π_m is given by

$$\hat{\pi}_m = 1 - \sum_{k=1}^{m-1} \hat{\pi}_k. \quad (4.2)$$

The variance of $\hat{\Pi}$ is given by

$$V(\hat{\Pi}) = (A^{-1})V(Z)(A^{-1})^t \quad (4.3)$$

and

$$V(\hat{\pi}_m) = \sum_{k=1}^{m-1} V(\hat{\pi}_k) + 2 \sum_{k < j=1}^{m-1} Cov(\hat{\pi}_k, \hat{\pi}_j) \quad (4.4)$$

where $V(Z)$ denotes the variance-covariance matrix of the scrambled responses which utilizes the higher order moments of the scrambling variables Z_i^l , $t = 1, 2, 3, \dots, m$.

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Appendix A: Theorems and Proofs

Theorem 2.1

An unbiased estimator of the population proportion π_1 is given by

$$\hat{\pi}_1 = \frac{\{(\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2)\} \left\{ \frac{1}{n} \sum_{i=1}^n Z_i - \theta_3 \right\} - (\theta_2 - \theta_3) \left\{ \frac{1}{n} \sum_{i=1}^n Z_i^2 - (\gamma_{002} + \theta_3^2) \right\}}{\Delta} \quad (2.6)$$

Theorem 2.1 Proof

Solving (2.2) and (2.4) for π_1 and using the method of moments proves the theorem.

Theorem 2.2

An unbiased estimator of the population proportion π_2 is given by

$$\hat{\pi}_2 = \frac{(\theta_1 - \theta_3) \left\{ \frac{1}{n} \sum_{i=1}^n Z_i^2 - (\gamma_{002} + \theta_3^2) \right\} - \{(\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2)\} \left\{ \frac{1}{n} \sum_{i=1}^n Z_i - \theta_3 \right\}}{\Delta} \quad (2.7)$$

Theorem 2.2 Proof

Solving (2.2) and (2.4) for π_2 and using the method of moments proves the theorem.

Theorem 2.3

An unbiased estimator of the population proportion π_3 is given by

$$\hat{\pi}_3 = 1 - \hat{\pi}_1 - \hat{\pi}_2. \quad (2.8)$$

Theorem 2.3 Proof

Theorem 2.3 is proven by taking expected values on both sides of (2.8).

Based on these theorems and proofs, the following lemmas are put forth.

Lemma 2.1

The variance of Z_i is given by

$$V(Z_i) = A_1\pi_1 + A_2\pi_2 + A_{11}\pi_1(1-\pi_1) + A_{22}\pi_2(1-\pi_2) + A_{12}\pi_1\pi_2 + A_{00} \quad (2.9)$$

where

$$A_1 = (\gamma_{200} - \gamma_{002}),$$

$$A_2 = (\gamma_{020} - \gamma_{002}),$$

$$A_{00} = \gamma_{002},$$

$$A_{11} = (\theta_1 - \theta_3)^2,$$

$$A_{22} = (\theta_2 - \theta_3)^2$$

and

$$A_{12} = -2(\theta_1 - \theta_3)(\theta_2 - \theta_3).$$

Lemma 2.2

The variance of Z_i^2 is given by

$$V(Z_i^2) = B_1\pi_1 + B_2\pi_2 + B_{11}\pi_1(1-\pi_1) + B_{22}\pi_2(1-\pi_2) + B_{12}\pi_1\pi_2 + B_{00} \quad (2.10)$$

where

$$B_1 = (\gamma_{400} - \gamma_{004}) + 4(\gamma_{300}\theta_1 - \gamma_{003}\theta_3) + 6(\gamma_{200}\theta_1^2 - \gamma_{002}\theta_3^2) + (\theta_1^4 - \theta_3^4) + (\gamma_{002} + \theta_3^2)^2 - (\gamma_{200} + \theta_1^2)^2$$

$$B_2 = (\gamma_{040} - \gamma_{004}) + 4(\gamma_{030}\theta_2 - \gamma_{003}\theta_3) + 6(\gamma_{020}\theta_2^2 - \gamma_{002}\theta_3^2) + (\theta_2^4 - \theta_3^4) + (\gamma_{002} + \theta_3^2) - (\gamma_{020} + \theta_2^2)^2$$

$$B_{11} = [(\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2)]^2,$$

$$B_{22} = [(\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2)]^2$$

$$B_{12} =$$

$$-2\{(\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2)\}\{(\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2)\}$$

and

$$B_{00} = (\gamma_{004} + 4\gamma_{003}\theta_3 + 4\gamma_{002}\theta_3^2 - \gamma_{002}^2).$$

Lemma 2.2 Proof

Based on the definition of variance,

$$\begin{aligned} V(Z_i^2) &= E(Z_i^4) - \{E(Z_i^2)\}^2 \\ &= (\gamma_{400} + 4\gamma_{300}\theta_1 + 6\gamma_{200}\theta_1^2 + \theta_1^4)\pi_1 \\ &\quad + (\gamma_{040} + 4\gamma_{030}\theta_2 + 6\gamma_{020}\theta_2^2 + \theta_2^4)\pi_2 \\ &\quad + (1-\pi_1-\pi_2)(\gamma_{004} + 4\gamma_{003}\theta_3 + 6\gamma_{002}\theta_3^2 + \theta_3^4) \\ &\quad - \left[\pi_1(\gamma_{200} + \theta_1^2) + \pi_2(\gamma_{020} + \theta_2^2) \right. \\ &\quad \left. + (1-\pi_1-\pi_2)(\gamma_{002} + \theta_3^2) \right]^2 \end{aligned}$$

which, on rearranging reduces to (2.10), and proves the lemma.

Lemma 2.3

The covariance between Z_i and Z_i^2 is given by

$$\begin{aligned} Cov(Z_i, Z_i^2) &= C_1\pi_1 + C_2\pi_2 + C_{11}\pi_1(1-\pi_1) \\ &\quad + C_{22}\pi_2(1-\pi_2) + C_{12}\pi_1\pi_2 + C_{00} \end{aligned} \quad (2.11)$$

where

$$\begin{aligned} C_1 &= (\gamma_{300} - \gamma_{003}) + 3(\theta_1\gamma_{200} - \theta_3\gamma_{002}) \\ &\quad + (\theta_1^3 - \theta_3^2) - \theta_3\{(\gamma_{200} + \theta_1^2) \\ &\quad - (\gamma_{002} + \theta_3^2)\} - (\theta_1 - \theta_3)(\gamma_{200} + \theta_1^2) \end{aligned}$$

$$\begin{aligned} C_2 &= (\gamma_{030} - \gamma_{003}) + 3(\theta_2\gamma_{020} - \theta_3\gamma_{002}) \\ &\quad + (\theta_2^3 - \theta_3^2) - \theta_3\{(\gamma_{020} + \theta_2^2) \\ &\quad - (\gamma_{002} + \theta_3^2)\} - (\theta_2 - \theta_3)(\gamma_{020} + \theta_2^2) \end{aligned}$$

$$C_{11} = (\theta_1 - \theta_3)\{(\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2)\},$$

$$C_{22} = (\theta_2 - \theta_3) \{(\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2)\}$$

$$C_{12} = (\theta_2 - \theta_3) \{(\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2)\} \\ + (\theta_1 - \theta_3) \{(\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2)\}$$

and

$$C_{00} = (\gamma_{003} + 2\theta_3\gamma_{002}).$$

Lemma 2.3 Proof

Based on the definition of covariance,

$$\begin{aligned} Cov(Z_i, Z_i^2) &= E(Z_i^3) - E(Z_i)E(Z_i^2) \\ &= (\gamma_{300} + 3\theta_1\gamma_{200} + \theta_1^3)\pi_1 \\ &\quad + (\gamma_{030} + 3\theta_2\gamma_{020} + \theta_2^3)\pi_2 \\ &\quad + (\gamma_{003} + 3\theta_3\gamma_{002} + \theta_3^3)(1 - \pi_1 - \pi_2) \\ &\quad - \left[\begin{aligned} &\{ \pi_1\theta_1 + \pi_2\theta_2 + (1 - \pi_1 - \pi_2)\theta_3 \} \\ &\times \left\{ \begin{aligned} &\pi_1(\gamma_{200} + \theta_1^2) + \pi_2(\gamma_{020} + \theta_2^2) \\ &+ (1 - \pi_1 - \pi_2)(\gamma_{002} + \theta_3^2) \end{aligned} \right\} \end{aligned} \right] \end{aligned}$$

which, on rearranging, reduces to (2.11) and proves the lemma.

Consider the following theorems:

Theorem 2.4

The variance of the unbiased estimator $\hat{\pi}_1$ of the population proportion π_1 is given by

$$V(\hat{\pi}_1) =$$

$$\begin{aligned} &\left[\begin{aligned} &\pi_1 \left\{ \begin{aligned} &\left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right)^2 A_1 + B_1(\theta_2 - \theta_3)^2 \\ &- 2(\theta_2 - \theta_3) \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) C_1 \end{aligned} \right\} \\ &+ \pi_2 \left\{ \begin{aligned} &\left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right)^2 A_2 + B_2(\theta_2 - \theta_3)^2 \\ &- 2(\theta_2 - \theta_3) \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) C_2 \end{aligned} \right\} \\ &+ \pi_1(1 - \pi_1) \left\{ \begin{aligned} &\left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) A_{11} + \\ &(\theta_2 - \theta_3)^2 B_{11} - 2(\theta_2 - \theta_3) \\ &\left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) C_{11} \end{aligned} \right\} \\ &+ \pi_2(1 - \pi_2) \left\{ \begin{aligned} &\left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) A_{22} \\ &+ (\theta_2 - \theta_3)^2 B_{22} - 2(\theta_2 - \theta_3) \\ &\left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) C_{22} \end{aligned} \right\} \\ &+ \pi_1\pi_2 \left\{ \begin{aligned} &\left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) A_{12} + \\ &(\theta_2 - \theta_3)^2 B_{12} - 2(\theta_2 - \theta_3) \\ &\left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) C_{12} \end{aligned} \right\} \\ &+ \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) A_{00} + \\ &(\theta_2 - \theta_3)^2 B_{00} - 2(\theta_2 - \theta_3) \\ &\left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) C_{00} \end{aligned} \right] \end{aligned}$$

(2.12)

Theorem 2.4 Proof

Based on the definition of variance,

$$V(\hat{\pi}_1) =$$

$$\begin{aligned} &\left[\begin{aligned} &\{ (\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \}^2 \sum_{i=1}^n V(Z_i) \\ &+ (\theta_2 - \theta_3)^2 \sum_{i=1}^n V(Z_i^2) - 2(\theta_2 - \theta_3) \{ (\gamma_{020} + \theta_2^2) \\ &- (\gamma_{002} + \theta_3^2) \} \sum_{i=1}^n Cov(Z_i, Z_i^2) \end{aligned} \right] \end{aligned}$$

Using the lemmas, the following theorems are put forth.

Theorem 2.5

The variance of the unbiased estimator $\hat{\pi}_2$ of the population proportion π_2 is given by

$$V(\hat{\pi}_2) = \frac{1}{n\Delta^2} \left[\begin{aligned} & \pi_1 \left\{ \begin{aligned} & A_1 \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right)^2 \\ & + B_1 (\theta_1 - \theta_3)^2 - 2(\theta_1 - \theta_3) \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) C_1 \end{aligned} \right\} \\ & + \pi_2 \left\{ \begin{aligned} & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right)^2 \\ & A_2 + (\theta_1 - \theta_3)^2 B_2 - 2(\theta_1 - \theta_3) \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) C_2 \end{aligned} \right\} \\ & + \pi_1(1 - \pi_1) \left\{ \begin{aligned} & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right)^2 \\ & A_{11} + (\theta_1 - \theta_3)^2 B_{11} - 2(\theta_1 - \theta_3) \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) C_{11} \end{aligned} \right\} \\ & + \pi_2(1 - \pi_2) \left\{ \begin{aligned} & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right)^2 \\ & A_{22} + (\theta_1 - \theta_3)^2 B_{22} - 2(\theta_1 - \theta_3) \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) C_{22} \end{aligned} \right\} \\ & + \pi_1 \pi_2 \left\{ \begin{aligned} & (\theta_1 - \theta_3)^2 B_{12} + \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right)^2 \\ & A_{12} - (\theta_1 - \theta_3) \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) C_{12} \end{aligned} \right\} \\ & + A_{00} \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right)^2 \\ & + B_{00} (\theta_1 - \theta_3)^2 - 2(\theta_1 - \theta_3) \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) C_{00} \end{aligned} \right] \quad (2.13)$$

Theorem 2.6

The covariance between the unbiased estimators $\hat{\pi}_1$ and $\hat{\pi}_2$ is given by

$$Cov(\hat{\pi}_1, \hat{\pi}_2) = \frac{1}{n\Delta^2} \left[\begin{aligned} & \pi_1 \left\{ \begin{aligned} & C_1 \Psi - B_1 (\theta_1 - \theta_3) (\theta_2 - \theta_3) \\ & - A_1 \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) \end{aligned} \right\} \\ & + \pi_2 \left\{ \begin{aligned} & C_2 \Psi - B_2 (\theta_1 - \theta_3) (\theta_2 - \theta_3) \\ & - A_2 \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) \end{aligned} \right\} \\ & + \pi_1(1 - \pi_1) \left\{ \begin{aligned} & C_{11} \Psi - B_{11} (\theta_1 - \theta_3) (\theta_2 - \theta_3) \\ & - A_{11} \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) \end{aligned} \right\} \\ & + \pi_2(1 - \pi_2) \left\{ \begin{aligned} & C_{22} \Psi - B_{22} (\theta_1 - \theta_3) (\theta_2 - \theta_3) \\ & - A_{22} \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) \end{aligned} \right\} \\ & + C_{00} \Psi - B_{00} (\theta_1 - \theta_3) (\theta_2 - \theta_3) \\ & - A_{00} \left\{ \begin{aligned} & \left((\gamma_{020} + \theta_2^2) \right) \left\{ (\gamma_{200} + \theta_1^2) \right\} \\ & \left[-(\gamma_{002} + \theta_3^2) \right] \left[-(\gamma_{002} + \theta_3^2) \right] \end{aligned} \right\} \end{aligned} \right] \quad (2.14)$$

where

$$\Psi = (\theta_1 - \theta_3) \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) + (\theta_2 - \theta_3) \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right)$$

Theorem 2.5 Proof

Based on the definition of variance,

$$V(\hat{\pi}_2) = \frac{1}{n^2 \Delta^2} \left[\begin{aligned} & (\theta_1 - \theta_3)^2 \sum_{i=1}^n V(Z_i^2) + \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right)^2 \sum_{i=1}^n V(Z_i) \\ & - 2(\theta_1 - \theta_3) \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) \\ & \sum_{i=1}^n Cov(Z_i, Z_i^2) \end{aligned} \right]$$

Theorem 2.6 Proof

Based on the definition of covariance,

$$\begin{aligned}
 \text{Cov}(\hat{\pi}_1, \hat{\pi}_2) &= \\
 &= \frac{\text{Cov} \left[\begin{aligned} & \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) \\ & \sum_{i=1}^n Z_i - (\theta_2 - \theta_3) \sum_{i=1}^n Z_i^2, (\theta_1 - \theta_3) \\ & \sum_{i=1}^n Z_i^2 - \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) \sum_{i=1}^n Z_i \end{aligned} \right]}{n^2 \Delta^2} \\
 &= \frac{1}{n^2 \Delta^2} \left[\begin{aligned} & (\theta_1 - \theta_3) \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) \text{Cov}(Z_i, Z_i^2) \\ & - (\theta_1 - \theta_3)(\theta_2 - \theta_3) \sum_{i=1}^n \text{Cov}(Z_i^2, Z_i^2) \\ & - \left((\gamma_{020} + \theta_2^2) - (\gamma_{002} + \theta_3^2) \right) \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) \\ & \sum_{i=1}^n \text{Cov}(Z_i, Z_i) + (\theta_2 - \theta_3) \\ & \left((\gamma_{200} + \theta_1^2) - (\gamma_{002} + \theta_3^2) \right) \sum_{i=1}^n \text{Cov}(Z_i, Z_i^2) \end{aligned} \right]
 \end{aligned}$$

These lemmas result in theorem 2.7.

Theorem 2.7

The variance of the unbiased estimator $\hat{\pi}_3$ of the parameter π_3 is given by

$$V(\hat{\pi}_3) = V(\hat{\pi}_1) + V(\hat{\pi}_2) + 2\text{Cov}(\hat{\pi}_1, \hat{\pi}_2) \quad (2.15)$$

Theorem 2.7 Proof

Theorem 2.7 is proved based on the definition of variance.

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Empirical Sampling from Permutation Space with Unique Patterns

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The exact distribution of a test statistic ultimately guarantees that the probability of a Type I error is exactly α . Several methods for estimating the exact distribution of a test statistic have evolved over the years with inherent computational problems and varying degrees of accuracy. The unique pattern of permutations resulting from using experimental data to sample within the permutation space without the risk of repeating permutations is identified. The method presented circumvents the theoretical requirements of asymptotic procedures and the computational difficulties associated with an exhaustive enumeration of permutations. Results show that time and space complexities are drastically reduced without compromising accuracy even when enumeration is not exhaustive provided error tolerance is achieved. The exact distribution of the Siegel-Tukey test statistic is examined as an illustration.

Key words: Algorithm, exact test, permutation test, bootstrap, resampling.

Introduction

The first edition of Fisher (1935) contains descriptions of two tests of significance that depend on permutation: Fisher's exact test for analyzing categorical data, and the permutation test for the difference between means. Many studies have been designed to confirm the asymptotic equivalence of permutation and classical tests (Ludbrook, 1994). Fisher wrote that "the statistician does not carry out this very simple and very tedious process, but his conclusions have no justification beyond the fact that they agree with those which could have been arrived at by this elementary method" (1936, p 59). Ernst (2004) noted that with fast computers there is little reason for a statistician not to carry out this very tedious process.

The main problem with permutation tests is that their null distributions are generally very difficult to express in closed form and to calculate exactly. This is because they depend

on a specific data set; thus they vary as the data varies in the sample space, however, for several test statistics involving ranks, the null distributions only need to be computed once. For large sample sizes, direct calculations are practically impossible due to the very large cardinality of associated permutation sample spaces. For example, a data set consisting of four treatments with five observations per treatment, $n_i = 5$, $i = 1(1)4$, demands as many as

$$\frac{\left(\sum_{i=1}^4 n_i\right)!}{\prod_{i=1}^4 (n_i!)} = \frac{20!}{5!5!5!5!} = 11,732,745,024$$

configurations for an exhaustive enumeration of all permutations. Pesarin (2001) stated that, unless sample sizes are very large, the approximation of such distributions by means of asymptotic arguments is not always appropriate. No general agreement exists regarding how large a sample should be before applying asymptotic approximation (Fahoome, 2000). Pesarin (2001) observed that the algorithms for exact calculations are generally based on direct calculus of upper tail probabilities; a strategy which may become highly impractical, if not

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impossible, in multivariate problems because there is no general computing routine useful to identify the critical regions. This was also observed by Hall and Weierserman (1997). In the early years of research into exact statistical inference, Scheffé (1943) clearly identified the fact that the permutation approach is the only way of constructing the exact distribution of a test statistic.

To avoid the computational difficulty in exact permutation tests, the conditional Monte Carlo (CMC) method was adopted by Pesarin (2001). In CMC replicate resampling is conducted without-replacement on the given data set, which is considered as playing the role of a finite population, provided that sample sizes are finite. According to Opdyke (2003), all existing permutation procedures developed to date can perform conventional Monte Carlo sampling without replacement within a sample but none can avoid the possibility of drawing the same sample more than once. The consideration given by Odiase and Ogbonmwan (2007) is an exception but involves a complete enumeration of all the distinct permutations, which becomes impracticable when the sample size is large.

In this study, the unique pattern of each permutation resulting from experimental data is identified and exploited in sampling from the permutation space without the attendant risk of repeating permutations. The method presented circumvents the elaborate theoretical requirements of asymptotic procedures and the logical and computational difficulties associated with an exhaustive enumeration of permutations.

Exhaustive Permutation Procedures

The process of obtaining permutations begins by choosing the test statistic T and the acceptable significance level α . Let $\pi_1, \pi_2, \dots, \pi_N$ be a set of all distinct permutations of the observations or ranks of the observations in the experiment. Compute the test statistic T_i for permutation π_i , that is, $T_i = T(\pi_i)$. Construct an empirical cumulative distribution for T as:

$$p_0 = p(T \leq T_i) = \frac{1}{N} \sum_{i=1}^N \psi(t_0 - T_i),$$

where

$$\psi(\cdot) = \begin{cases} 1, & \text{if } t_0 \geq T_i \\ 0, & \text{if } t_0 < T_i \end{cases}.$$

Under the empirical distribution, if $p_0 \leq \alpha$, reject the null hypothesis.

Paired Permutation

Given two paired samples $X = (x_1, x_2, \dots, x_n)$ and $Y = (y_1, y_2, \dots, y_n)$, suppose a sample of n units from the population distribution F_X is paired with a sample of n units from the population distribution F_Y and are simultaneously tested in an experiment with T as the test statistic. For k distinct values of the test statistic T , the probability distribution of the test statistic $T = (T_1, T_2, \dots, T_k)$ under the null hypothesis $H_0 : F_X = F_Y$ is given by

$$P(T_j = t_0 | H_0) = \sum_{i=1}^{f_j} \binom{2^{-n}}{i} = f_j \cdot \binom{2^{-n}}{1},$$

where f_j is the number of occurrences of T_j . For specified value of n and the level of significance α , the critical value c corresponds to a level closest to α . Ordering all the distinct occurrences of T in ascending order of magnitude, and if g is the position of the observed value of T , then the following significance level for the left tail of the distribution of the test statistic is

$$\alpha = P(T_g \leq c | H_0) = \sum_{j=1}^g \sum_{i=1}^{f_j} \binom{2^{-n}}{i} = \binom{2^{-n}}{1} \sum_{j=1}^g f_j$$

and, for the right tail,

$$\alpha = P(T_g \geq c | H_0) = \binom{2^{-n}}{k} \sum_{j=g}^k f_j.$$

For a two-tailed test, the left and right tails are summed. If the distribution of the test statistic is symmetric, then

$$\sum_{j=1}^g f_j = \sum_{j=k-g+1}^k f_j.$$

The distribution of the test statistic is obtained by tabulating the distinct values of the statistic against their probabilities of occurrence in the complete enumeration (see Odiase & Ogbonmwan, 2007a for a detailed description of the implementation of the paired permutation algorithm). Given a balanced two-sample layout as

$$\begin{pmatrix} x_1 & y_1 \\ x_2 & y_2 \\ \vdots & \vdots \\ x_n & y_n \end{pmatrix},$$

where $x_i \in X$ and $y_j \in Y$. If $n = 4$, then, for a two-sample problem, the number of permutations is $\sum_{i=0}^n \binom{n}{i} = 2^n$.

The test statistic is computed for each permutation in the complete enumeration of the distinct permutations. The distribution of the test statistic is obtained by tabulating the distinct values of the statistic against their probabilities of occurrence in the complete enumeration, where all the permutations are equally likely.

Considering consecutive number of pairs for a given experiment, the growth rate of the permutations from $n-1$ pairs to n pairs in a two-sample paired permutation experiment is

$\frac{2^n}{2^{n-1}} = 2$, meaning that it doubles each time a single pair of observations is added.

Independent Samples Experiment

Given a multi-sample experiment with $X_i = (X_{i1}, X_{i2}, \dots, X_{in_i})^T$, $i = 1(1)p$ and $X_N = (X_1, X_2, \dots, X_p)$. Under the null hypothesis, X_N

is composed of $N = \sum_{i=1}^p n_i$ independent and

identically distributed random variables. An exhaustive permutation of the observations

yields $\frac{N!}{\prod_{i=1}^p [(n_i)!]}$ permutations of the N variates

of p subsets of size n_i , $i = 1(1)p$, which are equally likely and each has the conditional

probability $\left(\frac{N!}{\prod_{i=1}^p [(n_i)!]} \right)^{-1}$. Odiase and

Ogbonmwan (2005a) showed that the number of permutations for a two-sample experiment is

$\sum_{i=0}^n \binom{n_1}{i} \binom{n_2}{i}$, $n = \min(n_1, n_2)$. After obtaining

the permutations of a two sample experiment, find the number of ways to permute any n_3 elements of the combined $(n_1 + n_2 + n_3)$ variates of the three treatments. This yields:

$$\binom{n_1 + n_2 + n_3}{n_3} \sum_{i=0}^n \binom{n_1}{i} \binom{n_2}{i} = \left(\sum_{r=1}^3 n_r \right) \sum_{i=0}^n \binom{n_1}{i} \binom{n_2}{i}.$$

By following the same procedure as for the case of three treatments, a complete enumeration of the distinct permutations for a four-treatment experiment yields:

$$\left(\sum_{r=1}^4 n_r \right) \left(\sum_{r=1}^3 n_r \right) \sum_{i=0}^n \binom{n_1}{i} \binom{n_2}{i} = \prod_{j=3}^4 \left(\sum_{r=1}^j n_r \right) \sum_{i=0}^n \binom{n_1}{i} \binom{n_2}{i}.$$

Continuing in this manner, for $p \geq 3$ treatments, the distinct permutations are enumerated through the expression

$$\prod_{j=3}^p \left(\sum_{r=1}^j n_r \right) \sum_{i=0}^n \binom{n_1}{i} \binom{n_2}{i},$$

but

$$\sum_{i=0}^n \binom{n_1}{i} \binom{n_2}{i} = \left(\sum_{r=1}^2 n_r \right).$$

Therefore, in a p -sample problem, the number of distinct permutations is $\prod_{j=1}^p \binom{\sum_{r=1}^j n_r}{n_j}$ (Odiase &

Ogbonmwan, 2005b). Observe that, for the balanced case, the number of distinct permutations is

$$\prod_{j=1}^p \binom{jn}{n} \sum_{i=0}^n \binom{n}{i}^2 = \prod_{j=1}^p \binom{jn}{n}.$$

Again, considering consecutive number of treatments for a given experiment, the growth rate of the permutations from $p-1$ treatments to p treatments is

$$\frac{\prod_{j=1}^p \binom{jn}{n}}{\prod_{j=1}^{p-1} \binom{jn}{n}} = \binom{np}{n}.$$

Repeated Measures (Block) Permutation

Repeated measures ANOVA tests the equality of means and is used when all members of a random sample are measured under varying conditions. In the repeated measures design, each trial represents the measurement of the same characteristic under a different condition. Given the layout of a multi-sample ($n \times k$) experiment as

$$\begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} \end{pmatrix},$$

where x_{ij} is an observation in the j^{th} treatment and the i^{th} block and the total number of observations in the experiment is nk . Rank the observations for each row from 1 (smallest x_{ij} on row i) to k (largest x_{ij} on row i). Let the layout of the ranks (r_{ij}) of the observations x_{ij} be

$$L_R = \begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1k} \\ r_{21} & r_{22} & \cdots & r_{2k} \\ \vdots & \vdots & \vdots & \vdots \\ r_{n1} & r_{n2} & \cdots & r_{nk} \end{pmatrix}.$$

The data are arranged in k columns (treatments) and n rows (blocks), where each block contains k repeated observations. Obviously, there are $k!$ possible arrangements or permutations of each block and due to multiplication of choices, the entire layout of the $n \times k$ experiment requires $(k!)^n$ permutations of the observations to yield the exact distribution of a test statistic, with the permutations equally likely and each having the conditional probability $(k!)^{-n}$.

The first step in developing permutation algorithm is to formulate an initial configuration of the ranks of the variates of an experiment by taking the trivial configuration

	<i>Tr.1</i>	<i>Tr.2</i>	<i>Tr.3</i>	...	<i>Tr.k</i>
<i>Block1</i>	1	2	3	...	k
<i>Block2</i>	1	2	3	...	k
<i>Block3</i>	1	2	3	...	k
$\vdots$	$\vdots$	$\vdots$	$\vdots$	...	$\vdots$
<i>Block n</i>	1	2	3	...	k

because any configuration of the ranks can engender all the distinct permutations. The test statistic is computed for each permutation in the complete enumeration of all the distinct permutations. The distribution of the test statistic is obtained by tabulating the distinct values of the test statistic against their probabilities of occurrence in the complete enumeration.

Considering two consecutive numbers of blocks for a given experiment, the growth rate of the permutations from $n-1$ blocks to n blocks

is $\frac{(k!)^n}{(k!)^{n-1}} = k!$ and the growth rate of the

permutations from $k-1$ treatments to k

treatments is $\frac{(k!)^n}{[(k-1)!]^n} = k^n$ and clearly, $k!$

grows faster than k^n for a fixed n , and for a fixed

$k, k!$ is constant while k^n explodes as n increases. Therefore, the growth rate of the permutations is higher for a unit increase in blocks than a unit increase in treatments for a fixed number of treatments and the reverse is the case when it is the number of blocks that is fixed.

Sampling Permutations with Unique Patterns

Given the layout of a two-sample experiment as

$$\begin{pmatrix} x_1 & y_1 \\ x_2 & y_2 \\ \vdots & \vdots \\ x_{1n_1} & y_{n_2} \end{pmatrix},$$

where x_i and y_i are the i^{th} observations of the independent random samples X and Y respectively, arrange the combined samples in ascending order of magnitude and rank all the $m = n_1 + n_2$ observations from 1 (smallest) to m (largest). Let the layout of the ranks (r_{ij}) of the observations in a two-sample layout be

$$L_R = \begin{pmatrix} r_{11} & r_{21} \\ r_{12} & r_{22} \\ \vdots & \vdots \\ r_{1n_1} & r_{2n_2} \end{pmatrix}.$$

Under the null hypothesis, L_R is composed of m independent and identically distributed random variables and hence conditioned on the observed data set. An exhaustive permutation of the ranks yields $N = \frac{m!}{n_1!n_2!}$ permutations of the m ranks

of the variates of two subsets of sizes n_1 and n_2 , which are equally likely, each having the conditional probability N^{-1} .

The unique pattern of each permutation resulting from experimental data is identified by adopting the first sample, for example, in a two-sample problem. This is carried out by concatenating the ranks or indices of observations in the experiment in a particular manner that makes the pattern unique for every distinct permutation. The unique patterns

obtained are therefore exploited in sampling from the permutation space without the risk of repeating permutations already sampled. The benefit of this approach is that – even when enumeration is not exhaustive – the distribution of a test statistic can be obtained within a reasonable level of accuracy with reduced time and space complexities. This sampling approach therefore circumvents the elaborate theoretical requirements of asymptotic procedures and the logical and computational difficulties associated with an exhaustive enumeration of permutations.

Methodology

Let the initial configuration of the ranks of the variate in a two-sample experiment be L_R . The entire permutation space can be spanned by any of the permutations (configurations) of the observations or ranks of observations. In a two-sample problem, only one of the samples is required to define each permutation because it is obvious that the remaining variates are in the second sample.

In a two-sample experiment

$$\begin{pmatrix} x_1 & y_1 \\ x_2 & y_2 \\ \vdots & \vdots \\ x_{1n_1} & y_{n_2} \end{pmatrix},$$

where x_i and y_i are the i^{th} observations of the independent random samples X and Y respectively, arrange the combined samples in ascending order of magnitude and rank all the $m = n_1 + n_2$ observations from 1 (smallest) to m (largest) to arrive at L_R . For the original permutation and subsequent permutations, sort X such that $x_1 \leq x_2 \leq \dots \leq x_{n_1}$.

The variates are identified by their indices (1, 2, ..., m) or actual ranks, which are employed in obtaining the unique patterns. Attach 0 in front of the first nine indices or ranks (01, 02, ..., 09) to make each number two digits, leaving 10, 11, ..., 99 as they are and treat all the numbers as strings so that it will be possible to manipulate the numbers. Concatenate the indices or ranks of X and store as a single constant value. This now becomes the pattern of the

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given layout of the observations. (Concatenation is a standard operation in computer programming languages. It is the operation of joining two character strings end to end. In programming languages, string concatenation is a binary operation usually accomplished by putting a concatenation operator between two strings or operands.)

After a unique pattern is obtained, a resampling without replacement is carried out to obtain a random sample of n_I variates from the original combined sample of m variates. This is achieved by deleting points already selected at random. Again, sort the resampled n_I variates and concatenate their indices or ranks to obtain a pattern. Compare this pattern with previously obtained patterns and store it only if it is unique, otherwise, resample without replacement again until a unique pattern is obtained. The chosen test statistic is computed for each unique permutation and the probability distribution of the test statistic is constructed. Finally, compute the cumulative probability distribution of the test statistic, T , under the null hypothesis and obtain the p -values such that the probability of making a Type I error is exactly α .

As an illustration, consider an $n \times k$ experiment with $n = 2$ treatments (X, Y) and $k = 5$ variates in each treatment could have the trivial configuration or permutation of ranks represented as

X	Y
1	6
2	7
3	8
4	9
5	10

Using the methodology presented, the permutation is written as

X	Y
01	06
02	07
03	08
04	09
05	10

a total of $\frac{10!}{5! \times 5!} = 252$ permutations are

required for an exhaustive enumeration of all the distinct or unique permutations. The process starts thus: The entire permutation space can be spanned by the trivial permutation (configurations) of the observations or ranks of observations, any other permutation from the permutation space can also be adopted to span all the unique permutations. In a two-sample problem, only one of the samples (X) is required to define each permutation because it is clear that the remaining variates are in the second sample.

The first permutation pattern is 0102030405. Assuming resampling from the permutation space yields $X = \{8, 3, 5, 2, 6\}$, then the second permutation pattern is obtained by first sorting to have $\{2, 3, 5, 6, 8\}$, leading to the pattern 0203050608. Resampling again, given $\{2, 10, 5, 9, 8\}$, the third permutation pattern is 0205080910. The resampling process continues until either all the patterns are enumerated for small samples or the error tolerance is achieved for large samples. See Table 1 for an exhaustive

enumeration of the $\frac{10!}{5! \times 5!} = 252$ permutation

patterns for this illustration.

For very small samples, an exhaustive enumeration of all the unique permutations is achieved with the sampling method described. When sample size is large, enumeration of permutations does not need to be exhaustive. Instead, a subset of the permutation space (for example, 2,000) is obtained and the probability distribution of the test statistic is constructed. Take a second sample of same size and fuse it into the earlier distribution to obtain an updated probability distribution and compare with the earlier distribution. With a given level of error

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Table 1: Exhaustive Enumeration of Unique Permutation Patterns for $n = 2, k = 5$

0102030405	0304050710	0103050709	0405070809	0304070810	0105060708
0203050608	0206070809	0105060910	0102030408	0203060708	0405060708
0106070809	0102030910	0102040910	0205080910	0102060810	0102030506
0104050809	0102050609	0102060709	0204050708	0304060708	0506080910
0104080910	0102030709	0304050709	0102040608	0206070810	0305060710
0104060708	0205060809	0104060809	0102030510	0204050610	0102070809
0203040708	0104060710	0306070809	0307080910	0102040609	0102040710
0507080910	0103040508	0103040810	0305080910	0103040507	0102040709
0203060810	0306070810	0203040510	0205070810	0105080910	0106080910
0102060710	0103050610	0204070910	0103050810	0203060809	0204050809
0102030409	0102030407	0204060708	0506070809	0102050910	0205070910
0304050910	0405060910	0102060809	0103060910	0104060709	0103040506
0203040508	0205060910	0205060810	0103060709	0204060910	0203040610
0304050708	0104070809	0103050710	0105060710	0102030509	0304050609
0102030607	0406080910	0304050809	0103040708	0203050910	0204080910
0203040810	0104070910	0102040509	0104050910	0203050609	0304070809
0103060710	0103040608	0406070809	0103050609	0107080910	0104070810
0106070810	0204050910	0305060708	0203040609	0102030609	0106070910
0405060710	0304060910	0304050610	0103040609	0102050809	0102040506
0203040506	0102030406	0104050607	0204070810	0103070810	0203040509
0102040610	0304060809	0102040810	0103050708	0405060709	0203060910
0203040607	0104050709	0204050709	0102080910	0206080910	0102030810
0205060710	0103040809	0103060708	0203060710	0405060809	0204060710
0104050609	0102060910	0104050710	0102070910	0103060810	0304080910
0103060809	0203050607	0102040507	0102030708	0203040709	0204050810
0105060709	0207080910	0304070910	0204050710	0203070809	0103040710
0102040508	0305060809	0103050809	0102030410	0103040607	0205060709
0105070810	0103040510	0405070910	0405060810	0607080910	0204060809
0102030710	0102070810	0203080910	0204060810	0406070910	0405070810
0203050809	0203060709	0204060709	0103080910	0105070809	0204050607
0102030507	0103070809	0102050607	0103050910	0104050810	0105070910
0203040608	0204050609	0104060810	0203040809	0103070910	0102040607
0103040610	0103050607	0206070910	0102040809	0506070910	0304060709
0305060810	0306080910	0203040710	0105060809	0102060708	0203050709
0102050710	0203070910	0304060710	0104060910	0304050608	0102030608
0203050610	0102030508	0102030809	0406070810	0103050608	0204070809
0102030610	0203040507	0405080910	0102040708	0105060810	0103040509
0305060910	0205070809	0103040709	0304050607	0203040910	0203050708
0306070910	0305070910	0102040510	0304060810	0305070809	0203070810
0204050608	0205060708	0103040910	0304050810	0407080910	0102050608
0305060709	0104050608	0104050610	0203050810	0506070810	0102050610
0305070810	0104050708	0203050710	0102050708	0102050709	0102050810

tolerance, if the error tolerance is exceeded, another sample is taken and fused into the last update of the probability distribution to obtain another update and again compared with the previous update of the probability distribution. This process is continued until the error tolerance is achieved. Compare for every occurrence of the test statistic in the last two updates using the error tolerance as a guide and proceed to update the probability distribution if the error tolerance is not met. Compute the cumulative probability distribution of the Test Statistic, T , under the null hypothesis and obtain the p-values such that the probability of making a type I error is exactly α .

Unique Permutation Pattern Test Procedure

Let $\pi_1, \pi_2, \dots, \pi_N$ be a set of all distinct permutations of the ranks of the data set in the experiment. The unique permutation pattern test procedure is as follows:

1. Read the original layout of observations.
2. Rank the combined observations of the experiment in (1) to obtain $L_R = \pi_1$ and compute the observed value of T statistic to obtain $T_1 = t_0$.
3. Store pattern of (1) or (2).
4. Obtain a distinct permutation π_i , of the ranks (L_R) from (3) by sampling without replacement.
5. Obtain pattern of (4) and compare with previous patterns. If different, store pattern, if already exists, go to (4).
6. Compute the T statistic $T_i = T(\pi_i)$, for permutation π_i in (5), where $i > 1$; update probability distribution.
7. Perform (4) to (6) for $i = 2, 3, \dots, k \leq N$. If sample size (N) is large,
 - a) Assume a level of error tolerance (0.00001) and take a subset of size $k = 1,000$ of the permutation space to obtain

the probability distribution of the test statistic.

- b) Take another subset of size k from the permutation space and fuse into the earlier probability distribution to obtain an updated distribution. Compare this distribution with the earlier distribution of the test statistic for every value of the test statistic.
 - c) If the error tolerance is exceeded for any value of the test statistic, go back to (b); continue this process until the error tolerance is achieved.
8. Construct the empirical cumulative probability distribution for the distinct values of T and extract critical values.

$$p_0 = p(T \leq T_i) = \frac{1}{k} \sum_{i=1}^k \psi(T_i - t_0),$$

where

$$\psi(T_i - t_0) = \begin{cases} 1, & \text{if } T_i \leq t_0 \\ 0, & \text{if } T_i > t_0 \end{cases}.$$

9. Under the empirical distribution, if $p_0 \leq \alpha$, reject the null hypothesis.

In a two-sample problem, only one of the samples is important in the generation of permutation patterns because it is unique for each permutation, that is,

$$\binom{m}{n_1} = \binom{m}{n_2} = \frac{m!}{n_1! n_2!}, \quad m = n_1 + n_2.$$

To provide exact critical values when ties occur, midranks are assigned as the ranks of tied observations, and the algorithm is implemented with r_{ij} as input, composed of actual ranks containing ties. Tabulated exact critical values of a test statistic are usually provided for experiments with distinct observations, because it will be practically difficult to consider all possible occurrences of ties and create tables of exact critical values for each occurrence of ties

for different sample sizes. This will result in several volumes of tables. In order to arrive at the critical values (see Table 2), the ranks of distinct observations (r_{ij}) were used as input in Algorithm for various sample sizes. See Appendix A for the unique permutation pattern algorithm. This algorithm identifies and compiles the unique permutation patterns of the layout of observations or rank of observations in a two-sample experiment. It is illustratively implemented to produce a table of critical values for the Siegel-Tukey test statistic

Siegel-Tukey Test

The Siegel-Tukey test is similar in procedure to the Wilcoxon Rank Sum test for difference in location. It is based on the logic that if two samples come from populations with the same median, the one with the greater variability will have more extreme scores. The hypotheses for a two-tailed test are:

H_0 : There is no difference in spread
between the two populations

versus

H_1 : There is some difference in spread
between the two populations.

The two samples are combined and ordered in ascending order of magnitude, keeping track of sample membership. For $m = n_1 + n_2$, the ranking proceeds as follows: $\alpha(1) = 1$, $\alpha(m) = 2$, $\alpha(m-1) = 3$, $\alpha(2) = 4$, $\alpha(3) = 5$, $\alpha(m-2) = 6$, $\alpha(m-3) = 7$, $\alpha(4) = 8$, the ranking continues to alternate from lowest to highest, ranking two scores at each end. It tests for differences in scale between two groups.

Critical Values for the Siegel-Tukey Test Statistic

Figures 1a-1b illustrate that the normal distribution will poorly approximate the exact distribution of the Siegel-Tukey (S-T) test statistic for very small sample sizes. As group sample size increases, the shape of the distribution of the S-T test begins to look more

like the normal distribution as shown in Figures 1c-1d. The critical values of the S-T test statistic shown in Table 2 were obtained from the enumeration of all distinct permutations of the ranks of the observations in an experiment ($m, n < 20$) combined with the idea of resampling while ensuring an error tolerance level ($m, n \geq 20$). These critical values ensure that the probability of a Type I error in decisions arising from the use of the S-T test is exactly α .

Results obtained from asymptotic procedures and resampling techniques are commonly adopted in several nonparametric tests as alternatives to tabulated exact critical values. Fahoome (2002) conducted a Monte Carlo study and recommended the asymptotic approximation of the S-T test when group sample sizes exceed 25, based on conservative estimates of $0.045 < \text{Type I error rate} < 0.055$ for $\alpha = 0.05$; other authors recommended higher or lower sample sizes.

Conclusion

The critical values for a test statistic are determined by cutting off the most extreme $100\alpha\%$ of the theoretical frequency distribution of the test statistic, where α is the level of significance (Siegel & Castellan, 1988). Classical methods require that the theoretical distribution of the test statistic should agree with a mathematically definable frequency distribution, this often leads to a probability of Type I error greater than α , particularly when sample sizes are small. The cost of such an error might be too high to risk. Therefore, the exact permutation paradigm methodology presented in this study is of value because it guarantees that the probability of a Type I error is exactly α with the attendant advantage of no distributional assumptions apart from the exchangeability of the observations. When sample sizes are large and it becomes practically difficult or impossible to construct the probability distribution, permutation sampling becomes very useful because it quickly converges to the actual distribution; Scheffe (1943) opined that this is the only sure way of constructing the exact distribution of a test statistic.

EMPIRICAL SAMPLING FROM PERMUTATION SPACE WITH UNIQUE PATTERNS

Figure 1: Exact Distribution of Siegel-Tukey Test Statistic (S-T) for Different Sample Sizes with their Large Sample Approximations (Z)

— S-T - - - - Z

(a)
 $n_1 = 4, n_2 = 4$

— S-T - - - - Z

(b)
 $n_1 = 6, n_2 = 6$

— S-T - - - - Z

(c)
 $n_1 = 8, n_2 = 8$

— S-T - - - - Z

(d)
 $n_1 = 15, n_2 = 15$

Figure 2: Distribution of Siegel-Tukey Test Statistic with Error Tolerance = 0.00001 for Different Sample Sizes

(a)
 $n_1 = 20, n_2 = 20$

(b)
 $n_1 = 30, n_2 = 30$

(c)
 $n_1 = 40, n_2 = 40$

(d)
 $n_1 = 50, n_2 = 50$

EMPIRICAL SAMPLING FROM PERMUTATION SPACE WITH UNIQUE PATTERNS

Figure 3: Distribution of Siegel-Tukey Test Statistic for Different Levels of Error Tolerance ($n_1 = 15, n_2 = 15$)

(a)
2 Iterations

(b)
5 Iterations

(c)
36 Iterations

(d)
339 Iterations

Figure 4: Distribution of Siegel-Tukey Test Statistic for Different Number Samples ($n_1 = 15, n_2 = 15$)

(a)
103 Iterations

(b)
82 Iterations

(c)
50 Iterations

(d)
36 Iterations

EMPIRICAL SAMPLING FROM PERMUTATION SPACE WITH UNIQUE PATTERNS

Table 2: Lower and Upper Critical Values for the Siegel-Tukey Test Statistic

Sample Size n_1 n_2	$ST_{0.9000}$	$ST_{0.9500}$	$ST_{0.9750}$	$ST_{0.9900}$	$ST_{0.9950}$	$ST_{0.9975}$	$ST_{0.9990}$
3 2	6 12						
3 3	7 14	6 15					
4 2	11 17						
4 3	12 20	11 21					
4 4	13 23	12 24	11 25				
5 2	17 23	16 24					
5 3	18 27	17 28	16 29				
5 4	20 30	18 32	17 33	16 34			
5 5	21 34	20 35	18 37	17 38	16 39	16 39	
6 2	23 31	22 32					
6 3	25 35	24 36	23 37				
6 4	27 39	25 41	24 42	23 43	22 44		
6 5	29 43	27 45	25 47	24 48	23 49	22 50	
6 6	31 47	29 49	27 51	25 53	24 54	23 55	
7 2	30 40	29 41					
7 3	33 44	31 46	30 47	29 48			
7 4	35 49	33 51	32 52	30 54	29 55		
7 5	37 54	35 56	34 57	32 59	30 61	29 62	
7 6	40 58	37 61	35 63	33 65	32 66	31 67	29 69
7 7	42 63	40 65	37 68	35 70	33 72	32 73	30 75
8 2	39 49	38 50	37 51				
8 3	42 54	40 56	39 57	37 59			
8 4	44 60	42 62	41 63	39 65	38 66	37 67	
8 5	47 65	45 67	43 69	41 71	39 73	38 74	37 75

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Table 2 (continued): Exact Critical Values for Siegel-Tukey Test Statistic

Sample Size n_1 n_2	$ST_{0.9000}$	$ST_{0.9500}$	$ST_{0.9750}$	$ST_{0.9900}$	$ST_{0.9950}$	$ST_{0.9975}$	$ST_{0.9990}$
8 6	50 70	47 73	45 75	43 77	41 79	40 80	38 82
8 7	53 75	50 78	47 81	44 84	43 85	41 87	39 89
8 8	56 80	52 84	50 86	46 90	44 92	43 93	41 95
9 2	48 60	47 61	46 62				
9 3	51 66	49 68	48 69	47 70	46 71		
9 4	55 71	52 74	50 76	49 77	47 79	46 80	
9 5	58 77	55 80	53 82	51 84	49 86	48 87	47 88
9 6	61 83	58 86	56 88	53 91	51 93	50 94	48 96
9 7	64 89	61 92	58 95	55 98	53 100	51 102	49 104
9 8	68 94	64 98	61 101	57 105	55 107	53 109	51 111
9 9	71 100	67 104	63 108	60 111	57 114	55 116	53 118
10 10	88 122	83 127	79 131	75 135	72 138	69 141	66 144
11 11	107 146	101 152	97 156	92 161	88 165	85 168	82 171
12 12	128 172	121 179	116 184	110 190	106 194	103 197	99 201
13 13	150 201	143 208	137 214	131 220	126 225	122 229	118 233
14 14	175 231	167 239	161 245	153 253	148 258	144 262	138 268
15 15	201 264	193 272	185 280	177 288	172 293	167 298	161 304
20 20	362 458	349 471	338 482	325 495	316 504	308 512	298 522
30 30	828 1002	804 1027	783 1047	759 1071	743 1088	728 1102	710 1121
40 40	1487 1754	1449 1791	1417 1824	1380 1861	1354 1886	1331 1910	1303 1937
50 50	2339 2711	2286 2764	2241 2809	2189 2861	2153 2898	2122 2930	2082 2970

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Appendix A: Unique Permutation Pattern Algorithm

This computer algorithm identifies and compiles the unique permutation patterns of the layout of observations or rank of observations in a two-sample experiment. It was implemented to produce a table of critical values for the Siegel-Tukey test statistic.

Algorithm (Permutation)

Two-Sample problem: Unique Permutation Patterns

Assign ranks to the observations based on sample size

```

1:  $N \leftarrow N1 + N2$ 
2: for  $I \leftarrow 1, N$  do
3:    $X_I \leftarrow I$ 
4:   if  $I \leq N1$  then
5:      $X2_I \leftarrow X_I$ 
6:   end if
7: end for
8:  $K \leftarrow 1$ 
   Determine the number of permutations to be sampled
9:  $P1 \leftarrow 1 : P2 \leftarrow 1 : P3 \leftarrow 1$ 
10: for  $I \leftarrow 1, N$  do
11:   if  $I \leq N1$  then
12:      $P1 \leftarrow P1 * I$ 
13:   end if
14:   if  $I > N1$  then
15:      $P2 \leftarrow P2 * (I - N1)$ 
16:   end if
17:    $P3 \leftarrow P3 * I$ 
18: end for
19:  $P \leftarrow P3 / (P1 * P2)$ 
20: Call Pattern
21: Compute Test Statistic  $PP$  and update frequency  $FREQ$ 
   Resample without replacement
22: for  $K \leftarrow 2, P$  do
23:    $CHECK \leftarrow 1$ 
24:   while  $CHECK \leftarrow 1$  do
25:     for  $I \leftarrow 1, N$  do
26:        $X1_I \leftarrow X_I$ 
27:     end for
28:     for  $I \leftarrow 1, N1$  do
29:        $NT \leftarrow N - I + 1$ 
30:        $S \leftarrow INT(NT * RND + 1)$ 
31:        $X2_I \leftarrow X1_S$ 
32:       for  $J \leftarrow S, NT$  do
33:          $X1_J \leftarrow X1_{J+1}$ 
34:       end for

```

Appendix A (continued): Unique Permutation Pattern Algorithm

```

35:     end for
36:     Call Pattern
        Ensure no repetition of permutations
37:      $CHECK \leftarrow 0$ 
38:     for  $I1 \leftarrow 1, K - 1$  do
39:         if  $PAT_K \leftarrow PAT_{I1}$  then
40:              $CHECK \leftarrow 1$ 
41:         end if
42:     end for
43:     if  $CHECK \leftarrow 1$  then
44:          $PAT_K \leftarrow ""$ 
45:     end if
46: end while
47: Compute Test Statistic  $PP$  and update frequency  $FREQ$ 
48: end for
49: Sort  $PP_I$  in ascending order for  $I \leftarrow 1, COUNT1$ 
50: PRINT  $N1, N2$ 
51:  $PV \leftarrow 0$ 
52: for  $I \leftarrow 1, COUNT1$  do
53:      $PDM \leftarrow FREQ_I / P$ 
54:      $PV \leftarrow PV + PDM$ 
55:     PRINT  $PP_I, FREQ_I, PDM, PV$ 
56: end for

```

Algorithm (Pattern)

```

1: Sort  $X2(I)$  for  $I \leftarrow 1, N1$  to have a unique pattern
2: for  $J \leftarrow 1, N1$  do
3:     if  $X2_J < 10$  then
4:          $PAT_K \leftarrow PAT_K + "0" + LTRIM(RTRIM(STR(X2_J)))$ 
5:     else  $PAT_K \leftarrow PAT_K + LTRIM(RTRIM(STR(X2_J)))$ 
6:     end if
7: end for

```


Appendix A (continued): Unique Permutation Pattern Algorithm

Algorithm (Permutation-Convergence)

Unique Permutation Patterns: Iterate to convergence
Assign ranks to the observations based on sample size

```

1:  $N \leftarrow N1 + N2$ 
2: for  $I \leftarrow 1, N$  do
3:    $X_I \leftarrow I$ 
4:   if  $I \leq N1$  then
5:      $X2_I \leftarrow X_I$ 
6:   end if
7: end for
8:  $BB \leftarrow 0$ 
9:  $CK \leftarrow 1$ 
10: Ensure error tolerance is achieved
11: while  $CK \leftarrow 1$  do
12:   for  $C0 \leftarrow 1, COUNT1$  do
13:      $FREQ_{C0} \leftarrow 0$ 
14:   end for
15:    $COUNT1 \leftarrow 0$ 
16:   for  $K \leftarrow 1, NN$  do
17:      $PAT_K \leftarrow ""$ 
18:   end for
19:    $BB \leftarrow BB + 1$ 
    Resample without replacement
20:   for  $K \leftarrow 1, NN$  do
21:      $CHECK \leftarrow 1$ 
      Ensure pattern is unique
22:     while  $CHECK \leftarrow 1$  do
23:       for  $I \leftarrow 1, N$  do
24:          $X1_I \leftarrow X_I$ 
25:       end for
26:       for  $I \leftarrow 1, N1$  do
27:          $NT \leftarrow N - I + 1$ 
28:          $S \leftarrow INT(NT * RND + 1)$ 
29:          $X2_I \leftarrow X1_S$ 
30:         for  $J \leftarrow S, NT$  do
31:            $X1_J \leftarrow X1_{J+1}$ 
32:         end for
33:       end for
34:       Sort  $X2_I$  to have a unique pattern

```

Appendix A (continued): Unique Permutation Pattern Algorithm

```

35:         Call Pattern
           Ensure no repetition of permutations
36:          $CHECK \leftarrow 0$ 
37:         for  $I1 \leftarrow 1, K - 1$  do
38:             if  $PAT_K \leftarrow PAT_{I1}$  then
39:                  $CHECK \leftarrow 1$ 
40:             end if
41:         end for
42:         if  $CHECK \leftarrow 1$  then
43:              $PAT_K \leftarrow ""$ 
44:         end if
45:     end while
46:     Compute Test Statistic  $PP$  and update frequency  $FREQ$ 
47: end for
48: Sort  $PP_I$  in ascending order for  $I \leftarrow 1, COUNT1$ 
   Merge and Update pdf
49: if  $BB > 1$  then
50:      $NP \leftarrow COUNT2 + COUNT1$ 
51:     for  $I \leftarrow 1, NP$  do
52:         if  $I \leq COUNT2$  then
53:              $UPD_I \leftarrow UPD1_I$ 
54:              $FREQ_I \leftarrow FREQ1_I$ 
55:         else
56:              $UPD_I \leftarrow PP_{I-COUNT2}$ 
57:              $FREQ_I \leftarrow FREQ2_{I-COUNT2}$ 
58:         end if
59:     end for
60:     for  $J \leftarrow 1, COUNT2$  do
61:         for  $I \leftarrow COUNT2 + 1, NP$  do
62:             if  $UPD_J \leftarrow UPD_I$  then
63:                  $FREQ_J \leftarrow FREQ_J + FREQ_I$ 
64:                 for  $T \leftarrow I, NP - 1$  do
65:                      $UPD_T \leftarrow UPD_{T+1}$ 
66:                      $FREQ_T \leftarrow FREQ_{T+1}$ 
67:                 end for
68:                  $NP \leftarrow NP - 1$ 
69:             end if
70:         end for
71:     end for
72:     Sort the update  $UPD$  in ascending order
73: else
    
```

Appendix A (continued): Unique Permutation Pattern Algorithm

```

74:       $NP \leftarrow COUNT1$ 
75:      for  $I2 \leftarrow 1, NP$  do
76:           $UPD_{I2} \leftarrow PP_{I2}$ 
77:           $FREQ_{I2} \leftarrow FREQ2_{I2}$ 
78:      end for
79:  end if
80:  Print Number of trials  $BB$ , Permutation Sample size  $NN$ , Sample1
     $N1$ , Sample2  $N2$ 
81:   $PV \leftarrow 0$ 
82:  for  $I \leftarrow 1, NP$  do
83:       $PDM_I \leftarrow FREQ_I / NN * BB$ 
84:       $PV \leftarrow PV + PDM_I$ 
85:      PRINT  $UPD_I, FREQ_I, PDM_I, PV$ 
86:  end for
    Check error tolerance
87:  if  $BB > 1$  then
88:       $CK \leftarrow 0$ 
89:      for  $I \leftarrow 1, COUNT2$  do
90:          for  $II \leftarrow 1, NP$  do
91:              if  $UPD1_I \leftarrow UPD_{II}$  And  $ABS(PDM1_I - PDM_{II}) >$ 
                 $TOL$  then
92:                   $CK \leftarrow 1$ 
93:              end if
94:          end for
95:      end for
96:  end if
    Store last iteration
97:  for  $I \leftarrow 1, NP$  do
98:       $UPD1_I \leftarrow UPD_I$ 
99:       $FREQ1_I \leftarrow FREQ_I$ 
100:      $PDM1_I \leftarrow PDM_I$ 
101:  end for
102:   $COUNT2 \leftarrow NP$ 
103: end while

```

A Weighted Exponential Detection Function Model for Line Transect Data

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A new parametric model is proposed for modeling the density function of perpendicular distances in line transects sampling. The model can be considered a weighted exponential model in the sense that it combines two exponential models with different weights. The proposed model is appealing because it is monotone decreasing with distance from transect line; in contrast to the classical exponential model, it satisfies the shoulder condition at the origin. Simulation results for a wide range of target densities show reasonable and good performances of the weighted exponential model in most considered cases compared to the classical exponential and the half-normal models.

Key words: Line transect sampling, exponential model, weighted exponential model, half-normal model.

Introduction

Transect methods, particularly line transect methods, are a practical and relatively inexpensive procedure for estimating the population density of certain objects in a given region; these methods have become a popular sampling scheme among ecologists. The estimation procedure can be achieved by walking distance L following a deterministic transect line, counting the number of objects being investigated and recording the perpendicular distance, X , from the object sighted to the path of the observer (line transect center). When objects are observed from a line transect with a detection function $g(x)$, the distance X to the observed object from a randomly placed transect will tend to have a probability density function (pdf) $f(x)$ of the same shape as $g(x)$, but scaled so that the area under $f(x)$ equals unity. Buckland, et al.

(2001) and Burnham, et al. (1980) are the key references for this distance sampling procedure.

The logical assumption related to the detection function $g(x)$ indicates that $g(x)$ is monotonically decreasing and satisfies the shape criterion (i.e., $g'(x) = 0$). Accordingly, $f(x)$ is in turn monotonically decreasing with $f'(0) = 0$. Burnham and Anderson (1976) gave the fundamental relation for estimating the density of objects in a specific area, which is expressed as

$$D = \frac{E(n)f(0)}{2L},$$

where $E(n)$ is the expected value of the number of detected objects. Given various assumptions (Burnham & Anderson, 1976) show that the general estimate for D is given by

$$\hat{D} = \frac{n\hat{f}(0)}{2L},$$

where $\hat{f}(0)$ is an appropriate sample estimator of $f(0)$ based on n observed perpendicular distances $x_1, x_2, \dots, x_n$. Thus, the key aspects in line transects sampling are the modeling of $f(x)$ and the estimation of $f(0)$.

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Let $f(x)$ be the unknown pdf of perpendicular distances $X_1, X_2, \dots, X_n$, which are usually assumed to be a random sample (Buckland, et al., 1993). A parametric approach involves assuming that $f(x)$ is a member of a family of proper pdf of a known functional form, but depends on an unknown parameter θ , where θ may take a vector value and should be estimated by using perpendicular distances. A variety of approaches to estimate θ will lead to $\hat{f}(0) = f(0, \hat{\theta})$.

A number of parametric models have been proposed for $f(x)$. The classical exponential model and the half normal model, each with one scale parameter, are the most prominent. Gates, et al. (1968) suggested the exponential model with detection function,

$$g_1(x) = e^{-x/\alpha}, \quad x \geq 0$$

and pdf,

$$f_1(x) = e^{-x/\alpha} / \alpha, \quad x \geq 0. \quad (1)$$

The maximum likelihood (ML) method indicates that the ML estimator of $f(0)$ is $\hat{f}_{1,ML}(0) = 1/\bar{X}$, where $\bar{X}$ is the sample mean. The detection function $g_1(x)$ (or the pdf $f_1(x)$) do not satisfy the shoulder condition which minimizes the importance of utilizing this model in line transect sampling. In contrast to the exponential model, the half normal model suggested by Hemingway (1971) satisfies the shoulder condition assumption. The half normal detection function is given by

$$g_2(x) = e^{-x^2/2\sigma^2}, \quad x \geq 0$$

and the pdf is,

$$f_2(x) = \frac{2}{\sigma\sqrt{2\pi}} e^{-x^2/2\sigma^2}, \quad x \geq 0. \quad (2)$$

The ML estimator of $f(0)$ is $\hat{f}_{2,ML}(0) = \left(\frac{2}{\pi T}\right)^{1/2}$ under the half normal

model, where $T = \sum_{i=1}^n x_i^2 / n$. Quinn and Gallucci (1980) derived the minimum variance unbiased estimator for $f(0)$ under Model (2), which is given by

$$\hat{f}_{2,MV}(0) = \frac{1}{\beta(n)} \left(\frac{2}{\pi T}\right)^{1/2},$$

where

$$\beta(n) = \frac{\Gamma((n-1)/2)}{\Gamma(n/2)} \left(\frac{n}{2}\right)^{1/2}.$$

Under Model (2), Zhang (2009) proposed the shrinkage estimator

$$\hat{f}_{2,SH}(0) = \frac{n-2}{n} \beta(n) \left(\frac{2}{\pi T}\right)^{1/2}.$$

The estimator $\hat{f}_{2,SH}(0)$ is biased for $f(0)$, but it achieves the smallest mean square error.

Comparing the estimators $\hat{f}_{2,ML}(0)$, $\hat{f}_{2,MV}(0)$ and $\hat{f}_{2,SH}(0)$ it is observed that

$$\begin{aligned} \hat{f}_{2,SH}(0) &= \frac{n-2}{n} \beta^2(n) \hat{f}_{2,MV}(0) \\ &= \frac{n-2}{n} \beta(n) \hat{f}_{2,ML}(0) \end{aligned}$$

Because $\beta(n) \rightarrow 1$ (Magnus, et al., 1966) and $\frac{n-2}{n} \rightarrow 1$ as $n \rightarrow \infty$, the three estimators are

asymptotically equivalent. A simulation study was performed using a finite sample for different target models; results indicate that the three estimators perform very similarly to each other, even for the target detection functions that are deviated from the half normal model. (For other parametric models with two parameters see: Burnham & Anderson (1976); Pollock, (1978);

Burnham, et al. (1980); Buckland (1985); Eidous (2004).

A weighted exponential model with one parameter is proposed to fit line transects data. Two estimators under this model are derived to estimate $f(0)$ and hence the density of objects, D . The small-sample properties of the new estimators were studied and compared to both the classical exponential and the half normal estimators via simulation techniques.

The Model

Let $X_1, X_2, \dots, X_n$ be n perpendicular distances (assumed to be independent and identically distributed) following the detection function $g(x; \theta, \gamma)$, where θ and γ are two unknown parameters. The detection function is proposed to be,

$$g(x; \theta, \gamma) = 2e^{-\theta x} - e^{-\gamma x}, \\ x \geq 0, \theta, \gamma > 0$$

According to this detection function, the probability of detecting an object given its perpendicular distance on the transect line is one (i.e., $g(0; \theta, \gamma) = 1$), which indicates that the probability of detecting on the line transect center is certain. However, the first derivative of $g(x; \theta, \gamma)$ at $x = 0$ is $-2\theta + \gamma$ (i.e. $g'(0; \theta, \gamma) = -2\theta + \gamma$), which indicates that $g(x; \theta, \gamma)$ do not satisfy the shoulder condition unless $\gamma = 2\theta$. Therefore, the detection function for the perpendicular distances that satisfies the shoulder condition is proposed to be,

$$g_3(x) = e^{-\theta x} (2 - e^{-\theta x}),$$

and the corresponding pdf is,

$$f_3(x) = \frac{2}{3\theta} e^{-\theta x} (2 - e^{-\theta x}), \quad x \geq 0, \theta > 0. \quad (3)$$

Because $g_3(0) = 1$, the parameter $f_3(0)$ is given by

$$f_3(0) = \frac{2}{3\theta}. \quad (4)$$

model (3) can be expressed in terms of $f_3(0)$ as

$$f_3(x) = f_3(0) e^{-3f_3(0)x/2} \left(2 - e^{-3f_3(0)x/2} \right), \\ x \geq 0 \quad (5)$$

It can be shown that the detection function $g_3(x)$ is monotonically decreasing in x . The first derivative of $g_3(x)$ is $g'_3(x) = 2\theta(e^{-2\theta x} - e^{-\theta x})$, which equals zero at $x = 0$; thus, $g_3(x)$ is monotonically decreasing for $x \in (0, \infty)$ if $2\theta(e^{-2\theta x} - e^{-\theta x}) < 0 \Rightarrow e^{-2\theta x} - e^{-\theta x} < 0 \Rightarrow e^{-2\theta x} < e^{-\theta x} \Rightarrow -2\theta x < -\theta x \Rightarrow 2\theta x > \theta x$, which is true for all $x > 0$ and $\theta > 0$. Accordingly $f_3(x)$ is monotonically decreasing for $x \in (0, \infty)$.

Moments and Maximum Likelihood Estimators

The parameter $f_3(0)$ in model (5) must be estimated. The expected value of X based on this model is $7/(9f_3(0))$, which gives $\hat{f}_{3,MO}(0) = 7/(9\bar{X})$ as the moment estimator for $f_3(0)$.

Although the moment estimator for $f_3(0)$ is given in a closed form, the maximum likelihood estimator must be calculated using a numerical method. The likelihood function $L(f)$ based on model (5) is

$$L(f) = \prod_{i=1}^n f_3(x_i) \\ = f_3(0)^n \exp(-3f_3(0) \sum_{i=1}^n \frac{x_i}{2}) \prod_{i=1}^n \left(2 - \exp(-\frac{3f_3(0)x_i}{2}) \right).$$

To find the maximum likelihood estimator of $f_3(0)$, the following equation must be solved

$$\frac{\partial \log L(f)}{\partial f} = 0,$$

where

$$\frac{\partial \log L(f)}{\partial f} = \frac{n}{f_3(0)} - \frac{3}{2} \sum_{i=1}^n x_i + \frac{3}{2} \sum_{i=1}^n \left(\frac{x_i}{2 \exp(3f_3(0)x_i/2) - 1} \right).$$

The maximum likelihood estimator can be found by using numerical methods such as the Newton-Raphson, and a Mathematica Program for carrying out the estimation procedure can be written. Let $\hat{f}_{3,ML}(0)$ be the maximum likelihood estimator of $f_3(0)$, then as $n \rightarrow \infty$, $\hat{f}_{3,ML}(0)$ is asymptotically $N(f_3(0), \sigma_f^2)$, where $\sigma_f^2 = \left\{ -E \left(\frac{d^2 \ln L(f)}{df^2} \right) \right\}^{-1}$. Using the transformation $u = 2 - \exp(-3f_3(0)x/2)$ results in,

$$\begin{aligned} -E \left(\frac{d^2 \ln L(f)}{df^2} \right) &= \frac{n}{f_3(0)^2} + \frac{9}{2} \sum_{i=1}^n E \left(\frac{X_i^2 \exp(-3f_3(0)X_i/2)}{(2 - \exp(-3f_3(0)X_i/2))^2} \right) \\ &= \frac{n}{f_3(0)^2} + \frac{4n}{3f_3(0)^2} \int_1^2 \frac{(2-u) \ln^2(2-u)}{u} du. \end{aligned}$$

The Mathematica Program was used to compute the last integral, which gives,

$$= \frac{0.80153 n}{f_3(0)^2}.$$

Therefore,

$$\sigma_f^2 = \frac{f_3(0)^2}{0.80153 n}.$$

Replacing $f_3(0)$ by $\hat{f}_{3,ML}(0)$ leads to the estimate $\hat{\sigma}_f^2$ of σ_f^2 and the approximate large-sample $(1 - \alpha)100\%$ confidence interval (C.I.) for $f_3(0)$ is given by

$$\hat{f}_{3,ML}(0) \pm Z_{\alpha/2} \sqrt{\hat{\sigma}_f^2}.$$

For example, if $\alpha = 0.05$, then $Z_{0.025} = 1.96$ and thus, a 95% C.I. for $f_3(0)$ is $\hat{f}_{3,ML}(0) \pm 2.18925 \hat{f}_{3,ML}(0) / \sqrt{n}$.

Methodology

To assess the performances of the proposed estimators $\hat{f}_{3,MO}(0)$ and $\hat{f}_{3,ML}(0)$ of $f(0)$ under the weighted exponential family, a simulation study was performed. For comparison, the classical exponential estimator $\hat{f}_{1,ML}(0)$ and the half normal estimator $\hat{f}_{2,ML}(0)$ were also considered. Four target models were chosen for inclusion in the simulation based on the criterion that they are representative of many different shapes that might occur in the field. These four models are:

- (1) Exponential Power (EP) Model (Pollock, 1978)

$$\begin{aligned} f(x) &= \frac{1}{\Gamma(1+1/\beta)} e^{-x^\beta}; \\ x &\geq 0, \quad \beta \geq 1 \end{aligned}$$

- (2) Hazard-Rate (HR) Model (Hayes and Buckland, 1983)

$$\begin{aligned} f(x) &= \frac{1}{\Gamma(1-1/\beta)} (1 - e^{-x^\beta}); \\ x &\geq 0, \quad \beta > 1 \end{aligned}$$

- (3) Beta (BE) Model (Eberhardt, 1968)

$$\begin{aligned} f(x) &= (1+\beta)(1-x)^\beta; \\ 0 &\leq x < 1, \quad \beta \geq 0 \end{aligned}$$

- (4) General Polynomial (GP) Model (Zhang, 2009)

$$\begin{aligned} f(x) &= \frac{10\Gamma(\beta)}{3\sqrt{\pi}\Gamma(\beta-1/2)} (1+(x/0.6)^2)^{-\beta} \\ x &\geq 0, \quad \beta > 1/2. \end{aligned}$$

Four models were selected from the following different models: EP, HR, BE and GP. For the EP model, parameter values $\beta = 1.0, 1.5, 2.0, 2.5$ and corresponding truncation points $w = 5.0, 3.0, 2.5, 2.0$. For the HR model with parameter values $\beta = 1.5, 2.0, 2.5, 3.0$ and corresponding truncation points $w = 20, 12, 8, 6$. The BE model parameter values $\beta = 1.5, 2.0, 2.5, 3.0$ and truncated point $w = 1.0$ for all cases. For the GP model parameter values $\beta = 0.6, 0.9, 1.9, 3.5$ and the truncated point $w = 3.0$ for all cases.

The 16 target models considered cover a wide range of perpendicular distance probability density functions that vary near zero from spike to flat. It should be noted that the EP model with $\beta = 1$ and the BE model with different values of β do not satisfy the shoulder condition assumption. These choices were made in order to assess the robustness of the considered estimators with respect to the violation of the shoulder condition assumption. Note also that the other considered models satisfy the shoulder condition assumption.

For each model 1,000 samples of perpendicular distances were randomly drawn for sample sizes $n = 50, 100, 200$. Table (1) reports the simulated value of the relative bias (RB) for each model and for each sample size,

$$RB = \frac{E(\hat{f}(0)) - f(0)}{f(0)},$$

and the relative mean error (RME)

$$RME = \frac{\sqrt{MSE(\hat{f}(0))}}{f(0)},$$

for each considered estimator.

Conclusion

Based on the simulation, several conclusions can be drawn by inspecting the results with respect to RB and RME .

- (1) The performance of the classical exponential estimator, $\hat{f}_{1,ML}(0)$ is effective when the target (underlying) model is exponential (EP with $\beta = 1$). In this case, the RB and RME associated with $\hat{f}_{1,ML}(0)$ were very small compared other considered estimators. However, the RB and RME of $\hat{f}_{1,ML}(0)$ become very large when the underlying model deviates from the exponential. The RME values of $\hat{f}_{1,ML}(0)$ range between 0.080 (EP with $\beta = 1$ and $n = 200$) and 0.732 (EP with $\beta = 2.5$ and $n = 50$).
- (2) The estimator $\hat{f}_{2,ML}(0)$ seems to be better than $\hat{f}_{1,ML}(0)$ for most considered cases. Regarding RME , $\hat{f}_{2,ML}(0)$ beats $\hat{f}_{1,ML}(0)$ for all considered cases except for (EP with $\beta = 1$ and HR with $\beta = 1.5$ and $\beta = 2$). Despite that HR satisfies the shoulder condition, it decreases very sharply away $x = 0$ when $\beta = 1.5$ and $\beta = 2$. This may explain the performances of $\hat{f}_{1,ML}(0)$ in these two cases. The performance of $\hat{f}_{2,ML}(0)$ is very good when the target model is half normal (EP with $\beta = 2$) and when the shoulder condition of the target model is very large (EP with $\beta = 2.5$ and HR with $\beta = 3$). Except for the cases: EP with $\beta = 1$, HR with $\beta = 1.5$ and $\beta = 2$, the performance of $\hat{f}_{2,ML}(0)$ is acceptable compared the other estimators. The RME values of $\hat{f}_{2,ML}(0)$ range from 0.052 (EP with $\beta = 2$ and $n = 200$) to 0.576 (EP with $\beta = 1.5$ and $n = 200$).

- (3) The RB and RME associated with the two proposed estimators $\hat{f}_{3,MO}(0)$ and $\hat{f}_{3,ML}(0)$ are very similar to each other in all considered cases. Therefore, $\hat{f}_{3,MO}(0)$ is recommended as opposed to $\hat{f}_{3,ML}(0)$ because the formal model takes a closed form, while $\hat{f}_{3,ML}(0)$ needs a numerical method to compute. Comparing the RME s of $\hat{f}_{3,MO}(0)$ and $\hat{f}_{2,ML}(0)$ it appears that $\hat{f}_{3,MO}(0)$ performs better than $\hat{f}_{2,ML}(0)$ in most cases. More specifically, if the shoulder condition of the target model seems to be large, then $\hat{f}_{2,ML}(0)$ beats $\hat{f}_{3,MO}(0)$ (e.g. EP with $\beta = 2, 2.5$ and HR with $\beta = 3$). Otherwise, $\hat{f}_{3,MO}(0)$ performs better than $\hat{f}_{2,ML}(0)$. The RME values of $\hat{f}_{3,MO}(0)$ range from 0.058 (GP with $\beta = 0.6$ and $n = 200$) to 0.357 (EP with $\beta = 2.5$ and $n = 50$). Comparing the range of RME for different estimators indicates that $\hat{f}_{3,MO}(0)$ is more stable than the other estimators.

Therefore, based on results in this study, it may be concluded that the weighted exponential model fits the line transect data reasonably and it can be recommended as a promising parametric model to estimate the parameter $f(0)$ and the population density D .

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WEIGHTED EXPONENTIAL DETECTION MODEL FOR LINE TRANSECT DATA

Table 1: RB and RME for Different Estimators when Data are Simulated from the Four Target Models

n	β	w	Estimator							
			$\hat{f}_{1,ML}(0)$		$\hat{f}_{2,ML}(0)$		$\hat{f}_{3,MO}(0)$		$\hat{f}_{3,ML}(0)$	
			RB	RME	RB	RME	RB	RME	RB	RME
Exponential Power (EP) Model										
50	1	5	0.055	0.154	-0.384	0.393	-0.179	0.211	-0.187	0.219
100			0.040	0.105	-0.393	0.397	-0.191	0.206	-0.187	0.204
200			0.041	0.080	-0.395	0.397	-0.190	0.198	-0.186	0.199
50	1.5	3	0.400	0.435	-0.133	0.166	0.089	0.159	0.089	0.155
100			0.391	0.408	-0.141	0.156	0.082	0.122	0.081	0.118
200			0.390	0.399	-0.142	0.149	0.081	0.103	0.078	0.102
50	2	2.5	0.593	0.617	0.017	0.104	0.239	0.274	0.248	0.281
100			0.590	0.602	0.015	0.073	0.236	0.254	0.243	0.261
200			0.580	0.586	0.008	0.052	0.229	0.238	0.233	0.242
50	2.5	2	0.711	0.732	0.118	0.155	0.331	0.357	0.345	0.373
100			0.697	0.708	0.109	0.132	0.320	0.334	0.330	0.343
200			0.695	0.700	0.105	0.117	0.318	0.325	0.326	0.331
Hazard Rate (HR) Model										
50	1.5	20	-0.120	0.199	-0.565	0.571	-0.316	0.339	-0.311	0.337
100			-0.126	0.169	-0.570	0.573	-0.320	0.332	-0.310	0.335
200			-0.131	0.152	-0.575	0.576	-0.324	0.329	-0.323	0.331
50	2	12	0.149	0.256	-0.409	0.427	-0.107	0.194	-0.128	0.215
100			0.126	0.187	-0.427	0.434	-0.124	0.164	-0.126	0.175
200			0.112	0.152	-0.437	0.441	-0.135	0.157	-0.127	0.149
50	2.5	8	0.387	0.443	-0.226	0.270	0.079	0.186	0.067	0.161
100			0.394	0.421	-0.231	0.252	0.084	0.143	0.083	0.139
200			0.374	0.386	-0.250	0.258	0.068	0.102	0.069	0.109
50	3	6	0.559	0.599	-0.074	0.169	0.213	0.270	0.236	0.294
100			0.559	0.579	-0.084	0.135	0.213	0.242	0.226	0.255
200			0.543	0.552	-0.099	0.122	0.200	0.215	0.213	0.227

Table 1 (continued): RB and RME for Different Estimators when Data are Simulated from the Four Target Models

n	β	w	Estimator							
			$\hat{f}_{1,ML}(0)$		$\hat{f}_{2,ML}(0)$		$\hat{f}_{3,MO}(0)$		$\hat{f}_{3,ML}(0)$	
			RB	RME	RB	RME	RB	RME	RB	RME
Beta (BE) Model										
50	1.5	1	0.410	0.436	-0.096	0.126	0.096	0.151	0.092	0.152
100			0.406	0.419	-0.099	0.115	0.093	0.124	0.103	0.134
200			0.403	0.410	-0.101	0.109	0.092	0.107	0.096	0.109
50	2	1	0.350	0.382	-0.148	0.171	0.050	0.130	0.067	0.134
100			0.336	0.352	-0.157	0.168	0.039	0.091	0.046	0.093
200			0.332	0.340	-0.158	0.163	0.036	0.066	0.041	0.072
50	2.5	1	0.297	0.332	-0.189	0.207	0.009	0.117	0.021	0.121
100			0.298	0.315	-0.189	0.198	0.010	0.080	0.010	0.075
200			0.289	0.298	-0.196	0.200	0.003	0.057	-0.000	0.054
50	3	1	0.263	0.301	-0.216	0.231	-0.018	0.115	-0.011	0.116
100			0.257	0.276	-0.221	0.229	-0.023	0.082	-0.023	0.080
200			0.256	0.267	-0.223	0.227	-0.023	0.061	-0.025	0.060
General Polynomial (GP) Model										
50	0.6	3	0.254	0.290	-0.220	0.243	0.030	0.117	0.033	0.123
100			0.245	0.262	-0.233	0.238	0.022	0.083	0.021	0.073
200			0.246	0.259	-0.217	0.229	0.018	0.058	0.014	0.061
50	0.9	3	0.189	0.243	-0.296	0.308	-0.075	0.141	-0.077	0.154
100			0.181	0.211	-0.302	0.308	-0.081	0.117	-0.095	0.128
200			0.170	0.187	-0.309	0.311	-0.090	0.108	-0.092	0.110
50	1.9	3	0.280	0.332	-0.262	0.289	-0.004	0.138	0.001	0.141
100			0.275	0.303	-0.276	0.289	-0.009	0.099	-0.011	0.101
200			0.267	0.283	-0.284	0.291	-0.015	0.074	-0.019	0.075
50	3.5	3	0.452	0.489	-0.118	0.174	0.129	0.194	0.121	0.191
100			0.435	0.454	-0.135	0.163	0.116	0.154	0.119	0.155
200			0.426	0.436	-0.140	0.154	0.109	0.130	0.120	0.142

Improved Estimator in the Presence of Multicollinearity

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The performances of two biased estimators for the general linear regression model under conditions of collinearity are examined and a new proposed ridge parameter is introduced. Using Mean Square Error (MSE) and Monte Carlo simulation, the resulting estimator's performance is evaluated and compared with the Ordinary Least Square (OLS) estimator and the Hoerl and Kennard (1970a) estimator. Results of the simulation study indicate that, with respect to MSE criteria, in all cases investigated the proposed estimator outperforms both the OLS and the Hoerl and Kennard estimators.

Key words: Regression, multicollinearity, ridge regression, Monte Carlo simulation.

Introduction

Multiple regression fits a model to predict a dependent variable (Y) from two or more independent variables (X):

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + e.$$

If the model fits the data well, the overall R^2 value will be high and the corresponding P value will be low. In addition to the overall P value, multiple regression also reports an individual P value for each independent variable; a low P value indicates that a particular independent variable significantly improves the fit of the model.

If the overall P value is very low, but all the individual P values are high, this indicates that a model fits the data well, even though none of the X variables has a statistically significant impact on predicting Y . This occurs when two or more variables are highly correlated. If both variables are removed from the model, the fit would be much worse; thus, the overall model fits the data but neither X variable makes a significant contribution when it is added to the

model last. When this occurs, the X variables are collinear and the results show multicollinearity, meaning the variables are related.

If the goal is simply to predict Y from a set of X variables, then multicollinearity is not problematic. The predictions will be accurate and the overall R^2 quantifies how well the model predicts the Y values. However, if the goal is to understand how the various X variables impact Y , then multicollinearity poses a big problem. These problems are summarized as:

- (1) The individual P values can be misleading, that is, a P value can be high, even though the variable is important.
- (2) The confidence intervals on the regression coefficients will be very wide – and may include zero – which indicates that a researcher cannot be confident whether an increase in X values is associated with an increase or decrease in Y values. In addition, wide confidence intervals can change the coefficients and/or their signs.

For these reasons, multicollinearity must be examined and removed. Different methods exist that can be used to reduce or to eliminate the impact of multicollinearity, examples include:

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- (1) Removing a variable: If one of the variables does not seem logically essential to the model, then removing it may be helpful.
- (2) Combining the variables; for example, if height and weight are collinear independent variables, then it would be logical to remove height and weight from the model and instead use a variable such as surface area (calculated from height and weight).
- (3) Increasing sample size: Another way to reduce the impact of collinearity is to increase sample size, this results in narrower confidence intervals, despite multicollinearity, with more data.
- (4) Using a standard technique called ridge regression: Ridge regression was originally developed to overcome multicollinearity.

Consider the standard linear regression model:

$$\vec{Y} = X\vec{\beta} + \vec{e}, \quad (1)$$

formulated to result in a $X'X$ in correlation form and where $X'Y$ is the vector of correlation coefficients of the dependent variable with each explanatory variable. Also assume that X is $n \times p$ of full rank $p < n$, $E(e) = 0$ and $E(ee') = \sigma^2 I_n$. The p - vector of the OLS estimator ($\vec{\beta}$), is then given by the solution of:

$$X'X\vec{\beta} = X'Y \quad (2)$$

so that,

$$\vec{\beta} = (X'X)^{-1} X'Y. \quad (3)$$

Clearly, $\vec{\beta}$ is an unbiased estimator of $\vec{\beta}$. There are many reasons why a data analyst is often not satisfied with OLS estimates. One of the reasons is prediction accuracy: OLS estimates often have low bias but large variance. Thus, prediction accuracy can occasionally be improved by shrinking some coefficients to zero.

In doing this, a little bias is sacrificed to reduce the variance of the predicted values and hence may improve overall prediction accuracy.

Many attempts have been made to improve the OLS estimator procedure. Hoerl and Kennard (1970a) suggested a new technique called ridge regression to improve OLS estimates. The ridge regression estimators $\vec{\beta}^*$, for a fixed $k > 0$, satisfy,

$$(X'X + kI_p)\vec{\beta}^* = X'Y, \quad (4)$$

so that,

$$\vec{\beta}^* = (X'X + kI_p)^{-1} X'Y, \quad (5)$$

as an alternative to the OLS estimator for use in the presence of multicollinearity, where I denotes an identity matrix, and k is a positive number known as ridge parameter, which must be estimated from the real data. The ridge regression MSE is given by:

$$\begin{aligned} MSE(\vec{\beta}^*) &= \sigma^2 \sum_{i=1}^p \frac{\lambda_i}{(\lambda_i + k_i)^2} + \sum_{i=1}^p \frac{k_i^2 \beta_i^2}{(\lambda_i + k_i)^2}, \\ &= \text{Variance} + (\text{Bias})^2, \end{aligned} \quad (6)$$

where σ^2 represents the error variance of the model given by (1). When the reduction in variance exceeds the square of the bias, ridge estimates are preferred.

When using ridge estimates, the choice of k -values in (5) is crucially important and several methods have been proposed for this purpose (see Hoerl & Kennard, 1970a; Saleh & Kibria, 1993; Singh & Tracy, 1999; Khalaf & Shuker, 2005; Alkhamisi & Shukur, 2008; Khalaf, 2011; Khalaf, 2011).

The Proposed Estimator

The general form of ridge regression suggested by Hoerl and Kennard (1970a) reduces $X'X$ to a diagonal matrix by applying an orthogonal transformation Q , thus,

$$Q(X'X)Q' = \Lambda,$$

where Q is a $p \times p$ orthogonal matrix, Λ is a diagonal matrix whose diagonal elements $\lambda_1, \lambda_2, \dots, \lambda_p$ are the eigenvalues of $X'X$. If $X^* = XQ'$ and $\alpha = Q\beta$, then model (1) may be rewritten as,

$$\vec{Y} = X^* \alpha + \vec{e},$$

where

$$(X^*)'(X^*) = \Lambda.$$

The general ridge estimation procedure is defined as,

$$\hat{\alpha}^* = ((X^*)'(X^*) + K)^{-1} (X^*)' \vec{Y}, \quad (7)$$

where K is a diagonal matrix with non-negative diagonal elements $k_1, k_2, \dots, k_p, k_i > 0$. It follows from Hoerl and Kennard (1970a) that the value of k_i which minimizes the MSE of $\hat{\alpha}^*$ given by:

$$MSE(\hat{\alpha}^*) = \sigma^2 \sum_{i=1}^p \frac{\lambda_i}{(\lambda_i + k_i)^2} + \sum_{i=1}^p \frac{k_i^2 \alpha_i^2}{(\lambda_i + k_i)^2},$$

is:

$$k_i = \frac{\sigma^2}{\alpha_i^2}, \quad (8)$$

where σ^2 represents the error variance of model (1) and α_i is the i^{th} element of $\vec{\alpha}$. Equation (8) gives a value of k_i that is fully dependent on the unknown σ^2 and α_i , and therefore must be estimated from observed data. Hoerl and Kennard (1970a) recommended replacing σ^2 and α_i by their corresponding unbiased estimators, that is:

$$\hat{k}_i = \frac{\hat{\sigma}^2}{\hat{\alpha}_i^2}, \quad (9)$$

where $\hat{\sigma}^2 = \frac{\sum_i e_i^2}{n-p}$ is the residual MSE, which is an unbiased estimator of σ^2 , and $\hat{\alpha}_i$ is the element of $\vec{\hat{\alpha}}$ which is an unbiased estimator of $\vec{\alpha}$. Hoerl and Kennard found that the best method for achieving a better estimator $\vec{\hat{\alpha}}^*$ is to use $k_i = k$ for all i , and they suggested k to be $\hat{k}_{HK}$ where:

$$\hat{k}_{HK} = \frac{\hat{\sigma}^2}{\max(\hat{\alpha}_i^2)}. \quad (10)$$

They showed that the estimator $\hat{k}_{HK}$ (HK) is sufficient to give ridge estimators with smaller MSEs than an OLS estimator. This article proposes a modification of the Hoerl and Kennard (1970a) estimator shown in (10) to obtain a new estimator, given by:

$$\begin{aligned} \hat{k}_{GK} &= \frac{\hat{\sigma}^2}{\max(\hat{\alpha}_i^2)} + \frac{1}{\frac{1}{2}(\lambda_{\max} + \lambda_{\min})}, \\ &= \frac{\hat{\sigma}^2}{\max(\hat{\alpha}_i^2)} + \frac{2}{(\lambda_{\max} + \lambda_{\min})}, \end{aligned} \quad (11)$$

where $\lambda_{\max}, \lambda_{\min}$, are the largest and smallest eigenvalues of the matrix $X'X$, respectively. This estimator will be denoted by GK. Because $\frac{2}{\lambda_{\max} + \lambda_{\min}} > 0$, then GK is greater than HK.

Monte Carlo Simulation

Monte Carlo simulation was used to investigate the properties of the considered estimators. It is convenient to make the comparison among the OLS estimator, HK estimator given by (10) and the new proposed GK estimator given by (11). These choices were made for many reasons: First is that; interest herein lies in studying the properties of the proposed GK estimator as an alternative to the OLS estimator in the presence of multicollinearity. Second, GK is a modified version of HK, so it is necessary to make a

comparison between them. Finally, the HK estimator was the first ridge estimator proposed among all other estimators, therefore, most studies comparing ridge estimators consider the HK estimator.

A comparison was made based on MSE criterion. Following McDonald and Galarneau (1975), Wichern and Churchill (1978), Gibbons (1981) and Kibria (2003), the explanatory variables were generated using the device:

$$\begin{aligned} x_{ij} &= (1 - \rho^2)^{\frac{1}{2}} z_{ij} + \rho z_{ip}, \\ i &= 1, 2, \dots, n, \\ j &= 1, 2, \dots, p. \end{aligned} \quad (12)$$

where z_{ij} are independent standard normal pseudo-random numbers, ρ is specified so that the correlation between any two explanatory variables is given by ρ^2 and p is the number of explanatory variables. Once more, the variables are standardized so that $X'X$ and $X'Y$ are in correlation forms. Four sets of correlations were considered corresponding to $\rho = 0.7, 0.8, 0.9$ and 0.99 . Using the condition number, $CN = \frac{\lambda_{\max}}{\lambda_{\min}}$, it can be shown that these values of ρ will include a wide range of low, moderate and high correlations between variables. The n observations for the dependent variable Y are determined by:

$$\begin{aligned} Y_i &= \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \dots + \beta_p X_{ip} + e_i, \\ i &= 1, 2, \dots, n \end{aligned}$$

where e_i are independent normal $(0, \sigma^2)$ pseudo-numbers and β_0 is considered identically zero without loss of generality. Three different sample sizes, $n = 20, 30, 50$ were used with 10, 15 and 20 explanatory variables, respectively. These choices of p were chosen to study the behavior of the estimators for small,

moderate and large number of explanatory variables.

The parameter values were chosen so that $\sum_{j=1}^p \beta_j^2 = 1$, which is a common restriction in simulation studies (see Muniz & Kibria, 2009). For given values of p, n and ρ , the experiment was repeated 5,000 times by generating 5,000 samples. For each replicate r ($r = 1, 2, \dots, 5,000$) the values of k different proposed estimators and the corresponding ridge estimators were calculated using:

$$\hat{\alpha}^* = (\Lambda + \hat{k}I)^{-1} X'^* \bar{Y}, \quad (13)$$

where $\hat{k} = HK, GK$. The MSE for the estimators were calculated as follows:

$$MSE(\hat{\alpha}^*) = \frac{1}{5000} \sum_{r=1}^{5000} (\bar{\alpha}_r^* - \bar{\alpha})' (\bar{\alpha}_r^* - \bar{\alpha}). \quad (14)$$

Results

The results of the simulations that compared the MSE to the other estimators are summarized in Tables 1-3. To compare the performances of the considered estimators, the MSE was calculated for each. The estimator that resulted in the minimum MSE was considered to be the best. The statistics package Minitab 14 was used for all calculations.

Tables 1-3 show that both HK and GK are better than the OLS estimator, and the GK estimator performs better than the HK estimator. This also reveals that for low correlation, $r = 0.7$, the performance of the GK estimator is slightly better than the HK estimator. Moreover, it was observed that, for given n and p , the MSE for all estimators increased as the correlation among the explanatory variables increased. Conversely, as the sample size and the number of explanatory variables increase, the MSE of all estimators decreased.

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Table 1: Estimated MSE and the values of CN with $p = 10$ and $n = 20$.

	ρ	0.99	0.9	0.8	0.7
	CN	980.58	90.17	44.24	18.93
Estimators	OLS	0.03877	0.02844	0.02147	0.01679
	HK	0.03453	0.02613	0.02015	0.01611
	GK	0.02820	0.02241	0.01826	0.01393

Table 2: Estimated MSE and the values of CN with $p = 15$ and $n = 30$.

	ρ	0.99	0.9	0.8	0.7
	CN	2834.43	255.92	89.68	64.19
Estimators	OLS	0.01886	0.01299	0.00933	0.00738
	HK	0.01822	0.01275	0.00922	0.00733
	GK	0.01641	0.01112	0.00875	0.00701

Table 3: Estimated MSE and the values of CN with $p = 20$ and $n = 50$.

	ρ	0.99	0.9	0.8	0.7
	CN	25266.30	2235.51	945.37	399.63
Estimators	OLS	0.01454	0.00922	0.00665	0.00505
	HK	0.01416	0.00910	0.00660	0.00503
	GK	0.00694	0.00436	0.00320	0.00488

Conclusion

Several procedures for constructing ridge estimators have been proposed in the literature. These procedures aim at a rule for selecting the constant k in equation (13). The best method for estimating k remains an unsolved problem and no constant value of k is certain to yield an estimator that is uniformly better in terms of MSE than the OLS estimators in all cases.

This study investigated the properties of a newly proposed method for estimating the ridge parameter (k) in the presence of

multicollinearity. The investigation used Monte Carlo experiments, where levels of correlation, numbers of explanatory variables and sample sizes were varied. Each combination was replicated 5,000 times. The evaluation of the new estimator was accomplished by comparing the MSE of this estimator with the OLS estimator and the Hoerl and Kennard (1970a) estimator. Results show that the proposed estimator uniformly dominates the other estimators.

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New Approximate Bayesian Confidence Intervals for the Coefficient of Variation of a Gaussian Distribution

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Confidence intervals are constructed for the coefficient of variation of a Gaussian distribution. Considering the square error and the Higgins-Tsokos loss functions, approximate Bayesian models are derived and compared to a published classical model. The models are shown to have great coverage accuracy. The classical model does not always yield the best confidence intervals; the proposed models often perform better.

Key words: Estimation, loss functions, confidence intervals, statistical analysis.

Introduction

A significant amount of research in Bayesian analysis and modeling has been published during the last thirty-five years. Bayesian analysis implies the exploitation of suitable prior information and the choice of a loss function in association with Bayes' Theorem. It is based on the notion that a parameter within a model is not merely an unknown quantity but rather behaves as a random variable that follows some distribution. In the area of life testing, it is 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) gave an excellent account of the use of Bayesian statistics in reliability

problems. As he pointed out, "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..." (Drake, 1966, p. 315-320).

This study considers a widely used and useful underlying model; that is, the normal underlying model characterized by

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2};$$

$$-\infty < x < \infty, -\infty < \mu < \infty, \sigma > 0. \quad (1)$$

For a given level of significance, the published classical model obtained by Miller (1991) considers the following confidence bounds for the coefficient of variation of a normal distribution.

$$L_M = \frac{S}{\bar{X}} - Z_{\alpha/2} \left[m^{-1} \left(\frac{S}{\bar{X}} \right)^2 \left(0.5 + \left(\frac{S}{\bar{X}} \right)^2 \right) \right]^{\frac{1}{2}}$$

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and

$$U_M = \frac{s}{\bar{X}} + Z_{\alpha/2} \left[m^{-1} \left(\frac{s}{\bar{X}} \right)^2 \left(0.5 + \left(\frac{s}{\bar{X}} \right)^2 \right) \right]^{\frac{1}{2}} \quad (2)$$

with $m=n-1$, where n is the sample size. This classical approach uses the Z-table to construct confidence intervals for a normal population coefficient of variation. This article relies only on observations under study to construct new approximate Bayesian confidence intervals for the coefficient of variation of a normal population.

Methodology

For model (1), the following results will be used to derive the approximate Bayesian confidence intervals for the coefficient of variation of a normal distribution: approximate Bayesian confidence bounds for a normal population variance (Camara 2003) and approximate Bayesian confidence bounds for a normal population mean (Camara, 2009). Although no specific analytical procedure is available that allows the identification of the appropriate loss function to be used, the most common is the square error loss function. One reason for selecting this loss function is due to its analytical tractability in Bayesian analysis. As this study shows, 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 compared to the classical model (2).

Square Loss Error Function

The popular square error loss function places a small weight on estimates near the true value and proportionately more weight on extreme deviations 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:

$$L_{SE}(\hat{\theta}, \theta) = \left(\hat{\theta} - \theta \right)^2 \quad (3)$$

Higgins-Tsokos Loss Function

The Higgins-Tsokos loss function places a heavy penalty on extreme over- or under-estimation. That is, it places an exponential weight on extreme errors. The Higgins-Tsokos loss function is defined as:

$$L_{HT}(\hat{\theta}, \theta) = \frac{f_1 e^{f_2(\hat{\theta}-\theta)} + f_2 e^{-f_1(\hat{\theta}-\theta)}}{f_1 + f_2} - 1,$$

$$f_1, f_2 > 0 \quad (4)$$

The Pareto prior was selected due to its mathematical tractability. The Pareto prior defined as follows:

$$f_1(\theta) = \frac{a}{b} \left(\frac{b}{\theta} \right)^{a+1}; \quad (5)$$

$$\theta \geq b > 0, \quad a > 0.$$

where $\theta = 1/\sigma^2$.

The use of good approximations of the Pareto prior (5) along with the square error loss and the Higgins-Tsokos loss leads to the approximate Bayesian confidence bounds for a normal population variance and positive mean (Camara, 2003). For the square error loss function

$$L_{\sigma^2(SE)} = \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n-2-2\ln(\alpha/2)}$$

and

$$U_{\sigma^2(SE)} = \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n-2-2\ln(1-\alpha/2)} \quad (6)$$

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For the Higgins-Tsokos loss function

$$L_{\sigma^2((HT))} = \frac{1}{\frac{n-1-2Ln(\alpha/2)}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{1}{f_1 + f_2} Ln \left(\frac{\sum_{i=1}^n (x_i - \bar{x})^2 + f_2}{\sum_{i=1}^n (x_i - \bar{x})^2 - f_1} \right)}$$

and

$$U_{\sigma^2(HT)} = \frac{1}{\frac{n-1-2Ln(1-\alpha/2)}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{1}{f_1 + f_2} Ln \left(\frac{\sum_{i=1}^n (x_i - \bar{x})^2 + f_2}{\sum_{i=1}^n (x_i - \bar{x})^2 - f_1} \right)} \quad (7)$$

The approximate Bayesian confidence interval for a positive normal population mean corresponding to the square error loss (Camara, 2009) is:

$$L_{\mu(SE)} = \left(s^2 + \bar{x}^2 - \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n-2-2\ln(1-\alpha/2)} \right)^{0.5}$$

and

$$U_{\mu(SE)} = \left(s^2 + \bar{x}^2 - \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{n-2-2\ln(\alpha/2)} \right)^{0.5} \quad (8)$$

The approximate Bayesian confidence bounds for a positive normal population mean corresponding to the Higgins-Tsokos loss function (Camara, 2009) is:

$$L_{\mu(HT)} = \left(s^2 - \bar{x}^2 - \frac{1}{\frac{n-1-2Ln(1-\frac{\alpha}{2})}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{1}{f_1 + f_2} Ln \left(\frac{\sum_{i=1}^n (x_i - \bar{x})^2 + f_2}{\sum_{i=1}^n (x_i - \bar{x})^2 - f_1} \right)} \right)^{0.5}$$

and

$$U_{\mu(HT)} = \left(s^2 + \bar{x}^2 - \frac{1}{\frac{n-1-2Ln(1-\frac{\alpha}{2})}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{1}{f_1 + f_2} Ln \left(\frac{\sum_{i=1}^n (x_i - \bar{x})^2 + f_2}{\sum_{i=1}^n (x_i - \bar{x})^2 - f_1} \right)} \right)^{0.5} \quad (9)$$

Using Equations (6), (7), (8) and (9), the approximate Bayesian confidence intervals are obtained for the coefficient of variation of a normal population corresponding to the square error loss function:

$$L_{C_v(SE)} = \left(\frac{n-1}{\left(1 + \left(\frac{\bar{x}}{s} \right)^2 \right) (n-2-2Ln(\alpha/2)) - n+1} \right)^{0.5}$$

and

$$U_{C_v(SE)} = \left(\frac{n-1}{\left(1 + \left(\frac{\bar{x}}{s} \right)^2 \right) (n-2-2Ln(1-\alpha/2)) - n+1} \right)^{0.5}$$

(10)

The approximate Bayesian confidence interval for the coefficient of variation of a normal population corresponding to the Higgins-Stokes Loss functions are:

$$L_{Cv}(HT) = \frac{1}{\left((s^2 + \bar{x}^2) \left(\frac{n-1-2Ln\left(\frac{\alpha}{2}\right)}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{1}{f_1 - f_2} Ln \left(\frac{\sum_{i=1}^n (x_i - \bar{x})^2 + f_2}{\sum_{i=1}^n (x_i - \bar{x})^2 + f_1} \right) \right) - 1 \right)^{0.5}}$$

and

$$U_{Cv}(HT) = \frac{1}{\left((s^2 + \bar{x}^2) \left(\frac{n-1-2Ln\left(1-\frac{\alpha}{2}\right)}{\sum_{i=1}^n (x_i - \bar{x})^2} - \frac{1}{f_1 - f_2} Ln \left(\frac{\sum_{i=1}^n (x_i - \bar{x})^2 + f_2}{\sum_{i=1}^n (x_i - \bar{x})^2 + f_1} \right) \right) - 1 \right)^{0.5}}$$

(11)

Results

To assess the proposed models, numerical results were obtained using SAS along with samples from normally distributed populations (Examples 1, 2, 3, 4, 7) as well as approximately normal populations (Examples 5, 6). Results were then compared to those obtained with the classical approach (2); for the Higgins-Tsokos loss function, $f_1 = 1$ and $f_2 = 1$ were considered. WC corresponds to the widths of the classical confidence intervals, and WSE and WHT denote the widths of the approximate Bayesian confidence intervals corresponding to the square error and the Higgins-Tsokos loss functions.

Example 1

Data: 24, 28, 22, 25, 24, 22, 29, 26, 25, 28, 19, 29 (Mann, 1998, p. 504).

Normal population distribution obtained with SAS:

Table 1: Classical (2) and Approximate Bayesian Confidence Intervals for the Population Coefficient of Variation Corresponding To Data Set 1

C.L.%	Approximate Bayesian Bounds (SE)	Approximate Bayesian Bounds (HT)	Classical Bounds I
80	0.1077-0.1291	0.1132-0.1276	0.0899-0.1587
90	0.1028-0.1298	0.1077-0.1291	0.0799-0.1687
95	0.0986-0.1301	0.1028-0.1298	0.0716-0.1770
99	0.0905-0.1303	0.0937-0.1303	0.0549-0.1937

C.L.%	Lengths of Approximate Bayesian Intervals (SE)	Lengths of Approximate Bayesian Intervals (HT)	$\frac{WC}{WSE}$	$\frac{WC}{WHT}$
80	0.0214	0.0144	3.215	4.778
90	0.0270	0.0214	3.289	4.150
95	0.0315	0.0270	3.346	3.904
99	0.0398	0.0366	3.487	3.792

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$$N(\mu = 25.083, \sigma = 3.1176)$$

The corresponding coefficient of variation is:

$$\bar{C}_v = \frac{\sigma}{\mu} = 0.124$$

Example 2

Data: 13, 11, 9, 12, 8, 10, 5, 10, 9, 12, 13 (Mann, 1998, p. 504).

Normal population distribution obtained with SAS:

$$N(\mu = 10.182, \sigma = 2.4008)$$

The corresponding coefficient of variation is:

$$\bar{C}_v = \frac{\sigma}{\mu} = 0.236$$

Example 3

Data: 16, 14, 11, 19, 14, 17, 13, 16, 17, 18, 19, 12 (Mann, 1998, p. 504).

Normal population distribution obtained with SAS:

$$N(\mu = 15.5, \sigma = 2.6799)$$

The corresponding coefficient of variation is:

$$\bar{C}_v = \frac{\sigma}{\mu} = 0.173$$

Example 4

Data: 27, 31, 25, 33, 21, 35, 30, 26, 25, 31, 33, 30, 28 (Mann, 1998, p. 504).

Normal population distribution obtained with SAS:

$$N(\mu = 28.846, \sigma = 3.9549)$$

The corresponding coefficient of variation is:

$$\bar{C}_v = \frac{\sigma}{\mu} = 0.137$$

Example 5

Data: 52, 33, 42, 44, 41, 50, 44, 51, 45, 38, 37, 40, 44, 50, 43 (McClave & Sincich, 1997, p. 301).

Normal population distribution obtained with SAS:

$$N(\mu = 43.6, \sigma = 5.4746)$$

The corresponding coefficient of variation is:

$$\bar{C}_v = \frac{\sigma}{\mu} = 0.126$$

Example 6

Data: 52, 43, 47, 56, 62, 53, 61, 50, 56, 52, 53, 60, 50, 48, 60, 55 (McClave & Sincich, 1997, p. 301).

Normal population distribution obtained with SAS:

$$N(\mu = 53.625, \sigma = 5.4145)$$

The corresponding coefficient of variation is:

$$\bar{C}_v = \frac{\sigma}{\mu} = 0.101$$

Example 7

The following observations were obtained from the collection of SAS data sets: 50, 65, 100, 45, 111, 32, 45, 28, 60, 66, 114, 134, 150, 120, 77, 108, 112, 113, 80, 77, 69, 91, 116, 122, 37, 51, 53, 131, 49, 69, 66, 46, 131, 103, 84, 78.

Normal population distribution obtained with SAS:

$$N(\mu = 82.861, \sigma = 33.226)$$

The corresponding coefficient of variation is:

$$\bar{C}_v = \frac{\sigma}{\mu} = 0.401$$

Table 2 Classical (2) and Approximate Bayesian Confidence Intervals for the Population Coefficient of Variation Corresponding To Data Set 2

C.L. %	Approximate Bayesian Bounds (SE)	Approximate Bayesian Bounds (HT)	Classical Bounds I
80	0.2007-0.2463	0.2122-0.2430	0.1647-0.3069
90	0.1908-0.2478	0.2007-0.2463	0.1441-0.3275
95	0.1823-0.2486	0.1908-0.2478	0.1269-0.3447
99	0.1662-0.2492	0.1724-0.2490	0.0924-0.3792

C.L. %	Lengths of Approximate Bayesian Intervals (SE)	Lengths of Approximate Bayesian Intervals (HT)	$\frac{WC}{WSE}$	$\frac{WC}{WHT}$
80	0.0456	0.0308	3.118	4.617
90	0.0570	0.0456	3.218	4.022
95	0.0663	0.0570	3.285	3.821
99	0.0830	0.0766	3.455	3.744

Table 3: Classical (2) and Approximate Bayesian Confidence Intervals for the Population Coefficient of Variation Corresponding To Data Set 3

C.L. %	Approximate Bayesian Bounds (SE)	Approximate Bayesian Bounds (HT)	Classical Bounds I
80	0.1495-0.1797	0.1573-0.1776	0.1243-0.2215
90	0.1427-0.1807	0.1495-0.1797	0.1103-0.2354
95	0.1368-0.1811	0.14273-0.1807	0.0985-0.2473
99	0.1255-0.1815	0.1300-0.1842	0.0750-0.2708

C.L. %	Lengths of Approximate Bayesian Intervals (SE)	Lengths of Approximate Bayesian Intervals (HT)	$\frac{WC}{WSE}$	$\frac{WC}{WHT}$
80	0.0302	0.0203	3.219	4.788
90	0.0380	0.0302	3.292	4.142
95	0.0443	0.0380	3.359	3.916
99	0.0560	0.0542	3.496	3.613

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Table 4: Classical (2) and Approximate Bayesian Confidence Intervals for the Population Coefficient of Variation Corresponding To Data Set 4

C.L.%	Approximate Bayesian Bounds (SE)	Approximate Bayesian Bounds (HT)	Classical Bounds I
80	0.1200-0.1419	0.1258-0.1404	0.1006-0.1736
90	0.1150-0.1426	0.1200-0.1419	0.0901-0.18414
95	0.1104-0.1430	0.1149-0.1426	0.0812-0.1930
99	0.1018-0.1433	0.1052-0.1432	0.0636-0.2107

C.L.%	Lengths of Approximate Bayesian Intervals (SE)	Lengths of Approximate Bayesian Intervals (HT)	$\frac{WC}{WSE}$	$\frac{WC}{WHT}$
80	0.0219	0.0146	3.333	5.000
90	0.0276	0.0219	3.406	4.292
95	0.0326	0.0277	3.429	4.036
99	0.0415	0.0380	3.545	3.871

Table 5: Classical (2) and Approximate Bayesian Confidence Intervals for the Population Coefficient of Variation Corresponding To Data Set 5

C.L.%	Approximate Bayesian Bounds (SE)	Approximate Bayesian Bounds (HT)	Classical Bounds I
80	0.1118-0.1293	0.1166-0.1282	0.09472-0.1564
90	0.1076-0.1299	0.1118-0.1293	0.08580-0.1653
95	0.1039-0.1301	0.1076-0.1299	0.0783-0.1728
99	0.0964-0.1303	0.0994-0.1303	0.0634-0.1877

C.L.%	Lengths of Approximate Bayesian Intervals (SE)	Lengths of Approximate Bayesian Intervals (HT)	$\frac{WC}{WSE}$	$\frac{WC}{WHT}$
80	0.0175	0.0116	3.526	5.314
90	0.0223	0.0175	3.565	4.543
95	0.0262	0.0223	3.607	4.238
99	0.0339	0.0309	3.667	4.023

Table 6: Classical (2) and Approximate Bayesian Confidence Intervals for the Population Coefficient of Variation Corresponding To Data Set 6

C.L.%	Approximate Bayesian Bounds (SE)	Approximate Bayesian Bounds (HT)	Classical Bounds I
80	0.0906-0.1038	0.0942-0.1029	0.0771-0.1248
90	0.0874-0.1042	0.0906-0.1038	0.0702-0.1317
95	0.0845-0.1044	0.0874-0.1042	0.0645-0.1375
99	0.0787-0.1045	0.0810-0.1045	0.0529-0.1490

C.L.%	Lengths of Approximate Bayesian Intervals (SE)	Lengths of Approximate Bayesian Intervals (HT)	$\frac{WC}{WSE}$	$\frac{WC}{WHT}$
80	0.0132	0.0087	3.614	5.483
90	0.0168	0.0132	3.661	4.659
95	0.0199	0.0168	3.668	4.345
99	0.0258	0.0235	3.725	4.089

Table 7: Classical (2) and Approximate Bayesian Confidence Intervals for the Population Coefficient of Variation Corresponding To Data Set 7

C.L.%	Approximate Bayesian Bounds (SE)	Approximate Bayesian Bounds (HT)	Classical Bounds I
80	0.3790-0.4063	0.3870-0.4047	0.3305-0.4715
90	0.3714-0.4071	0.3790-0.4063	0.3101-0.4919
95	0.3643-0.4075	0.3714-0.4071	0.2930-0.5090
99	0.3492-0.4077	0.3598-0.4077	0.2588-0.5431

C.L.%	Lengths of Approximate Bayesian Intervals (SE)	Lengths of Approximate Bayesian Intervals (HT)	$\frac{WC}{WSE}$	$\frac{WC}{WHT}$
80	0.0273	0.0177	5.165	7.966
90	0.0357	0.0273	5.092	6.660
95	0.0432	0.0357	5.000	6.050
99	0.0585	0.0479	4.860	5.935

BAYESIAN CONFIDENCE INTERVALS FOR THE GAUSSIAN DISTRIBUTION

Each of the seven randomly selected samples shows that the proposed approximate Bayesian confidence intervals contain the population coefficient of variation. The models are also strictly included in their counterparts obtained with classical approach (2). For each of the seven examples, the proposed approximate Bayesian approach has greater coverage accuracy than its classical counterpart (2).

Conclusion

New approximate Bayesian confidence intervals for the coefficient of variation of a normal population under two different loss functions were derived. The loss functions employed were the square error and the Higgins-Tsokos. Based on the above numerical results the following conclusions are put forth:

- The proposed approach and models rely only on the observations under study, contrary to the classical approach (2) that uses the standard normal distribution. The classical approach (2) used to constructing confidence intervals for the coefficient of variation of a normal population does not always perform better than the approximate Bayesian approach. In fact, in each of the examples provided, the obtained approximate Bayesian confidence intervals had greater coverage accuracy than those obtained with the classical approach (2). Each of the obtained approximate Bayesian confidence intervals contains the population coefficient of variation, and is strictly included in its classical counterpart obtained with the classical approach (2).
- With the proposed approach, approximate Bayesian confidence intervals for a normal population coefficient of variation may be obtained for any level of significance and any sample size.
- The approximate Bayesian approach under the square error loss function does not always yield the best approximate Bayesian results. In fact, in the examples provided, the Higgins-Tsokos loss function performs better.

- Bayesian analysis contributes to reinforcing well-known statistical theories such as the estimation theory.

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Parameter Estimation with Mixture Item Response Theory Models: A Monte Carlo Comparison of Maximum Likelihood and Bayesian Methods

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The Mixture Item Response Theory (MixIRT) can be used to identify latent classes of examinees in data as well as to estimate item parameters such as difficulty and discrimination for each of the groups. Parameter estimation via maximum likelihood (MLE) and Bayesian estimation based on the Markov Chain Monte Carlo (MCMC) are compared for classification accuracy and parameter estimation bias for difficulty and discrimination. Standard error magnitude and coverage rates were compared across number of items, number of latent groups, group size ratio, total sample size and underlying item response model. Results show that MCMC provides more accurate group membership recovery across conditions and more accurate parameter estimates for smaller samples and fewer items. MLE produces narrower confidence intervals than MCMC and more accurate parameter estimates for larger samples and more items. Implications of these results for research and practice are discussed.

Key words: Mixture item response theory, differential item functioning, Bayesian estimation, Markov chain Monte Carlo estimation, maximum likelihood estimation.

Introduction

Mixture item response theory (MixIRT) has become an increasingly popular tool for investigating a variety of issues in educational and psychological assessment (Cohen & Bolt, 2005; Bolt, Cohen & Wollack, 2001). Use of the MixIRT model in a variety of contexts has been described in detail by a number of authors (Cohen & Bolt, 2005; von Davier & Yamamoto, 2004; von Davier & Rost, 1995; Mislevy & Verhelst, 1990; Rost, 1990; Yamamoto, 1987). For example, MixIRT has been recommended for identifying subsets of a population (latent

classes) which are characterized by different item response models for a particular measure or instrument (Li, et al., 2009). In this context, psychometricians have used MixIRT to detect and characterize differential item functioning (DIF) (Cohen & Bolt, 2005; De Ayala, et al., 2002; Bolt, Cohen & Wollack, 2002, 2001). This simulation study compares the parameter estimation accuracy for two methods of estimation used with MixIRT: Maximum Likelihood Estimation (MLE) and Bayesian estimation using the Markov Chain Monte Carlo (MCMC) approach.

Prior research has demonstrated the utility of the MixIRT framework given its ability to identify differentially responding subgroups that exist organically in the data. This approach stands in contrast to the assumption that differential response patterns are inherently linked to easily identified grouping variables (e.g., gender) and that all (or most) members of such intact groups will demonstrate very similar responses to items; an assumption which underlies other statistical models used for similar purposes. For example, in the detection of DIF using standard methods such as logistic

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regression or the Mantel-Haenszel test, comparisons of item response patterns are made between known groups such as males and females. However, recent work in the area of DIF has demonstrated that the causes of DIF are often complex and not so clearly tied to easily identified groups (Cohen & Bolt, 2005). In such cases, the utility of the MixIRT approach – and its sometimes superiority – has been demonstrated in gaining a deeper understanding into differential item response patterns such as those associated with DIF (Maij-de Meij, Kelderman & van der Flier, 2010; Samuelson, 2008; Cohen, Cho & Kim, 2005; Rost, 1990).

The MixIRT model, which combines the powerful statistical tools of latent class analysis (LCA) and item response theory (IRT), assumes that a population is composed of a finite number of latent examinee classes that can be differentiated based upon their item response patterns (Rost, 1997). In turn, these different response patterns will manifest themselves as differences in parameters of the item response model associated with each group. The 2-parameter MixIRT (Mix2PL) model for dichotomous data takes the following form:

$$P(U = 1 | g, \theta_{ig}) = \frac{e^{(a_{jg}(\theta_{ig} - b_{jg}))}}{1 + e^{(a_{jg}(\theta_{ig} - b_{jg}))}} \quad (1)$$

Here latent class membership ($g = 1, 2, \dots, G$), within class difficulty for item j (b_{jg}), within class discrimination for item j (a_{jg}), and the within class level on the latent trait being measured for person i (θ_{ig}) are all model parameters to be estimated. In addition, each survey respondent is placed in a latent class, and the proportions of individuals in each class (π_g), are also estimated,

under the constraint that $\sum_{g=1}^G \pi_g = 1$. Variants of

this model including a pseudo-chance parameter (Mix3PL) and excluding both pseudo-chance and constraining discrimination to be equivalent across items (Mix1PL) are also available, as in the standard IRT context. The focus of this study is on dichotomous items for which chance responding is not applicable, such as behavior inventories; for this reason only the Mix1PL and Mix2PL models are examined.

The item parameter values carry the same meaning in the MixIRT context as in the more general IRT framework; thus, item difficulty provides information regarding the likelihood that an individual will endorse an item (or answer it correctly in the context of cognitive assessment), discrimination indicates how well the item differentiates between individuals with different levels of the construct being measured and pseudo-guessing is a measure of the likelihood that an examinee would respond to the item correctly due solely to chance (de Ayala, 2009).

When there are class differences in the item difficulty and discrimination parameter values, researchers conclude that members of the latent classes perform differently on the specific item (Cohen & Bolt, 2005). For example, assume that the results of the analysis indicate the presence of two distinct latent classes in the population. In this case, if a specific item for latent class 1 has a higher value for b_{jg} than class 2, it is known that the item is more difficult for class 1; this in turn may provide insights into the types of individuals who tend to be in that class. Similarly, if latent class 2 has a higher a_{jg} value on an item compared to class 1, it can be concluded that the item is better able to differentiate among individuals with different levels of the latent trait for class 2 than for class 1. This approach to using MixIRT models has been particularly evident in the identification and characterization of DIF for achievement tests (Cohen & Bolt, 2005), though it has also been used to identify different usage patterns of the not sure category in personality inventories (Maij-de Meij, Kelderman & van der Flier, 2008) and to identify individuals engaging in impression management in organizational surveys (Eid & Zickar, 2007).

Parameter Estimation

In the literature, model parameter estimation for MixIRT models has been examined using both MLE (Willse, 2011) and MCMC methods in the Bayesian context (von Davier & Rost, 2007). Excellent discussions regarding the technical details of both approaches are present in the literature; the interested reader is referred to von Davier and Carstensen (2007) for a thorough treatment of a number of MixIRT models available. Although

prior applied work has used both methods, there has been very little research empirically comparing the performance of the two estimation techniques to one another.

Based upon these prior applications, each approach has been shown to have specific advantages and disadvantages in practice. For example, MCMC has proven useful with complex MixIRT models because it does not require integration of the likelihood function (as does MLE) which can be extremely difficult when it is necessary to estimate many parameters (Junker, 1999).

Conversely, the MCMC approach is often very time consuming to implement (sometimes taking 10 days or more to fit a single model), and may encounter difficulties in converging to solutions for individual parameters (Li, et al., 2009). The issue of time is non-trivial when dealing with MixIRT models, as several different latent class solutions must typically be fit and then compared in order to determine which is optimal for the data at hand (Li, et al., 2009). MLE does not usually require such large amounts of time as MCMC and MLE has been used successfully in estimating MixIRT models (von Davier & Rost, 2007); however, MLE can mistakenly converge on localized, rather than general maximum likelihood solutions, leading to suboptimal model parameter estimates. This problem can be overcome through the use of multiple random starting values, such as the 10 random starts used in this study (Rost, 1991). Of concern, though, is that using more starting values and increasing the maximum number of iterations in order to increase the probability of obtaining optimal fit, also increases the time necessary for the model to converge and provide parameter estimates.

Although relatively little work has been done explicitly comparing the performance of MLE and MCMC estimation techniques in the context of MixIRT models, Li, et al. (2009) conducted a simulation study in which they examined the performance of MCMC primarily in terms of identifying the optimal model selection criterion for dichotomous item response data. However, as a part of this study, MixIRT parameter estimation was also examined. Results of their research indicated

that item parameter recovery was worse in the presence of more latent classes and better when there were more items and/or more examinees. Recovery of latent class membership was generally greater than 80%, with the most accurate results for the Mix2PL model and the least accurate for the Mix3PL.

Cho and Cohen (2010) expanded on this work by investigating item parameter recovery for the multilevel Mix1PL model, in which information at both the student (level 1) and school (level 2) levels were taken into consideration. The estimation used in this simulation study was also MCMC and the model was restricted to the 1-Parameter Logistic form. The authors reported that recovery of both the item difficulty estimates and group membership was good for the MCMC methodology used in the study. A study by Willse (2011) examined the performance of a joint maximum likelihood estimator for the Rasch MixIRT model. He reported the results of a simulation study that showed good parameter recovery for group specific item difficulty values. No other simulation work examining the accuracy of parameter estimates in the MixIRT context was identified in the literature.

The goal of this simulation study is to compare the parameter recovery performance of the MLE and MCMC estimation procedures in the context of the MixIRT model for dichotomous item response data. Prior simulation work in this area has focused primarily on MCMC estimation and has not directly compared the ability of this approach and MLE in terms of parameter recovery accuracy, both for the items and for latent class membership. In addition, this work adds the additional simulation conditions of group size ratio, which has not been previously examined. Thus, this study adds to the literature by directly comparing these two popular methods of estimation across a range of conditions for dichotomous item response data. Prior applied work in this area has shown both methods to be potentially useful in many cases. However, given that both have distinct certain practical advantages in terms of their relative abilities to converge on the optimal solution and the time needed to use each; it would be helpful to understand whether one technique provides any

methodological advantages over the other and, if so, under what conditions. If one approach does provide greater parameter estimation accuracy, researchers might be able to make decisions regarding which to use in light of this and the aforementioned practical concerns. Given that such a direct comparison has not been previously published, it is believed that this work will add valuable information to the literature on MixIRT models.

Methodology

The simulation study used to compare the parameter estimation accuracy for MLE and MCMC, involved the manipulation of several factors that have been shown pertinent in previous research. A total of 50 replications per combination of manipulated conditions were generated. The two estimation methods were fit using Mplus version 6.1 (Muthén & Muthén, 2011). Several of the simulation conditions used in this study were based on those reported in Li, et al. (2009). These were selected for use because they were used previously and have been shown to be related to the performance of the MCMC estimator.

Thus, given that something is known about how the MCMC approach performs under the various conditions, it was determined that they would be particularly informative for the comparison of this method and MLE. It should be noted that the simulating item parameter values were drawn from item responses to a behavioral checklist given to adolescents through the auspices of the 2009 administration of the Youth Risk Behavior Survey (Centers for Disease Control, 2009). A MixIRT study involving these items was published by Finch and Pierson (2011) in which they report results for four latent classes based on 16,000 adolescents' responses (yes or no) to items asking about participation in a variety of risky sexual and substance use behaviors. These data were fit with a Mix2PL model. The population item parameter values used in the generation of simulated data for the current study were drawn from this earlier work and are shown in Table 1.

Manipulated Conditions

A total of 2, 3, and 4 latent classes were simulated with sample sizes of 400, 1,000 and

2,000 examinees. Group sizes were either equal or unequal. In the unequal case for two groups, the ratio was 75/25, for three groups the ratio was 50/25/25 and for four groups the ratio was 40/20/20/20. Two models were simulated, the Mix1PL and Mix2PL, and the appropriate model was fit for each replication. Specifically, when the Mix2PL model was used to generate the data, the Mix2PL model was fit to each simulated dataset. Finally, three conditions were simulated for the number of items, 5, 15 and 30. These were intended to simulate very short, moderate and somewhat longer instruments. The underlying latent trait was simulated to be unidimensional from the $N(0,1)$ distribution.

In order to differentiate the groups in the simulations, the item discrimination and item difficulty parameter values for the groups were made to differ (Table 1 shows the values for each group). For the 5 item condition, the first 5 item parameter sets were used, and for the 30 item condition, the 15 item set was used twice, in keeping with the methodology laid out in Li, et al. (2009). The outcome variables of interest were the proportion of correctly placed individuals into the latent classes, the estimation bias for item difficulty and discrimination, mean standard error for parameters across replications and the coverage rates for the item parameters. In order to place all items on the same metric prior to estimating the outcome variables, methods outlined by Lloyd and Hoover (1980) were utilized.

Model Convergence Issues

Researchers using the MCMC approach to estimation must ensure that each time an analysis is run the results converge to the optimal solution. As a part of this, a burn-in period must be established, which means identifying a number of draws from the posterior distribution that will be ignored as the estimator seeks to converge to the solution for each parameter. After the burn-in has been established, samples are then drawn from subsequent values in the posterior in order to obtain the final parameter estimate. Based upon earlier work in this area, particularly that of Li, et al. (2009) and Cho and Cohen (2010), as well as examination of auto-correlation plots from several of the simulated datasets, 10,000

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Table 1: Item Difficulty and Discrimination Parameters Used In the Monte Carlo Simulations

Item	Difficulty			
	Class 1	Class 2	Class 3	Class 4
1	2.817	1.188	-2.522	1.824
2	-1.447	0.099	0.306	1.054
3	-2.507	-0.835	-2.002	2.819
4	0.268	-1.022	-0.547	3.177
5	1.743	-0.001	-2.569	2.535
6	-0.699	-1.525	1.248	1.847
7	0.022	0.206	-0.262	2.025
8	1.025	0.729	-1.627	2.059
9	1.201	0.747	-1.766	2.037
10	1.444	1.348	-2.398	2.422
11	1.299	0.867	-2.085	2.207
12	1.056	0.681	-1.725	2.233
13	0.713	0.626	-1.048	1.948
14	1.154	0.352	-1.536	2.212
15	0.546	0.001	-0.851	1.868
Item	Discrimination			
	Class 1	Class 2	Class 3	Class 4
1	0.096	1.735	0.083	0.689
2	0.025	1.549	2.812	1.203
3	0.236	1.146	0.057	0.351
4	1.207	0.568	1.009	0.928
5	0.845	0.279	0.547	0.483
6	0.923	1.339	0.629	0.632
7	0.918	2.105	0.836	1.062
8	1.857	3.198	1.654	2.459
9	1.075	2.106	0.722	0.978
10	1.415	0.512	2.133	3.304
11	2.477	0.163	1.765	0.853
12	1.606	2.189	1.359	2.752
13	0.432	1.918	0.529	0.547
14	2.151	1.212	1.643	2.359
15	1.029	2.130	1.150	1.009

iterations were used as the burn-in, 10,000 post burn-in values were used to obtain parameter estimates with MCMC and thinning of the posterior draws was set at 50.

Each method presented some difficulties in terms of convergence. The MLE approach had difficulty converging for the smallest sample size condition (400). Therefore additional simulations were run until the necessary 50 converged replicates were obtained for MLE. With respect to MCMC, difficulty was encountered in obtaining convergence for the 5 item condition for some of the replications. Thus, as with the MLE method, additional replications were run until the requisite 50 converged solutions were obtained. Although it was recognized that both conditions causing these problems (400 examinees and 5 items) might generally be viewed as problematic in practice, it is important to learn as much as possible about the relative performance of these two methods, including under relatively difficult circumstances such as these, given that such conditions are not uncommon in actual research practice, particularly for behavioral inventories and short mental health screening instruments.

Label Switching

An issue of some importance in any study involving latent class analysis is that of label switching, in which a given latent class might take one number (e.g., 1) in one case, and another number (e.g., 2) in another case. In reality, however, the group is constituted of the same individuals or type of individuals. In a simulation study involving MCMC estimation, label switching consists of two separate problems. First, within the context of Bayesian analysis, label switching can occur across repeated sampling from the posterior distribution within a single analysis. In order to detect this type of label switching, it is necessary to monitor the posterior densities of group membership. A multimodal distribution would be indicative of such label switching. During the simulation the densities were monitored and multimodal solutions did not present themselves, thus this type of label switching was eliminated as a concern.

The second type of label switching occurs across replications of a simulation study

and is not limited to MCMC but can also occur for MLE. Essentially, it involves changing the arbitrary group label as described, but in this case from one replication to another. For this study, the methodology described in Cho, Cohen and Kim (2006) was used. Namely, the item parameter estimates from the individual sample replications were compared with those used to generate the data and the group labels from the sample replications were changed to match those to which they most closely conformed from the model generation groups.

Results

Classification Accuracy

In order to identify statistically significant effects among the manipulated factors described, a repeated measures analysis of variance (ANOVA) was used. The within replication variable was method, and the between replication variables were the manipulated factors including number of items, sample size, number of groups, group size ratio and the underlying model. The dependent variable was the mean classification accuracy across replications. In addition to statistical significance, effect sizes were also calculated for all main effects and interactions.

ANOVA results for the classification accuracy outcome variable indicate that the method of estimation interacted significantly with number of items ($F < 0.001$, $\eta^2 = 0.363$), number of subjects ($F = -0.025$, $\eta^2 = 0.07$), group size ratio ($F = 0.006$, $\eta^2 = 0.117$) and number of groups ($F = 0.003$, $\eta^2 = 0.108$). In addition, method ($F < 0.001$, $\eta^2 = 0.721$) itself was statistically significant. Table 2 shows the classification accuracy rates for each of the manipulated variables by method. Across all other conditions, the MCMC approach yielded more accurate group classification than did MLE. This difference was most noticeable for fewer items, with the gap between the two estimation techniques narrowing as the number of items increased, in large part due to improvements in the accuracy of MLE. In addition, the MLE approach was more accurate at classifying individuals when the groups were of equal size, whereas the MCMC was largely impervious to the group size ratio. Across

conditions MCMC yielded similar rates of correct classification, which were uniformly higher than 0.9, whereas MLE was much more likely to be influenced by the manipulated conditions and rarely had correct classification rates greater than 0.9.

Item Discrimination Parameter Estimation

As with the classification accuracy results, ANOVA was used to identify significant study effects with regard to bias in the estimation of the item discrimination parameter.

The interaction terms of method by number of items ($F = 0.025$, $\eta^2 = 0.07$) and method by number of groups ($F < 0.001$, $\eta^2 = 0.147$) were significantly related to bias in the a parameter estimate. Table 3 shows the mean bias results across replications for these two terms. Regardless of the number of items, the Bayesian method provided estimates of a with bias under 0.15 in all cases. By contrast, MLE yielded very biased estimates in the case of 5 items, had comparable bias to the Bayesian for 15 items,

Table 2: Latent Class Classification Accuracy by Method, Number of Items, Number of Groups, Sample Size, Group Size Ratio and Underlying Model

Items	MLE	MCMC
5	0.761	0.939
15	0.889	0.972
30	0.916	0.991
Sample Size		
400	0.852	0.971
1,000	0.845	0.969
2,000	0.827	0.947
Groups		
2	0.831	0.949
3	0.880	0.970
4	0.820	0.972
Group Ratio		
Equal	0.841	0.963
Unequal	0.715	0.950
Model		
1PL	0.844	0.951
2PL	0.822	0.969

MIXTURE ITEM RESPONSE THEORY MODEL PARAMETER ESTIMATION

and had lower bias for 30 items. With respect to the number of groups, item discrimination bias for MLE increased concomitantly with increasing number of groups. In contrast, estimation accuracy for the Bayesian approach seemed largely unaffected by the number of groups in terms of the absolute size of bias, though for 4 groups the estimates were somewhat underestimated whereas for 2 and 3 groups they were somewhat overestimated.

In addition to parameter estimation bias, the coverage rates for the discrimination parameters were also estimated. These coverage rates represent the proportion of simulation replications for which the nominal 95% confidence interval actually contained the true population value of a : ideally they would be 0.95. The results of the ANOVA indicated that the main effect of method ($F < 0.001$, $\eta^2 =$

0.762), as well as the interaction of method by number of items ($F < 0.001$, $\eta^2 = 0.339$) were statistically significant. Table 4 includes the coverage rates for each method by the number of items.

Across conditions, the coverage rates for the MCMC estimates were near 1.0 and were much higher than those of the MLE method. The latter estimation approach had higher coverage for tests with a larger number of items, though in no case were these rates comparable to those of the MCMC approach and they were generally lower than the nominal 0.95 level. The standard errors of these estimates also appear in Table 4, and show that those associated with MCMC were larger than those from MLE. These larger standard errors resulted in wider confidence intervals for the MCMC estimates, which contributed in part to the higher coverage rates for this approach.

Table 3: Item Discrimination Bias by Method, Number of Items and Number of Groups

Items	MLE	MCMC
5	0.307	-0.133
15	-0.084	-0.082
30	0.074	0.149
Groups		
2	0.097	0.118
3	0.276	0.105
4	0.302	-0.080

Table 4: Item Discrimination Coverage Rates (Mean Standard Error across Replications) By Method and Number of Items

Items	MLE	MCMC
5	0.663 (0.394)	0.991 (0.902)
15	0.788 (0.378)	1.000 (0.886)
30	0.886 (0.366)	1.000 (0.865)

Item Difficulty Parameter Estimation

The ANOVA results for the item difficulty parameter bias revealed that only the interaction of method by number of groups was statistically significant ($F = 0.013$, $\eta^2 = 0.082$). Table 5 includes the b bias results for this interaction term. For both methods, underestimation bias of the b parameter increased concomitantly with increases in the number of groups. The significant interaction appears to be a function of the fact that for 2 groups, the bias in the MCMC estimator was somewhat smaller than that of MLE; however, for 3 groups this pattern was reversed and for 4 groups the bias of the two methods was comparable.

The ANOVA for the b parameter coverage rates showed that the main effect of method ($F < 0.001$, $\eta^2 = 0.768$) and the interaction of method by number of items ($F < 0.001$, $\eta^2 = 0.263$) were the two significant terms in this model. Table 6 includes the coverage rates for b by method and number of items. Item difficulty coverage rates were uniformly 1.0 for the MCMC estimator, whereas for MLE these rates were below the nominal 0.95 level except for the 30 item condition. An

examination of the average standard error for these estimates, also shown in Table 6, reveals that the MCMC estimator had a substantially larger standard error than did MLE, which in turn led to wider confidence intervals. Therefore, although the coverage rates for the MCMC approach were higher than those of MLE, the associated intervals were also wider, just as was the case for item discrimination.

Conclusion

It is hoped that the results of this study will prove useful to researchers and practitioners interested in using the MixIRT approach in order to gain a greater understanding of their data, whether in the context of characterizing DIF, or identifying specific item response profile groups, as was the case for the study upon which this work was built, or gaining further insights into the interplay of personality and item response profiles. In all of these cases, accurate estimation of item response and group membership parameters is crucial to obtaining useful results that can inform policy and practice. Prior applied research has focused on two different estimation methods, MCMC within the Bayesian framework, and MLE, and

Table 5: Item Difficulty Bias by Method and Number of Groups

Groups	MLE	MCMC
2	-0.029	-0.019
3	-0.031	-0.038
4	-0.057	-0.055

Table 6: Item Difficulty Parameter Coverage Rates (Mean Standard Error across Replications) by Method and Number of Items

Items	MLE	MCMC
5	0.620 (0.205)	1.00 (0.607)
15	0.814 (0.195)	1.00 (0.598)
30	0.959 (0.188)	1.00 (0.587)

has shown that both approaches appear to be useful for specific situations. In addition, a very brief simulation literature demonstrated some support for the MCMC technique in terms of parameter estimation, though no direct comparisons with MLE were made. At the same time, these earlier authors noted that the MCMC approach often requires a very lengthy time period in order to complete a single analysis (Li, et al., 2009), a fact which has also been reported by other authors. Therefore, while previous work indicates that the MCMC estimation approach might hold promise in terms of parameter estimation, the logistics of using it in many real world situations might limit its practical value. Given that there has been little simulation work examining MixIRT in general, and no studies that could be found comparing the two major parameter estimation approaches with one another, this the current study should prove informative to practitioners considering the use of the MixIRT paradigm in research.

Study results herein indicate that for correctly identifying which group an individual belongs to, the MCMC approach would seem to be more effective. Across virtually all conditions simulated, it was more accurate than MLE in terms of correct group identification. Across all simulated conditions, MCMC correctly classified respondents in over 96% of cases, whereas MLE was correct only 84% of the time. Furthermore, there was very little variation in the rates of accuracy for MCMC across manipulated conditions, however, for MLE the accuracy rates varied greatly, particularly as a function of the number of items. Thus, for researchers whose primary goal is to gain insights into the types of respondents present in the population, it would seem that MCMC is the preferable estimation approach.

For researchers who are most interested in the accuracy and precision of class specific item difficulty and discrimination values, the results of the study are somewhat more ambiguous. It seems that with respect to item discrimination estimates, the MCMC approach might provide somewhat less biased estimates for shorter instruments. By contrast, item discrimination bias was lower for MLE when the instrument contained 30 items. With respect to item difficulty, the length of the instrument was

not as salient as the number of latent classes, such that the presence of more groups was associated with greater item difficulty bias for both methods. It is possible that this relationship was due in part to the smaller number of individuals in the groups that was present when the number of groups increased.

In terms of estimate precision as measured by the average standard error value across replications and the coverage rates, MLE appears to have fared somewhat better than MCMC. It is true that the coverage rates for MCMC were uniformly higher than those of MLE, but this appears to have been due in the main to the larger standard errors associated with the Bayesian estimates. Thus, researchers using MCMC can be reasonably sure that the credible intervals for the estimates contain the population parameter value, but they also must be aware that these intervals will generally be wide. Such wide intervals may not be terribly informative to researchers interested in obtaining fairly precise estimates of the item difficulty and discrimination values.

Recommendations for Practice

Based on study results, some general recommendations for practice can be developed. First, when there are many items, the MLE approach might be optimal. With 30 items, MLE produced somewhat more accurate item parameter estimates than did MCMC and it had group classification accuracy rates above 90% (though this was lower than that of MCMC). In addition to the more accurate item parameter estimation in the presence of 30 items, MLE estimates were also more precise than those of MCMC, as witnessed in the narrower confidence intervals. However, when an instrument consists of very few items, MLE should probably be avoided, as it produced substantially more biased estimates than MCMC and will be less accurate in terms of classifying respondents. When researchers suspect that more than 3 groups are present, MCMC would also seem to be a better choice, particularly with regard to estimating item discrimination parameters. Such is not the case for item difficulty, which was compromised with equal severity for both estimation approaches for 4 groups. In short, situations in which many items are available to

describe many examinees and few groups are ideal for the use of MLE, whereas cases in which the number of items is small and/or the number of groups is large may be better suited to MCMC. All of these recommendations must be considered in light of the fact that the MCMC estimation will probably take substantially more time than will MLE.

Finally, with respect to using MixIRT models with relatively small samples as previously discussed, with a sample size of 400 individuals, both estimation methods had difficulty reaching convergence for many of the replications in the study. This was particularly an issue for MLE, though the Bayesian approach was also less successful for an N of 400 than for the larger sample sizes; thus, in practice researchers might find that they are unable to obtain useful estimates for this small sample size regardless of the method used. This problem was particularly acute for a larger number of groups in conjunction with the smaller sample size, because the number of individuals in each group became small. Therefore, one other recommendation for practice to come out of this study is that – for samples of 400 or fewer – MixIRT may not be particularly viable, except perhaps for the simplest models.

Limitations and Areas for Future Research

As with any research, this study has some limitations which impact interpretations of the results that must be acknowledged. First, the Mix3PL model was not included in the study. This decision was made consciously, as the focus of the study was on instruments that are common in psychology, such as behavior inventories and personality assessments, for which chance responding is a negligible issue. In addition, the item parameter values used to generate the data were based on a behavior inventory. That this focus is believed to be appropriate for research in psychology, but it does limit the findings for those interested in cognitive assessments where chance responses to items are an issue. Future research should include a Mix3PL model. In addition, the current study examined a limited range of unequal group size conditions. Although this is the first study in this area to manipulate group sizes, it is recognized that more work in this area needs to

be conducted and thus a wider range of unequal group size conditions should be simulated. In addition, it is believed that the settings of the MCMC and MLE techniques used in this study were in keeping with recommended practice, it would be helpful if a wider array of values for the burn-in period and post burn-in iterations for MCMC were used and if more conditions in terms of number of random starts and convergence criteria were investigated for MLE. Such research would provide more information regarding the optimal settings for use with these estimators.

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Statistical Inferences for Lomax Distribution Based on Record Values (Bayesian and Classical)

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A maximum likelihood estimation (MLE) based on records is obtained and a proper prior distribution to attain a Bayes estimation (both informative and non-informative) based on records for quadratic loss and squared error loss functions is also calculated. The study considers the shortest confidence interval and Highest Posterior Distribution confidence interval based on records, and using Mean Square Error MSE criteria for point estimation and length criteria for interval estimation, their appropriateness to each other is examined.

Key words: Lomax distribution; record values, maximum likelihood estimation, method of moment, Bayesian estimation, shortest interval, highest posterior density (HPD) interval, quadratic loss function, squared error loss function, prior density, posterior density, simulation, MSE.

Introduction

Let $X_1, X_2, X_3, \dots$ be a sequence of independent and identically (iid) random variable with cumulative distribution (cdf) function $F(x)$ and probability density (pdf) $f(x)$ For $n \geq 1$ define

$$T(1) = 1, T(n+1) \\ = \min \left\{ j : X_j \geq X_{T(n)} \right\}.$$

The sequence $\{X_{T(n)}\}_{n=1}^{\infty}$ is known as an upper record value statistic and the sequence $\{T(n)\}_{n=1}^{\infty}$ is known as a record time sequence (Arnold, Balakrishnan & Nagaraja, 1998). Chandler (1952) was one of the first to study record theory and he defined a mathematical model for record values. Record values arise naturally in many applications involving data

relating to weather, sports, economics and life testing studies. Many authors have studied records and their associated statistics as well as inference-based testing on records. Some of the best examples may be found in the works of Balakrishnan, Arnold, Nagaraja (1998), Ahsanullah (1998) and Nevzorov (1946).

Sevgi, et al. (2005) examined the relationship between order statistics and records. Mohammad (2002) and Balakrishnan (1994) examined the recurrent relations between the moments for the generalized exponential and Lomax distributions. Ahsanullah (1974) studied record values received from Lomax distribution, and Ahsanullah and Holland (1994) discussed both scale and location estimation of the distribution of generalized extreme values based on records. Asgharzadeh (2009) discussed both MLE and Bayesian estimation based on record values and Chan (1998) presents interval estimation according to records for groups of scales and locations. Soliman and Abd Ellah (2006) compared Bayesian and Non-Bayesian estimation based on records.

The Lomax distribution plays an important role in reliability. Consider the one-parameter Lomax distribution with pdf

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$$f(x; \theta) = \frac{1}{\theta} (1+x)^{-\left(\frac{1}{\theta}+1\right)} \quad x \geq 0, \theta > 0, \quad (1)$$

and cdf

$$F(x; \theta) = 1 - (1+x)^{-\frac{1}{\theta}} \quad x \geq 0, \theta > 0.$$

An application of the Lomax distribution in receiver operating characteristic (ROC) was presented by Campbell and Ratnaparkhi (1993). Distributional properties and recurrence relation moments of record values was studied by Balakrishnan (1994) and Ahsanullah (1991). Much work has been done with respect to estimating the parameters using both classical and Bayesian techniques, and parametric and nonparametric inference based on record values have also been studied extensively (for example, see Ahmadi, et al., 2009; Soliman & Al-Aboud, 2008; Baklizi, 2008).

This study has several components: It considers Lomax parameter estimation based on record values. It estimates the parameter θ using maximum likelihood and method of moment (MME) based on record values. It uses an appropriate selection of density function for a prior distribution to derive a Bayesian estimation based on record values. For the latter, by applying an appropriate selection for the prior density, the society parameter is controlled; this means that the Mean Square Error (MSE) of the Bayesian estimation is controlled by controlling the parameters of this distribution. Finally, it derives the shortest interval estimation and Highest Posterior Density (HPD) interval estimation based on record values. Examples are used to illustrate the various components.

Point Estimation of θ Parameter: The Method of Maximum Likelihood Estimation

If $X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}$ represents the first n upper record values from the Lomax distribution in (1), then the joint distribution of $X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}$ is

$$f(x_{T(1)}, x_{T(2)}, \dots, x_{T(n)}) = f(x_{T(n)}; \theta) \prod_{i=1}^{n-1} h(x_{T(i)}; \theta), \quad (2)$$

where

$$h(x_{T(i)}; \theta) = \frac{f(x_{T(i)})}{1 - F(x_{T(i)})}.$$

Thus, for the Lomax distribution,

$$f(x_{T(1)}, x_{T(2)}, \dots, x_{T(n)}) = \theta^{-n} \frac{(1+x_{T(n)})^{-\frac{1}{\theta}}}{\prod_{i=1}^n (1+x_{T(i)})}, \quad (3)$$

and the log likelihood function is

$$L = -n \ln \theta - \left(\frac{1}{\theta} \right) \ln(1+x_{T(n)}) - \sum_{i=1}^n \ln(1+x_{T(i)}). \quad (4)$$

The maximum likelihood estimation (MLE) based on records can be obtained from (4) as

$$-\frac{n}{\theta} + \frac{\ln(1+x_{T(n)})}{\theta^2} = 0$$

and

$$\hat{\theta} = \frac{\ln(1+x_{T(n)})}{n}. \quad (5)$$

Using (2), the marginal pdf of $X_{T(n)}$ can be derived as

$$f(x_{T(n)}) = \frac{1}{\theta^n (n-1)!} (1+x_{T(n)})^{-\left(\frac{1}{\theta}+1\right)} (\ln(1+x_{T(n)}))^{n-1}, \quad (6)$$

therefore,

$$(\hat{\theta}_{MLE}) = \theta, \text{Var}(\hat{\theta}_{MLE}) = \frac{\theta^2}{n}.$$

conversely, if (3) is rewritten as

$$f(x_{T(1)}, x_{T(2)}, \dots, x_{T(n)}) = \exp(-n \ln \theta - \frac{1}{\theta} \ln(1 + x_{T(n)}) - \sum_{i=1}^n \ln(1 + x_{T(i)})),$$

then $\ln(1 + x_n)$ is a complete sufficient statistic for parameter θ . Therefore $\hat{\theta}_{MLE}$ based on record is the equal to the Uniformly Minimum-Variance Unbiased Estimator (UMVUE) for parameter θ .

Point Estimation of θ Parameter: The Method of Moment Estimation

The MME, first introduced by Pearson (1894), was one of the first methods used to estimate the society parameter θ (for additional details and an example see Pearson, 1894). The Lomax parameter θ is estimated by the MME based on record values by using the density function (6), which results in

$$E(X_{T(n)}) = \frac{1}{(1-\theta)^n} - 1.$$

Next, solving the equation

$$E(X_{T(n)}) = \bar{X}$$

yields a MME based on record values, where $\bar{X}$ is average of the n first records $(X_{T(1)}, X_{T(2)}, \dots, X_{T(n)})$. Thus,

$$\hat{\theta}_{MME} = 1 - \frac{1}{(1 + \bar{X})^{\frac{1}{n}}}.$$

Bayesian Estimation of θ Parameter

The Bayesian estimator of θ is obtained based on record values under the two following loss functions:

$$L(\hat{\theta}, \theta) = \left(\frac{\hat{\theta}}{\theta} - 1 \right)^2, \quad (7)$$

and

$$L(\hat{\theta}, \theta) = (\hat{\theta} - \theta)^2, \quad (8)$$

where $\hat{\theta}$ is an estimator of θ . Assuming an inverse Weibull distribution $IWD(\gamma, \beta, c=1)$, the prior for θ is conjugated as

$$\pi(\theta) = \frac{1}{\Gamma(\gamma)\beta} \left(\frac{\beta}{\theta} \right)^{\gamma+1} \exp\left(-\frac{\beta}{\theta}\right), \quad (9)$$

such that

$$E(\theta) = \frac{\beta}{\gamma-1},$$

$$Var(\theta) = \frac{\beta^2}{(\gamma-1)^2(\gamma-2)}$$

where $\gamma > 0, \beta > 0$. Note that $\frac{1}{\theta} \sim \text{gamma}(\gamma, \beta)$. This prior density has an advantage over other priors because it is easy to use and the parameter (γ, β) can be chosen such that prior precision for the true value of θ is fulfilled because Bayesian estimations are functions of (γ, β) , therefore, the precision of the Bayesian estimations cannot be controlled by altering the prior distribution parameters. Combining likelihood function (3) with prior density (9), the posterior density of θ is obtained as

$$\pi(\theta|x) = \left\{ \frac{1}{\Gamma(n+\gamma) \left[\ln(1+x_{T(n)}) + \beta \right]} \left(\frac{\ln(1+x_{T(n)}) + \beta}{\theta} \right)^{n+\gamma-1} \times \exp\left(-\frac{\ln(1+x_{T(n)}) + \beta}{\theta}\right) \right\}$$

where $x = x_{T(1)}, \dots, x_{T(n)}$, $\theta > 0$. Note that

$$\left(\frac{1}{\theta} | x_{T(1)}, \dots, x_{T(n)}\right) \sim \text{gamma}\left(n + \gamma, \beta + \text{Ln}(1 + x_{T(n)})\right).$$

Bayesian Estimator of θ Under Quadratic Loss Function

The posterior distribution of θ is $IWD(n + \gamma, \beta + \text{Ln}(1 + x_n), c = 1)$, where IWD is Inverse Weibull Distribution (in other words $IWD = \frac{1}{W}$ where W is a Weibull variable) and the Bayes estimator of θ is based on record values under a quadratic loss function (7), for example $\hat{\theta}_{b,1}$, as given by Berger (1985) is

$$\begin{aligned} \hat{\theta}_{b,1} &= \frac{E\left(\omega(\theta)\mu(\theta) | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}\right)}{E\left(\omega(\theta) | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}\right)} \\ &= \frac{E\left(\frac{1}{\theta} | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}\right)}{E\left(\frac{1}{\theta^2} | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}\right)} \\ &= \frac{\beta + \text{Ln}(1 + x_{T(n)})}{n + \gamma + 1}. \end{aligned} \quad (10)$$

Bayesian Estimator of θ Under Squared Error Loss Function

Considering the posterior distribution of θ and loss function (8), the Bayes estimator based on record values, for example, $\hat{\theta}_{b,2}$, is given as (Berger, 1985):

$$\begin{aligned} \hat{\theta}_{b,2} &= E\left(\mu(\theta) | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}\right) \\ &= E\left(\theta | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}\right) \\ &= \frac{\text{Ln}(1 + x_{T(n)}) + \beta}{n + \gamma - 1}. \end{aligned}$$

As a result, the Bayesian estimation is formed as a differentia combination of both prior distribution and sample distribution as:

$$\hat{\theta}_{b,2} = \frac{n}{n + \gamma - 1} \frac{\text{Ln}(1 + x_{T(n)})}{n} + \frac{\gamma - 1}{n + \gamma - 1} \frac{\beta}{\gamma - 1}. \quad (11)$$

Interval Estimation of θ Based on Record Values: The Shortest Interval Estimation

To obtain the shortest $(1 - \alpha)\%$ confidence interval estimation based on record values, a pivot quantity is chosen as a function of a minimal sufficient statistic for parameter θ ($\hat{\theta}_{MLE}$) such that

$$Q = \frac{2 \text{Ln}(1 + X_{T(n)})}{\theta}.$$

From (6) it is clear that the distribution of Q is χ_{2n} for any constants a and b , hence,

$$\begin{aligned} P(a < Q < b) &= \int_a^b f_Q(t) dt \\ &= 1 - \alpha. \end{aligned} \quad (12)$$

Algebraic manipulation results in the confidence interval

$$\frac{2 \text{Ln}(1 + x_{T(n)})}{b} < \theta < \frac{2 \text{Ln}(1 + x_{T(n)})}{a},$$

thus, the length of interval is obtained as

$$L = 2 \text{Ln}(1 + x_{T(n)}) \left[\frac{1}{a} - \frac{1}{b} \right]. \quad (13)$$

To minimize (13) and satisfy (12), a and b are selected using the Lagrange multipliers method

$$\begin{aligned} \psi(a, b, \lambda) &= \\ &= 2 \text{Ln}(1 + x_{T(n)}) \left(\frac{1}{a} - \frac{1}{b} \right) + \lambda \left(\int_a^b f_Q(t) dt - (1 - \alpha) \right). \end{aligned}$$

After derivation by λ , a , and b , the following results:

$$\left\{ \begin{array}{l} \int_a^b f_Q(t) dt = 1 - \alpha \\ \frac{-2 \ln(1 + x_{T(n)})}{a^2} - \lambda f(a) = 0 \\ \frac{2 \ln(1 + x_{T(n)})}{b^2} + \lambda f(b) = 0 \end{array} \right. \Rightarrow \left\{ \begin{array}{l} \int_a^b f_Q(t) dt = 1 - \alpha \\ a^2 f_Q(a) = b^2 f_Q(b) \end{array} \right.$$

Accordingly, a and b must satisfy (14) to yield the shortest interval estimation for θ :

$$\begin{aligned} P(a < Q < b) &= \int_a^b f_Q(t) dt \\ &= 1 - \alpha, a^2 f_Q(a) \\ &= b^2 f_Q(b) \end{aligned} \quad (14)$$

Interval Estimation of θ Based on Record Values: Highest Posterior Density (HPD) θ Estimation

After obtaining the posterior distribution $\pi(\theta | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)})$, the problem of the likelihood that the parameter θ lies within the interval $[c_L, c_U]$ arises. Bayesians call the interval based on the posterior distribution a credible interval; the interval $[c_L, c_U]$ is said to be a $(1 - \alpha)\%$ credible interval for θ if

$$\int_{c_L}^{c_U} \pi(\theta | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}) d\theta = 1 - \alpha. \quad (15)$$

The Highest Posterior Density (HPD) region is given by $\{A : \pi(\theta | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}) \geq c\}$ where c is chosen so that

$$\begin{aligned} \int_{c_L}^{c_U} \pi(\theta | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}) d\theta &= 1 - \alpha \\ \pi(c_L | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}) &= \pi(c_U | X_{T(1)}, X_{T(2)}, \dots, X_{T(n)}) \end{aligned} \quad (16)$$

The HPD interval estimation is optimal in the sense that it results in the shortest interval. Let $\lambda = \frac{1}{\theta}$, by this assumption the posterior distribution of λ is Gamma $(n + \gamma, \ln(1 + x_n) + \beta)$. After algebraic manipulation, an HPD estimation $(1 - \alpha)\%$ for parameter θ based on records is given by

$$\begin{aligned} \frac{\Gamma^*(n + \gamma, A c_L, A c_U)}{\Gamma(n + \gamma)} &= 1 - \alpha, \left(\frac{c_L}{c_U} \right)^{n + \gamma - 1} \\ &= \exp(c_L A - c_U A), \end{aligned} \quad (17)$$

where $A = \beta + \ln(1 + x_{T(n)})$ and Γ^* is the generalized incomplete Gamma function. Therefore HPD interval estimation based on record values can be obtained as:

$$\theta \in \left[\frac{1}{c_U}, \frac{1}{c_L} \right]. \quad (18)$$

Simulation and Examples

MSE and Bias

To illustrate the estimation techniques developed, consider the following simulated data from the Lomax distribution:

3.286379	2.652416	1.325698
1.895476	16.420820	10.123657
1.254875	14.852147	12.985314
11.684235	15.365742	1085.950045
50.254198	850.569874	32.154875
950.548796	2423.065086	1.989562
84.254187	1240.325487	7372.085167
2.658474	352.325469	6524.123548
15.987455	33.659874	5487.214587
1.235478	3658.125489	9083.239327
48.236584	6985.125489	6.325698
448.125634	8754.215487	47739.689056
125.258643	25.365987	12543.2158746
25413.125487	256.326598	1254.365241
1.36548	16845.362545	25.326874
6985.125469	7.365214	121942.356923

LOMAX DISTRIBUTION INFERENCES FROM BAYESIAN AND CLASSICAL VALUES

This data was obtained by using the transformation $x_i = \frac{1}{(1-u_i)^\theta} - 1$, where u_i is a uniformly distributed random variable. If only the upper record values have been observed, these are:

3.286379	7372.085167
16.420820	9083.239327
1085.950045	47739.689056
2423.065086	121942.356923

for a non-informative prior distribution with $\gamma=0, \beta=1$, and $\gamma=8, \beta=7.56$ for an informative prior distribution. Results from equations (5), (10) and (11) for the parameter θ computed for $n=4, 5, 6, 7, 8$ are presented in Table1.

Interval Estimation

Results from using equations (14) and (15) for the parameter, $\lambda = \frac{1}{\theta}$ computed for $n=4, 5, 6, 7, 8$ are presented in Tables 2 and 3.

Table 1: Estimation, Bias and MSE

Number of Records (n=)		Estimate	Bias	MSE
4	$\hat{\theta}_{MLE}$	1.948300	0	0.9489683
5		1.781118	0	0.6344765
6		1.519049	0	0.3845852
7		1.539077	0	0.3383940
8		1.463914	0	0.2678805
4	$\hat{\theta}_{b,1}$ Non-Informative	1.758640	-0.18966006	0.6433108
5		1.650932	-0.13018638	0.4575572
6		1.444899	-0.07414991	0.2880506
7		1.471692	-0.06738463	0.2636236
8		1.412368	-0.05154600	0.2143157
4	$\hat{\theta}_{b,2}$ Non-Informative	2.931067	0.9827668	2.6528857
5		2.476398	0.6952796	1.4747832
6		2.022859	0.5308099	0.8076270
7		1.962257	0.4231795	0.6396728
8		1.815902	0.3519877	0.4737801
4	$\hat{\theta}_{b,1}$ Informative	1.181015	-0.7672848	0.6785692
5		1.176114	-0.6050046	0.4469587
6		1.111620	-0.4074296	0.2275325
7		1.145846	-0.3932308	0.2194012
8		1.133607	-0.3303074	0.1684260
4	$\hat{\theta}_{b,2}$ Informative	1.395746	-0.5525547	0.4308002
5		1.372133	-0.4089857	0.2774215
6		1.282638	-0.2364112	0.1378137
7		1.309539	-0.2295385	0.1372864
8		1.284754	-0.1791599	0.1082954

Table2: Shortest $(1 - \alpha)\%$ Confidence Interval Estimation Based On Record Values

Number of Records (n=)	Interval		Length	$(1 - \alpha)\%$ Confidence
4	0.7071710	4.549181	3.842010	90%
5	0.7314714	3.743103	3.011632	
6	0.6822589	2.965349	2.283090	
7	0.7401722	2.843073	2.102900	
8	0.7432804	2.589680	1.846400	
4	0.6255906	5.766975	5.141384	95%
5	0.6532331	4.580130	3.930780	
6	0.6139227	3.545798	2.931875	
7	0.6765692	3.340115	2.669904	
8	0.6765692	3.001246	2.324677	
4	0.5012662	9.505643	9.003677	99%
5	0.5321775	7.002903	6.470725	
6	0.5064018	5.142492	4.636090	
7	0.5586008	4.663650	4.104764	
8	0.5689107	4.069324	3.500414	

Table3: Highest Posterior Distribution (HPD) $(1 - \alpha)\%$ Interval Estimation Based On Record Statistics

Number of Records (n=)	$\lambda \in (\lambda_L, \lambda_U)$		$\theta \in [\frac{1}{\lambda_U}, \frac{1}{\lambda_L}]$		Length	$(1 - \alpha)\%$ Confidence
4	0.414500	1.137700	0.878966	2.412545	1.533579	90%
5	0.430000	1.140900	0.876501	2.325581	1.449080	
6	0.472900	1.196200	0.835980	2.114612	1.278631	
7	0.467300	1.164000	0.859100	2.139900	1.280846	
8	0.483600	1.173200	0.852369	2.067825	1.215455	
4	0.3668000.	1.237600	0.808015	2.726281	1.918266	95%
5	383300	1.236500	0.808734	2.608923	1.800188	
6	0.423500	1.293800	0.772917	2.361275	1.588358	
7	0.421100	1.254100	0.797384	2.374733	1.577384	
8	0.437700	1.260800	0.793147	2.284670	1.491523	
4	0.295500	1.416700	0.705865	3.384095	2.678229	99%
5	0.312600	1.407700	0.710378	3.198976	2.488598	
6	0.348500	1.468000	0.681198	2.869400	2.188242	
7	0.350100	1.415400	0.706514	2.856327	2.149813	
8	0.366900	1.417600	0.705417	2.725538	2.020121	

Figure 1: MSE's of the Estimators $\hat{\theta}_{MLE}$, $\hat{\theta}_{b,1}$, and $\hat{\theta}_{b,2}$ Informative and Non-Informative

Figure 2: Lengths of the Shortest Interval and Highest Posterior Distribution (HPD) Estimations Based on Record Statistics for 90% Confidence for $n=4,5,6,7,8$ and confidence=90

Figure 3: Lengths of the Shortest Interval and Highest Posterior Distribution (HPD) Estimations Based on Record Statistics for 95% Confidence

Figure 4: Lengths of the Shortest Interval and Highest Posterior Distribution (HPD) Estimations Based on Record Statistics for 99% Confidence

Figure 5: Lengths of the Shortest Interval and Highest Posterior Distribution (HPD) Estimations Based on Record Statistics for 90%, 95% and 99% Confidence

Conclusion

MLE and Bayesian estimations based on record values were obtained. For the Bayes estimations, in order to control the passive parameter of society, the prior distribution was assumed to be Gamma. In addition, Bayes estimations were obtained for two types of loss functions and, with a view of prior estimation, using an informative posterior density function, HPD estimations were obtained in a theoretic way (see Table 3). Conversely, the shortest confidence interval was obtained using a MLE based on records and equation (14) (Tate & Klett, 1959); see Table 2 for results.

Theoretical results of the study are explained numerically by simulation in the following ways: Table 1 shows that an informative Bayesian estimation based on

records under squared error loss function has the lowest MSE compared to the informative Bayesian estimation, which is based on records under a quadratic loss function with a non-informative Bayesian estimation under a squared error loss function.. This is also compared to a MLE based on records; comparisons are shown in Figure 1. Confidence intervals and their lengths for record numbers 4, 5, 6, 7, 8 and confidence levels 90%, 95% and 99% were obtained. The longer the n , the shorter the interval distance (see Table 3). Comparing Tables 2 and 3, it the point at which HPD estimations have a shorter length than the confidence interval with optimal length is observed. This comparison is illustrated in Figures 2, 3 and 4 for various confidence levels; Figure 5 shows the comparison for all levels.

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Inverted Exponential Distribution Under a Bayesian Viewpoint

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The objective of this study was to examine the properties of Bayes estimators of the parameter, reliability function and hazard rate under the symmetric and asymmetric loss functions for the inverted exponential model. The Bayes predictive interval and the Bayes estimate of shift point are also determined. A simulation study was carried out to study the properties of the Bayes estimators.

Key words: Bayes estimators, LINEX loss function, squared error loss function, prediction limits.

Introduction

The exponential distribution is frequently used in lifetime data analysis, but its suitability is restricted to constant hazard (failure) rates. For situations where a failure rate is monotonically increasing or decreasing, the two-parameter Weibull and the Gamma distributions are popular for analyzing lifetime data. Both distributions have increasing and decreasing hazard rates depending on the shape parameter. However, one of the major disadvantages of the Gamma distribution is that its distribution and survival functions cannot be expressed in a closed form if the shape parameter is not an integer. Moreover, there are terms involving the incomplete Gamma function, thus, it is necessary to obtain distribution, survival or hazard functions by numerical integration. This makes the Gamma distribution less popular compared to the Weibull distribution, which has a closed form for the hazard and survival functions, but the Weibull distribution also has disadvantages. Bain & Engelhardt (1991) demonstrated that the maximum likelihood estimators of the Weibull distribution might not behave properly for all parametric ranges.

Recently two new distributions have been introduced: the generalized Exponential (two - parameter) and the inverted Exponential (one - parameter) distributions. The generalized

exponential distribution can be used effectively in situations where a skewed distribution is needed. Gupta & Kundu (1999, 2002) and Raqab & Ahsanullah (2001) investigated several properties of the two parameter generalized exponential distribution.

It is remarkable that most of the Bayesian inference procedures have been developed with the usual squared error loss function (SELF), which is symmetrical and associates equal importance to losses due to overestimation and underestimation of equal magnitude. However, such a restriction may be unrealistic in the most situations of practical importance. For example, in estimating reliability and hazard rate functions, an overestimation is usually much more serious than an underestimation. The use of a symmetrical loss function in Bayesian framework might be inappropriate (Parsian & Kirmani, 2002).

A useful asymmetric loss function known as the LINEX loss function (LLF) was introduced by Varian (1975) and has been used in several studies. The LLF for any parameter θ is given by

$$L(\bar{\Delta}) = e^{a\bar{\Delta}} - a\bar{\Delta} - 1; \bar{\Delta} = \hat{\theta} - \theta \quad (1.1)$$

where $a(\neq 0)$ is the shape parameter and $\hat{\theta}$ is any estimate of the parameter θ .

The sign and magnitude of 'a' represents the direction and degree of

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asymmetry respectively. The positive (negative) value of 'a' is used when overestimation is more (less) serious than underestimation. The LLF (1.1) is approximately squared error and almost symmetric if $|a|$ is near zero. Many authors have discussed estimation procedures under a LLF criterion, however a few recently presented studies using Bayesian and/or LLF criterions, for example see Xu & Shi (2004), Ahmadi, et al. (2005), Son & Oh (2006), Singh, et al. (2007) and Prakash (2011).

Present article examine the properties of Bayes estimators for the r^{th} power of the parameter θ , reliability function, hazard rate and the shift point. Both the symmetric (SELF) and asymmetric (LLF) loss functions were considered and the behavior of the future observations is predicted in terms of the predictive interval.

The Model and the Prior Distributions

The model considered is the inverted Exponential distribution with a distribution function

$$F(x; \theta) = e^{-1/x\theta}; \quad x > 0, \theta > 0. \quad (2.1)$$

This distribution has no finite moments. The reliability function and hazard rate for a specific mission time $t(>0)$ are obtained as

$$\psi(t) = 1 - e^{-1/t\theta}$$

and

$$\rho(t) = \frac{1}{t^2\theta} (e^{1/t\theta} - 1)^{-1}.$$

If $x_1, x_2, \dots, x_n$ are n independent random samples from model (2.1), then the likelihood function is obtained as

$$L(x_1, x_2, \dots, x_n | \theta) = \frac{1}{\theta^2} \prod_{i=1}^n x_i^{-2} \exp\left(-\frac{T_n}{\theta}\right),$$

$$T_n = \left\{ \sum_{i=1}^n x_i^{-1} \right\}. \quad (2.2)$$

The maximum likelihood estimate (MLE) of the parameter θ is $\hat{\theta} = \frac{1}{n} T_n$. Further,

$x_i^{-1}; i=1, 2, \dots, n$ are iid Exponential with parameter θ , and the distribution of T_n is a Gamma distribution with a probability density function (pdf)

$$f(T_n) = \frac{T_n^{n-1}}{\Gamma n} e^{-\frac{T_n}{\theta}} \theta^{-n}; \quad T_n > 0. \quad (2.3)$$

It is assumed that, from a Bayesian viewpoint, there is clearly no way in which it can be stated that one prior is better than another (Arnold & Press, 1983). More frequently the case is that attention to a given flexible family of priors is restricted and a prior is chosen from that family. Thus, in present case the conjugate prior of the parameter θ is considered as inverted Gamma distribution and is given as:

$$g_1(\theta) = \frac{\beta^\alpha}{\Gamma \alpha} \theta^{-(\alpha+1)} e^{-\frac{\beta}{\theta}}; \quad \alpha > 0, \beta > 0. \quad (2.4)$$

Further, in a situation where a researcher has no or very little prior information about the parameter θ , a family of priors defined as

$$g_2(\theta) = \theta^{-\delta}; \quad \delta > 0, \quad (2.5)$$

If $\delta = 0$ a diffuse prior is obtained, and if $\delta = 1$ a non-informative prior is obtained. The posterior density of θ under the prior $g_1(\theta)$ is given by

$$Z_1(\theta) = \frac{(T_n + \beta)^{\alpha+n}}{\Gamma(\alpha+n)} e^{-\frac{(T_n + \beta)}{\theta}} \theta^{-(\alpha+n+1)}. \quad (2.6)$$

This is an inverted Gamma distribution with parameters $(\alpha+n)$ and $(T_n + \beta)$. Similarly, the posterior density of θ corresponding to $g_2(\theta)$ is

$$Z_2(\theta) = \frac{(T_n)^{\delta+n-1}}{\Gamma(\delta+n-1)} e^{-\frac{T_n}{\theta}} \theta^{-(\delta+n)}. \quad (2.7)$$

Bayes Prediction Limits

Predicting the nature of the future behavior of an observation when sufficient information regarding the past and present behavior of an event or an observation are known or given is an important problem in lifetime models. Statistical prediction limits have many applications in quality control and reliability problems and the determination of these limits has been extensively investigated. It may be desirable to obtain confidence limits not only for any parameter of a distribution, but also for a future observation drawn from the same model. Such limits are called prediction limits.

If a $100\varepsilon\%$ prediction limit for an additional observation is desired, for example Y , given a random sample $\underline{X} = (x_1, x_2, \dots, x_n)$ from model (2.1), the problem is equivalent to determining the region $R(\underline{X})$ such that $R(\underline{X})$ covers the average proportion ε of the distribution of Y .

A wealth of literature is available regarding predictive inference for future failure distributions; examples of studies involving predictive inference for future observations include: Aitchison & Dunsmore (1975), Bain (1978), Sinha (1990), Raqab (1997), Cramer & Kamps (1998), Raqab & Madi (2002), Ahmed et al. (2007) and Prakash & Prasad (2010).

In the context of prediction, it may be stated that (l, u) is a $100(1-\varepsilon)\%$ prediction interval for a future observation Y if

$$\Pr(l \leq Y \leq u) = 1 - \varepsilon; \quad (3.1)$$

where l and u are the lower and upper prediction limits for the random variable Y , and $1-\varepsilon$ is termed the confidence prediction coefficient.

The predictive distribution of a future observation Y may be obtained from model (2.1) by simplifying

$$h(y|\underline{X}) = \int_{\theta} f(y|\theta) \cdot Z_1(\theta) d\theta$$

$$\Rightarrow h(y|\underline{X}) = (n+\alpha)y^{-2} \frac{(T_n + \beta)^{n+\alpha}}{(T_n + \beta + y^{-1})^{n+\alpha+1}}, \quad (3.2)$$

and $100(1-\varepsilon)\%$ equal tail prediction interval is obtained by solving

$$\int_0^l h(y|\underline{X}) dy = \int_u^{\infty} h(y|\underline{X}) dy = \frac{\varepsilon}{2}. \quad (3.3)$$

Hence, the Bayes prediction limits and length of the Bayes predictive interval are obtained as

$$l = \left[(T_n + \beta) \left\{ \left(\frac{\varepsilon}{2} \right)^{-1/(n+\alpha)} - 1 \right\} \right]^{-1}, \quad (3.4)$$

$$u = \left[(T_n + \beta) \left\{ \left(1 - \frac{\varepsilon}{2} \right)^{-1/(n+\alpha)} - 1 \right\} \right]^{-1} \quad (3.5)$$

and

$$I = u - l. \quad (3.6)$$

Bayes Estimators for Reliability Function and Hazard Rate

The Bayes estimates of $\psi(t)$ and $\rho(t)$ under the SELF corresponding to the posterior $Z_1(\theta)$ are obtained as

$$\psi_1 = E_p(\psi(t)) = 1 - \left(1 + \frac{1}{t(T_n + \beta)} \right)^{-(n+\alpha)} \quad (4.1)$$

and

$$\begin{aligned} \rho_1 &= E_p(\rho(t)) = \frac{1}{t^2} I(0, \infty, \rho_{s1}); \\ \rho_{s1} &= z(e^{z/t} - 1)^{-1}, \end{aligned} \quad (4.2)$$

where

$$I(z_1, z_2, f_z) = \frac{(T_n + \beta)^{\alpha+n}}{\Gamma(\alpha+n)} \int_{z_1}^{z_2} f_z \cdot e^{-(T_n + \beta)z} z^{\alpha+n-1} dz.$$

Here f_z is a function of z and suffix P indicates the expectation taken under posterior density.

Similarly, the Bayes estimators of the reliability function and hazard rate under the LLF-criterion corresponding to the posterior $Z_1(\theta)$ are obtained by solving

$$\begin{aligned} \psi_2 &= -\frac{1}{a} \ln E_p(e^{-a\psi(t)}) \\ &= -\frac{1}{a} \ln(e^{-a} I(0, \infty, \psi_{L1})), \\ \psi_{L1} &= \exp(ae^{-z/t}) \end{aligned}$$

and

$$\begin{aligned} \rho_2 &= -\frac{1}{a} \ln E_p(e^{-a\rho(t)}) \\ &= -\frac{1}{a} \ln I(0, \infty, \rho_{L1}), \\ \rho_{L1} &= \exp\left(\frac{a}{t^2} \rho_{S1}\right). \end{aligned}$$

The expressions of the risks for these estimators under the SELF and the LLF loss criterions are $R_{(S)}(\psi_i)$, $R_{(L)}(\psi_i)$, $R_{(S)}(\rho_i)$ and $R_{(L)}(\rho_i)$; $i=1, 2$. Note that these do not exist in closed form. However, a numerical study has been carried out in later section.

The Bayes Estimator for Shift Point

In order to obtain information about their endurance, manufactured items such as mechanical or electronic components, are often put to life tests and life times are observed periodically. Physical systems manufacturing different items are often subject to random fluctuations and it may happen that, at some point, there is a change in the parameter. The objective of this study was to determine when

and where this change starts occurring; this is called the shift point inference problem. Bayesian modeling may play an important role in the study of such shift point problems (Broemeling & Tsurumi, 1987; Jani & Pandya, 1999).

Consider first a sequence of independent random sample of size n such as $x_1, x_2, \dots, x_m, x_{m+1}, \dots, x_n$ from model (2.1) with a reliability function $\psi_1(t)$ at mission time $t(>0)$. If it is later found that there was a change in the system at some point in time m , this will be reflected in the sequence after x_m by a change in the reliability $\psi_2(t)$ at mission time t .

Thus, from model (2.1), the pdf of the random samples $x_1, x_2, \dots, x_m$ of size m is given by

$$\begin{aligned} f(x_i; \theta_1) &= \frac{1}{\theta_1 x_i^2} \exp\left(-\frac{1}{\theta_1 x_i}\right); \\ i &= 1, 2, \dots, m, \theta_1 > 0. \end{aligned} \quad (5.1)$$

Similarly, the remaining $x_{m+1}, x_{m+2}, \dots, x_n$ components of size $(n-m)$ follow model (2.1) with the pdf

$$\begin{aligned} f(x_i; \theta_2) &= \frac{1}{\theta_2 x_i^2} \exp\left(-\frac{1}{\theta_2 x_i}\right); \\ i &= m+1, m+2, \dots, n, \theta_2 > 0. \end{aligned} \quad (5.2)$$

If prior information regarding the parameter is considered as the conjugate prior, then prior $g_1(\theta)$ is redefined as

$$\begin{aligned} g_3(\theta_i) &= \frac{\beta^\alpha}{\Gamma \alpha} \theta_i^{-(\alpha+1)} e^{-\frac{\beta}{\theta_i}}; \\ \alpha &> 0, \beta > 0, i = 1, 2. \end{aligned} \quad (5.3)$$

Further, the prior distribution for shift point m is considered to be discrete uniform over the set $\{1, 2, \dots, n-1\}$. Hence, the joint posterior density for the parameters θ_1, θ_2 and m is

$$Z_3(\theta_1, \theta_2, m) = k^{-1} \exp\left(-\frac{\omega_1}{\theta_1} - \frac{\omega_2}{\theta_2}\right) \theta_1^{-m-\alpha-1} \theta_2^{-n+m-\alpha-1};$$

(5.4)

where

$$k^{-1} = \sum_{m=1}^{n-1} \Delta,$$

$$\Delta = \left(\frac{\Gamma(m+\alpha) \Gamma(n-m+\alpha)}{\omega_1^{m+\alpha} \omega_2^{n-m+\alpha}} \right),$$

$$\omega_1 = \beta + \sum_{i=1}^m x_i^{-1}$$

and

$$\omega_2 = \beta + \sum_{i=m+1}^n x_i^{-1}.$$

This case may be verified without considering shift point situations with $\theta_1 = \theta_2$.

The marginal posterior density for shift point m is

$$Z_4(m) = k^{-1} \Delta. \quad (5.5)$$

Therefore, the Bayes estimator for shift point m under the SELF and LLF are obtained respectively as (suffixes S and L indicates the loss criterion selected as the SELF and LLF respectively)

$$\hat{m}_S = k^{-1} \sum_{m=1}^{n-1} (m\Delta)$$

and

$$\hat{m}_L = -\frac{1}{a} \ln \left\{ k^{-1} \sum_{m=1}^{n-1} (e^{-am} \Delta) \right\}. \quad (5.6)$$

If no further information regarding θ_i ; $i=1, 2$ is available and they are assumed as *a priori* independent random variables, then the non-informative prior is considered from (2.7) with ($\delta=1$) such that

$$g_4(\theta_i) = \frac{1}{\theta_i}; i=1, 2,$$

The Bayes estimators for shift point m under SELF and LLF are obtained from (5.6) by replacing $\beta=0=\alpha$ as:

$$\hat{m}'_S = k_1^{-1} \sum_{m=1}^{n-1} (m\Delta')$$

and

$$\hat{m}'_L = -\frac{1}{a} \ln \left\{ k_1^{-1} \sum_{m=1}^{n-1} (e^{-am} \Delta') \right\}. \quad (5.7)$$

where

$$k_1^{-1} = \sum_{m=1}^{n-1} \Delta',$$

$$\Delta' = \frac{\Gamma m \Gamma(n-m)}{\omega_3^m \omega_4^{n-m}},$$

$$\omega_3 = \sum_{i=1}^m x_i^{-1}$$

and

$$\omega_4 = \sum_{i=m+1}^n x_i^{-1}.$$

The Bayes Estimator for Parameter θ

The Bayes estimator for θ^r (r being any integer) obtained corresponding to the posterior $Z_1(\theta)$ under the SELF is

$$\hat{\theta}_S^r = \frac{\Gamma(n+\alpha-r)}{\Gamma(n+\alpha)} (T_n + \beta)^r. \quad (6.1)$$

In particular, the Bayes estimators for the parameters $\theta(r=1)$ and $\frac{1}{\theta}(r=-1)$ are given respectively as

$$\hat{\theta}_S = \frac{T_n + \beta}{n + \alpha - 1}$$

and

$$\hat{\theta}_s^{-1} = \frac{n + \alpha}{T_n + \beta} \quad (6.2)$$

Similarly, the Bayes estimator for θ^r under the LLF is obtained with respect to the posterior $Z_1(\theta)$ by solving

$$\hat{\theta}_L^r = -\frac{1}{a} \ln I(0, \infty, e^{-a\theta^r}). \quad (6.3)$$

The Bayes estimator for parameter θ does not exist in a closed form. However, the Bayes estimator for $\frac{1}{\theta}$ is given as

$$\hat{\theta}_L^{-1} = \left(\frac{n + \alpha}{a} \right) \ln \left(1 + \frac{a}{T_n + \beta} \right). \quad (6.4)$$

Note that, all results discussed thus hold for the posterior distribution $Z_2(\theta)$ if $\alpha(=\delta-1)$ and $\beta(=0)$ are substituted.

Numerical Analysis

To assess and study the properties of the proposed Bayes estimators and prediction interval, the random samples are generated as follows:

1. For the given values of prior parameters α and β , generate θ using the prior density $g_1(\theta)$. The values of α and β are chosen to maintain the prior variance at 1.00 and the considered values are $(\beta, \alpha) = (02, 03)$, $(10, 06)$ and $(30, 11)$.
2. Using θ obtained in (1), generate 10,000 random samples size $n = 5, 10, 15$ from the considered model (2.1).

Bayes Prediction Interval

The Bayes prediction intervals were obtained with the level of significance $\varepsilon = 99\%, 95\%, 90\%$ and results are presented in Table 1. The intervals tend to be wider as the sample size n increases when other parametric

values are fixed. The opposite trend was observed when a combination of the prior parameters increases. It is also noted that when the confidence level decreases the intervals also decrease.

Bayes Estimators for Reliability Function

Results for $a = 0.50, 1.00, 1.50$ and $t = 2.50$ (hours) are presented in Table 2. As Table 2 shows, the risk of Bayes estimators ψ_1 and ψ_2 decrease as sample size n increases under both loss criteria, SELF and LLF. In addition, the risk of ψ_1 increases as 'a' increases under a LLF loss criterion. A similar trend was observed for ψ_2 when 'a' increases under both loss criteria. A decreasing trend in risk was observed when a set of prior parameters increased only for ψ_1 under both loss criterions with other fixed parametric values. The magnitude of the risk is nominal for both estimators under the LLF.

Bayes Estimators for Hazard Rate

The numerical findings are presented in Table 3 for a similar set of values of 'a' and t. The performances of Bayes estimators ρ_1 and ρ_2 are similar to the Bayes estimators of the reliability functions ψ_1 and ψ_2 when sample size n or 'a' increase respectively. The magnitude of the risk is nominal for both estimators under the LLF loss criterion.

Bayes Estimators for Shift Point

For a similar set of values considered earlier with $a = 0.25, 0.50, 1.00, 1.50$, samples were generated for $n = 10, 15, 20$ and results are presented in Tables 4 and 5. It was observed that, when sample size n increases, the magnitude of the Bayes estimator (under SELF) increases but the increment in magnitude is nominal (robust). Further, an opposite trend was observed when values of the set of prior parameters increase. Similar properties have been noted for the Bayes estimate of the shift point under LLF, and a decreasing trend in the

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magnitude of the estimate has also been observed when 'a' increases.

Bayes Estimators for the r^{th} Power of the Parameter

The numerical findings presented in Tables 6 and 7 are for $a = 0.50, 1.00, 1.50$ and $r = \pm 1, \pm 2$. Based on results show in the tables it may be concluded that the magnitude of the risk increases (decreases) when $a(n)$ increases when other parametric values are fixed. The increasing trend in the magnitude has also been observed when prior parameters increase (only for $r = -1, -2$). Further, the magnitude of the risk is smaller for these estimators under the LLF.

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Table 1: Bayes Prediction Limits

n	β, α	$\varepsilon = 99\%$		$\varepsilon = 95\%$		$\varepsilon = 90\%$	
		l	u	l	u	l	u
05	02,03	1.2272	1.2648	1.2662	1.4722	1.2825	1.7349
	10,06	0.8442	0.8697	0.9292	1.0784	0.8212	1.1070
	30,11	0.5941	0.6118	0.5458	0.6326	0.5265	0.7077
10	02,03	2.2409	2.3083	2.0216	2.3447	1.3851	1.8645
	10,06	1.3329	1.3727	1.2600	1.4604	1.0571	1.4209
	30,11	0.8032	0.8271	0.7453	0.8631	0.6920	0.9287
15	02,03	2.0570	2.1284	2.7406	3.1751	1.7060	2.2914
	10,06	1.4661	1.5097	1.4084	1.6311	1.3485	1.8098
	30,11	0.8807	0.9068	0.9548	1.1052	0.7790	1.0445

Table 2: Risks for Bayes Estimate of Reliability Function

n	a	β, α	ψ_1	$R_s(\psi_1)$	$R_L(\psi_1)$	ψ_2	$R_s(\psi_2)$	$R_L(\psi_2)$
05	0.50	02,03	0.1125	14.7296	1.0523	0.0123	14.7012	1.0502
		10,06	0.0903	14.7612	1.0541	0.0780	14.8141	1.0607
		30,11	0.0584	14.8300	1.0578	0.0055	14.2740	1.0266
	1.00	02,03	0.1059	14.7296	2.8066	0.2646	14.7132	2.8041
		10,06	0.0818	14.7612	2.8106	0.1418	14.8245	2.8180
		30,11	0.0559	14.8300	2.8191	0.0567	14.5478	2.7834
	1.50	02,03	0.1190	14.7296	4.6586	0.2088	14.7194	4.6564
		10,06	0.0847	14.7612	4.6647	0.1302	14.8335	4.6724
		30,11	0.0561	14.8300	4.6777	0.0339	14.6418	4.6416
10	0.50	02,03	0.1827	5.9753	0.4270	0.8166	6.0077	0.4283
		10,06	0.1179	5.9827	0.4274	1.3328	5.8511	0.4193
		30,11	0.0768	6.0081	0.4288	0.5438	5.1131	0.3785
	1.00	02,03	0.1348	5.9753	1.1389	0.2641	6.0863	1.1399
		10,06	0.1057	5.9827	1.1398	0.6477	5.9076	1.1298
		30,11	0.0729	6.0081	1.1429	0.2365	5.5525	1.0852
	1.50	02,03	0.1668	5.9753	1.8905	0.0643	6.1807	1.8912
		10,06	0.1119	5.9827	1.8919	0.5157	5.9292	1.8813
		30,11	0.0734	6.0081	1.8967	0.0950	5.7037	1.8382
15	0.50	02,03	0.1932	0.4478	0.0321	1.5324	0.4472	0.0372
		10,06	0.1434	0.4489	0.0321	1.0564	0.5884	0.0393
		30,11	0.0856	0.4517	0.0323	0.8032	0.3951	0.0291
	1.00	02,03	0.2639	0.4478	0.0856	0.3801	0.4658	0.0913
		10,06	0.1468	0.4489	0.0857	0.3046	0.6159	0.0938
		30,11	0.0824	0.4517	0.0861	0.2365	0.4217	0.0822
	1.50	02,03	0.2005	0.4478	0.1421	0.7962	0.4796	0.1480
		10,06	0.1315	0.4489	0.1423	0.2168	0.6929	0.1505
		30,11	0.0870	0.4517	0.1429	0.0306	0.4310	0.1388

INVERTED EXPONENTIAL DISTRIBUTION UNDER A BAYESIAN VIEWPOINT

Table 3: Risks for Bayes Estimate of Hazard Rate

n	a	β, α	ρ_1	$R_s(\rho_1)$	$R_L(\rho_1)$	ρ_2	$R_s(\rho_2)$	$R_L(\rho_2)$
05	0.50	02,03	0.1181	14.1954	1.0230	0.3540	14.1651	1.0208
		10,06	0.1238	14.1827	1.0223	0.0195	14.2119	1.0294
		30,11	0.1398	14.2215	1.0244	0.1485	13.6402	0.9914
	1.00	02,03	0.1411	14.1954	2.7397	0.1463	14.1760	2.7368
		10,06	0.1216	14.1827	2.7381	0.3392	14.2227	2.7464
		30,11	0.1291	14.2215	2.7430	0.1184	13.9077	2.7026
	1.50	02,03	0.1157	14.1954	4.5564	0.0612	14.1813	4.5534
		10,06	0.1148	14.1827	4.5540	0.2712	14.2315	4.5631
		30,11	0.1317	14.2215	4.5615	0.1289	13.9996	4.5181
10	0.50	02,03	0.1944	5.7601	0.4152	0.0918	5.7696	0.4169
		10,06	0.0770	5.7694	0.4157	1.2395	5.6419	0.4077
		30,11	0.1676	5.8155	0.4182	0.3497	4.8807	0.3650
	1.00	02,03	0.1936	5.7601	1.1119	0.1672	5.7782	1.1138
		10,06	0.0883	5.7694	1.1130	0.6489	5.6963	1.1031
		30,11	0.1692	5.8155	1.1189	0.1737	5.3099	1.0537
	1.50	02,03	0.1841	5.7601	1.8493	0.1399	5.7825	1.8514
		10,06	0.0745	5.7694	1.8510	0.4315	5.7171	1.8404
		30,11	0.1730	5.8155	1.8599	0.0694	5.4577	1.7899
15	0.50	02,03	0.1314	0.4286	0.0310	1.1623	0.5327	0.0364
		10,06	0.1164	0.4258	0.0308	0.3103	0.4731	0.0386
		30,11	0.1303	0.4386	0.0316	0.5889	0.3813	0.0283
	1.00	02,03	0.2328	0.4286	0.0832	0.8862	0.5482	0.0897
		10,06	0.1980	0.4258	0.0828	0.0166	0.5017	0.0921
		30,11	0.1870	0.4386	0.0844	0.0024	0.4074	0.0804
	1.50	02,03	0.0677	0.4286	0.1384	0.5436	0.5566	0.1455
		10,06	0.1858	0.4258	0.1379	0.3606	0.5479	0.1479
		30,11	0.1560	0.4386	0.1403	0.0739	0.4165	0.1360

Table 4: Bayes Estimate of Shift Point Under SELF

Prior Density	$(\beta, \alpha) \downarrow n \rightarrow$	10	15	20
Conjugate	02,03	4.9919	5.0069	5.0169
	10,06	4.9493	4.9641	4.9740
	30,11	4.4590	4.4724	4.4813
Non-Informative	00,00	4.8946	4.9112	4.9472

Table 5: Bayes Estimate of Shift Point Under LLF

Prior Density	n	$(\beta, \alpha) \downarrow a \rightarrow$	0.25	0.50	1.00	1.50
Conjugate Prior	10	02,03	4.0051	3.2058	3.1096	3.0163
		10,06	3.7951	3.1965	3.1006	3.0076
		30,11	3.7196	3.1806	3.0852	2.9926
	15	02,03	4.2321	3.6035	3.4954	3.3905
		10,06	3.8554	3.2342	3.1372	3.0431
		30,11	3.7907	3.2191	3.1225	3.0288
	20	02,03	4.5051	3.7436	3.6313	3.5224
		10,06	3.8615	3.3673	3.2663	3.1683
		30,11	3.8356	3.3249	3.2252	3.1284
Non-Informative Prior	10	00,00	3.9477	3.2412	3.1440	3.0497
	15	00,00	4.0255	4.0184	3.9657	3.8467
	20	00,00	4.0926	4.0783	4.0424	3.9502

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Table 6: Risks for the Bayes Estimate of θ^r

n	a	β, α	$r = -2$				$r = 2$			
			$R_{(S)}(\hat{\theta}_S^r)$	$R_{(L)}(\hat{\theta}_S^r)$	$R_{(S)}(\hat{\theta}_L^r)$	$R_{(L)}(\hat{\theta}_L^r)$	$R_{(S)}(\hat{\theta}_S^r)$	$R_{(L)}(\hat{\theta}_S^r)$	$R_{(S)}(\hat{\theta}_L^r)$	$R_{(L)}(\hat{\theta}_L^r)$
05	0.50	02,03	13.288	0.9700	13.343	0.9726	10.285	4.5467	1.6360	1.9821
		10,06	13.719	0.9961	13.804	1.0061	11.384	7.0496	0.7671	1.5262
		30,11	14.246	1.0258	13.706	0.9949	14.270	9.1108	2.0452	2.9854
	1.00	02,03	13.288	2.6178	13.440	2.6363	10.285	6.0364	2.3876	2.5377
		10,06	13.719	2.6776	13.816	2.6959	11.384	9.8003	1.6753	2.2181
		30,11	14.246	2.7460	13.981	2.7115	14.270	9.7628	5.7040	3.6989
	1.50	02,03	13.288	4.4315	13.518	4.4154	10.285	8.4251	7.7043	2.8013
		10,06	13.719	4.4615	13.859	4.4899	11.384	11.112	6.9306	2.4745
		30,11	14.246	4.5661	14.082	4.5336	14.270	10.550	5.9482	4.2190
10	0.50	02,03	5.4663	0.3986	5.4705	0.3995	3.9248	0.9999	0.1222	0.0180
		10,06	5.5413	0.4029	5.3734	0.3929	3.6741	0.9096	0.2512	0.0331
		30,11	5.7225	0.4131	4.8579	0.3637	9.1533	3.4073	0.6589	0.8112
	1.00	02,03	5.4663	1.0738	5.4805	1.0754	3.9248	1.2036	0.1302	0.0354
		10,06	5.5413	1.0838	5.4371	1.0701	3.6741	8.8628	0.2709	0.0474
		30,11	5.7225	1.1071	5.2914	1.0512	9.1533	4.6310	0.6659	0.8903
	1.50	02,03	5.4663	1.3599	5.4858	1.7949	3.9248	2.0292	0.1518	0.1044
		10,06	5.5413	1.8063	5.4661	1.7915	3.6741	9.0630	0.2838	0.0675
		30,11	5.7225	1.8419	5.4438	1.7871	9.1533	5.4232	0.7181	0.9334
15	0.50	02,03	0.3864	0.0286	0.4302	0.0342	0.0087	0.0009	0.0368	0.0038
		10,06	0.3975	0.0292	0.4434	0.0364	0.0045	0.0005	0.0443	0.0045
		30,11	0.4208	0.0306	0.3550	0.0267	0.1127	0.0203	0.0034	0.0004
	1.00	02,03	0.3864	0.0666	0.4416	0.0847	0.0087	0.0028	0.0462	0.0097
		10,06	0.3975	0.0791	0.4818	0.0873	0.0045	0.0017	0.0628	0.0104
		30,11	0.4208	0.0822	0.3807	0.0769	0.1127	0.1251	0.0045	0.0019
	1.50	02,03	0.3864	0.1225	0.4565	0.1379	0.0087	0.0054	0.0525	0.0182
		10,06	0.3975	0.1322	0.5402	0.1406	0.0045	0.0034	0.0737	0.0178
		30,11	0.4208	0.1369	0.3900	0.1307	0.1127	0.4628	0.0070	0.0062

Table 7: Risks for the Bayes Estimate of θ^r

n	a	β, α	$r = -1$				$r = 1$			
			$R_{(S)}(\hat{\theta}_S^r)$	$R_{(L)}(\hat{\theta}_S^r)$	$R_{(S)}(\hat{\theta}_L^r)$	$R_{(L)}(\hat{\theta}_L^r)$	$R_{(S)}(\hat{\theta}_S^r)$	$R_{(L)}(\hat{\theta}_S^r)$	$R_{(S)}(\hat{\theta}_L^r)$	$R_{(L)}(\hat{\theta}_L^r)$
05	0.50	02,03	12.002	0.8972	12.029	0.8983	2.0144	0.1875	2.3556	0.2156
		10,06	12.224	0.9110	12.332	0.9193	1.6934	0.1622	2.1786	0.2043
		30,11	12.723	0.9401	12.246	0.9116	0.7526	0.0784	0.7404	0.0763
	1.00	02,03	12.002	2.4474	12.082	2.4583	2.0144	0.5928	2.7107	0.7636
		10,06	12.224	2.4806	12.333	2.4953	1.6934	0.5180	2.4282	0.7162
		30,11	12.723	2.5485	12.510	2.5191	0.7526	0.2664	1.0455	0.3536
	1.50	02,03	12.002	4.1081	12.129	4.1356	2.0144	1.1044	3.0264	1.5302
		10,06	12.224	4.1595	12.337	4.1834	1.6934	0.9617	2.6799	1.4354
		30,11	12.723	4.2639	12.610	4.2399	0.7526	0.5180	1.3107	0.8213
10	0.50	02,03	4.8368	0.3626	4.8418	0.3629	0.9737	0.0933	1.2338	0.1153
		10,06	4.8905	0.3657	4.7321	0.3559	0.9049	0.0880	1.1338	0.1057
		30,11	5.0740	0.3764	4.2866	0.3297	0.5090	0.0525	0.2913	0.0298
	1.00	02,03	4.8368	0.9901	4.8420	0.9903	0.9737	0.2977	1.3538	0.3923
		10,06	4.8905	0.9976	4.7943	0.9843	0.9049	0.2833	1.2602	0.3689
		30,11	5.0740	1.0225	4.6961	0.9708	0.5090	0.1769	0.4723	0.1598
	1.50	02,03	4.8368	1.6626	4.8461	1.6646	0.9737	0.5517	1.4573	0.7545
		10,06	4.8905	1.6742	4.8244	1.6604	0.9049	0.5279	1.3707	0.7208
		30,11	5.0740	1.7125	4.8414	1.6639	0.5090	0.3412	0.6191	0.3880
15	0.50	02,03	0.3405	0.0259	0.3434	0.0312	0.1351	0.0121	0.1536	0.0164
		10,06	0.3488	0.0264	0.4113	0.0333	0.1200	0.0110	0.2155	0.0179
		30,11	0.3695	0.0276	0.3085	0.0239	0.0756	0.0073	0.0843	0.0080
	1.00	02,03	0.3405	0.0713	0.3881	0.0778	0.1351	0.0369	0.1644	0.0427
		10,06	0.3488	0.0725	0.4367	0.0803	0.1200	0.0338	0.2174	0.0445
		30,11	0.3695	0.0754	0.3326	0.0702	0.0756	0.0236	0.1025	0.0298
	1.50	02,03	0.3405	0.1203	0.3939	0.1273	0.1351	0.0659	0.1861	0.0728
		10,06	0.3488	0.1221	0.4865	0.1300	0.1200	0.0608	0.2617	0.0746
		30,11	0.3695	0.1265	0.3414	0.1205	0.0756	0.0438	0.1117	0.0578

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Steady State Probabilities of a Three Preemptive Single Server Queue

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A three preemptive priority queuing system is considered where customers with three priorities joined a queue according to a Poisson process. A customer with higher priority needs to enter the service immediately upon arrival. The recursive formulas approach was extended to determine the steady state probabilities of such a priority queuing system.

Key words: Poisson process, recursive formulas based approach, steady state probabilities, three preemptive queues.

Introduction

Queuing systems are used frequently and represent adequate models in many real life aspects. Examples of queuing systems include job processing, production lines, service centers (such as ATM machines), bus stations, phone calls and network service. Consider an M/M/1 queuing system where customers arrive to a service facility with one server; the arrival process is Poisson with rate λ , and the service time distribution is exponential with rate μ . If $\rho(=\lambda/\mu)<1$, then the system is in a steady state and steady state probabilities exist. Determining performance measures for M/M/1 is simple and can be found in most elementary queuing system texts, such as Gross and Harries (1998).

Priority queues form a large class of queuing models where arrival customers are distinguished according to their importance. The customer with higher priority should be served before those of lower priorities. Examples include analysis of computer and communication systems, mobile phone

networks, ambulances and surgeries. The performance analysis of multi-server queues with multiple classes of customers often experiences difficulty because the state space needed to capture the system behavior grows infinitely in multiple dimensions; Marks (1973) and Cidon and Sidi (1990) proposed different approaches to obtain the steady state probabilities of such systems.

Two Levels Priority Queues

Consider an M/M/1 with two priority levels of customers: high and low. The high priority customers need to be served ahead of the low priority customers. The arrival process is Poisson with rates λ_1 and λ_2 for high and low priority customers, respectively. Also, the service time distribution is exponential with rates μ_1 and μ_2 for high and low priority customers, respectively. The service discipline within each priority level is first in, first out (FIFO).

Preemptive queues indicate that a customer with high priority must be served upon arriving unless there are already high priority customers in the queue or in service, that is., ahead of any low priority customers in the system. Thus, upon arrival of a high priority customer, if the customer in service is low priority then he/she is ejected from service and the high priority customer is serviced; the low priority customer returns to the service center and re-starts service from the beginning. Non-preemptive queues are defined as those where a

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customer in service cannot be ejected from service upon the arrival of high priority customer.

Steady State Probabilities of Priority Queuing Systems

The steady state probabilities of queuing systems can be determined with ease when the queue is stable, however, it is not an easy task in the case of infinite queues, when the system has a very large number of states or when ρ (the intensity factor) approaches 1 (Smith, 2002). Different approaches have been proposed in the literature to find steady state probabilities. Some are based on generating functions, difference equations or direct algebraic manipulations (Mark, 1973; Cidon & Sidi, 1990). In their work, Smith (2002) and Osogami, et al. (2004) considered approaches based on manipulating queuing systems as Markov chains.

The limiting distribution of a Markov chain can be interpreted as a steady state probability. Another approach is termed indirect; this approach is based on identifying the stationary distribution of a Markov chain associated with the number of customers at a moment when a customer finishes service and leaves the system. The limiting distribution of the Markov chain is the steady state probability of the corresponding queuing system. Many authors have used this indirect approach in the literature (Osogami, et al.; 2004; Sheskin, 1985). Gail, et al. (1992) considered a Markov chain with two priorities and multiple servers: again, when the queue length is infinite, determining the stationary distribution of a Markov chain becomes challenging.

Heyman (1990) proposed an approach to ascertain approximate values of a stationary distribution of an infinite stochastic matrix in one dimension. Heyman's approach was extended to the case of two dimensional state space Markov chains and applied to a non-preemptive queuing system (Alawneh, 1995). The truncated approach was used by Alawneh (2011) to determine approximate values of the steady state probabilities of M/M/2 with infinite queues; results were compared with approaches put forth by Flatto and McKean (1977) and Flatto and Han (1977). This article presents an extension of a recursive formula based approach

that may be used to find the steady state probabilities of three preemptive priority levels queuing system with one server.

Steady State Probabilities of Two Preemptive Priority Queue

Marks (1973) was the first to study non-preemptive queuing systems. He developed a computational approach based on recursion formulas to determine the exact values of both preemptive and non-preemptive systems. Cidon & Sidi (1990) developed a recursive formula based on a moment generating function to find the same probabilities. However, as model complexity increases, the required algebraic manipulations become more tedious. Pasternack and Drezener (1998) proposed a recursive formula based on difference equations to establish exact probabilities for priority queues; their technique requires less computation than Mark's (1973). Smith (2002) and Pasternack and Drezener (1998) proposed an alternate approach for use when a system is finite but the expected number of customers is large.

A recursive formula approach introduced in the literature to determine the exact values of the steady state probabilities of M/M/1 for customers with two priorities – high and low – was provided by Marks (1973). Consider an M/M/1 where arrival customers are classified into two types according to their priority of obtaining service: high and low. Four possible cases are possible for the state space: both $m = 0$ and $n = 0$, only $m = 0$, only $n = 0$; or $(n, m) \neq (0, 0)$. Figure 1 illustrates the general case when both m and n are nonzero; that is, $(n, m) \neq (0, 0)$. The other three cases may be obtained by using an appropriate substitution of n and/or m .

Let P_{nm} be the probability of having n high and m low priority customers in the system at the moment when one customer finishes his service and leaves the system, where n and m are non-negative integers. The steady state probability is determined by solving equations (White & Christie, 1958):

$$\mu_1 P(1,0) - \mu_2 P(0,1) = \lambda P(0,0) \quad (1)$$

Figure 1: Special Case of a State Diagram of M/M/1 with Two Priorities

$$\mu_1 P(n+1, 0) - \lambda_1 P(n-1, 0) = (\lambda + \mu_1) P(n, 0) \quad (2)$$

$$\left[\begin{array}{c} \mu_1 P(1, m) + \mu_1 P(1, m) \\ + \mu_2 P(1, m+1) + \lambda_2 P(0, m-1) \end{array} \right] = (\lambda + \mu_2) P(0, m) \quad (3)$$

$$\left[\begin{array}{c} \mu_1 P(n+1, m) + \lambda_2 P(n, m-1) \mu \\ + \lambda_2 P(n-1, m) \end{array} \right] = (\lambda + \mu_1) P(n, m) \quad (4)$$

for $n, m = 0, 1, 2, \dots$

The following ten-step algorithm was developed by Marks (1973) and may be used to solve equations (1) to (4) in order to determine the steady state probabilities of two preemptive queues:

1. Calculate $P_{00} = 1 - \rho_1 - \rho_2$.
2. Set $B_{00} = p_{00}$.
3. Set $m = 1$.

4. Calculate B_{11} as:

$$B_{11} = \frac{1}{[\beta - \alpha]} \gamma p_2 B_{00}, \quad (5)$$

where $0 < \gamma < \infty$.

5. Calculate B_{01} as:

$$B_{01} = \frac{[\beta - 1]}{\gamma} B_{00}, \quad (6)$$

where

$$\beta = \frac{1}{2} \left[(\rho_1 + \gamma p_2 + 1) + \sqrt{(\rho_1 + \gamma p_2 + 1)^2 - 4\rho_1} \right]. \quad (7)$$

6. Increase m by one.
7. Calculate B_{im} for $i = m, m-1, \dots, 1$, using the equation:

$$B_{im} = \left[\frac{1}{\beta - \alpha} i \right] \left\{ \rho^2 B_{i-1, m-1} + \sum_{k=i+1}^{k=m} \binom{K}{i-1} \left[\alpha + \beta(-1)^{k-i+1} \right] B_{kml} \right\} \quad (8)$$

for $i = m, m-1, \dots, 1; m \geq 1$.

8. Calculate B_{0m} using:

$$B_{0m} = \left(\frac{\omega}{\gamma} \right) B_{0, m-1} - \rho_2 B_{0, m-2} - \left(\frac{\alpha}{\gamma} \right) \sum_{k=0}^{m-1} B_{k, m-1}$$

and

$$\beta, \alpha = \frac{1}{2} \left[(\rho_1 + \rho_2 + 1) \pm \sqrt{(\rho_1 + \rho_2 + 1)^2 - 4\rho_1} \right],$$

where $0 < \alpha < 1, \beta > 1, \omega = \rho_1 + \rho_2 + \gamma$.

(9)

9. Repeat steps 6 through 8 until all necessary coefficients are obtained.

10. Calculate the state probabilities P_{nm} using the formula:

$$P_{nm} = \alpha^n \sum_{k=0}^{k=m} B_{km} \eta^k, \quad (10)$$

$$n \geq 0, m \geq 0.$$

Steady State Probabilities of Three Preemptive M/M/1 Queue

Next, the recursive formula approach is extended to the case where there are three preemptive priority levels. In this case, customers are classified according to their priorities into three types or classes. Type I, the highest priority, is followed by Type II, and lastly Type III, which is without priority. Assuming a preemptive priority, meaning customers with higher priority enter service upon arrival and ahead of any customer from a lower priority. In addition, a customer from the higher priority may eject any lower priority

customer in service. The state space of the queuing system depends on the number of customers from each priority level in the system – both in the queue and in service. If n, m and l are the number of each priority level in the system, then all n, m and l are nonnegative integers. Eight possible cases for the state space may be considered based on n, m and l . Figure 2 illustrates the most general case when n, m and l are all positive; the other seven cases may be obtained by appropriate substitutions of the values of n, m and l .

If λ_i for $i = 1, 2, 3$ is the arrival rate from each priority level and μ_i is the service rate for each priority level, for $i = 1, 2, 3$, then

$$\rho_i = \frac{\lambda_i}{\mu_i} \text{ for } i=1, 2, 3,$$

and λ and μ are defined as: $\lambda = \lambda_1 + \lambda_2 + \lambda_3$ and $\mu = \mu_1 + \mu_2 + \mu_3$, respectively.

Steady state equations are derived from Figure 2 as follows:

$$\mu_1 P_{0,1,0} + \mu_2 P_{0,1,0} + \mu_3 P_{0,0,1} = \lambda P_{0,0,0} \quad (11)$$

$$\mu_1 P_{n+1,0,0} + \lambda_1 P_{n-1,0,0} = (\lambda + \mu_1) P_{n,0,0} \quad (12)$$

$$\mu_1 P_{1,n,0} + \mu_2 P_{0,n+1,0} + \lambda_2 P_{0,n-1,0} = (\lambda + \mu_3) P_{0,n} \quad (13)$$

$$\mu_1 P_{1,0,l} + \mu_2 P_{0,1,l} + \mu_3 P_{0,0,l+1} + \lambda_3 P_{0,0,l-1} = (\lambda + \mu_3) P_{0,0,l} \quad (14)$$

$$\mu_1 P_{n,m,0} + \lambda_1 P_{n-1,m,0} + \lambda_2 P_{n-1,m,0} = (\lambda + \mu_1) P_{n,m,0} \quad (15)$$

$$\mu_1 P_{n+1,0,l} + \lambda_1 P_{n-1,0,l} + \lambda_3 P_{n-1,0,l-1} = (\lambda + \mu_1) P_{n,0,l} \quad (16)$$

Figure 2: Special Case of the State Diagram of M/M/1 with Three Priorities

$$\mu_1 P_{1,m,l} + \lambda_2 P_{0,m-1,l} + \mu_2 P_{0,m+1,l} + \lambda_3 P_{0,m,l-1} = (\lambda + \mu_3) P_{0,m,l} \quad (17)$$

$$\mu_1 P_{n+1,m,l} + \lambda_1 P_{n-1,m,l} + \lambda_2 P_{n,m-1,l} + \lambda_3 P_{n,m,l-1} = (\lambda + \mu_1) P_{n,m,l} \quad (18)$$

and

$$\sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} P_{l,m,n} = 1 \quad (19)$$

Defining $EP_{n,m,l} = P_{n+1,m,l}$ where E is a difference operator and rewriting (2) using the difference operator E results in:

$$(\mu_1 E^2 - (\lambda + \mu_1)E + \lambda_1)P_{l,0,0} = 0 \\ = \Psi(E)P_{l,0,0} \quad (20)$$

where

$$\Psi(E) = (\mu_1 E^2 - (\lambda + \mu_1)E + \lambda_1). \quad (21)$$

Substituting $m = 1$ and rewriting (18) using difference operator E results in:

$$\mu_1 P_{n+1,1,l} + \lambda_1 P_{n-1,1,l} + \lambda_2 P_{n,0,l} + \lambda_3 P_{n,0,l-1} = (\lambda + \mu_1) P_{n,0,l} \quad (22)$$

and

$$\Psi(E)P_{n,1,m} = -\lambda_3 P_{n,0,l-1} - \lambda_2 P_{n,0,l} \quad (23)$$

Using mathematical induction, for $n = 0$,

$$\Psi(E)P_{n,1,0} = -\lambda_2 P_{n,0,0} \quad (24)$$

and for $n = 1$,

$$\Psi(E)P_{n,1,1} = -\lambda_3 P_{n,0,0} - \lambda_2 P_{n,0,1}, \quad (25)$$

$$P_{n,1,0} = B^{100} r^n + B_{101} n r^n \quad (26)$$

and

$$P_{n,1,0} = B_{110} r^n + B_{111} n r^n + B_{112} n^2 r n. \quad (27)$$

STEADY STATE PROBABILITIES OF THREE PREEMPTIVE SINGLE SERVER QUEUE

Thus the general solution is

$$P_{n,1,l} = r^n \sum_{j=0}^{n+1} B_{i,m,j} n^j \quad (28)$$

and, the general solution for the steady state probabilities is

$$P_{n,m,l} = r^n \sum_{j=0}^{n+m} B_{i,m,j} n^j, \quad (29)$$

which shows that a recursive formula approach may be used to determine the steady state probabilities of a three preemptive queue.

Expected Number of Customers and the Average Waiting Time in M/M/1

To compare an M/M/1 with three priority levels but without priority according to the expected number of customers and average waiting time in the queue, let L_{iq} , $i = 1, 2, 3$ be the expected number of customers (average queue length) from the i^{th} priority level in the queue, and let W_{iq} be the average waiting time for the i^{th} priority level. The number of expected customers in the queue from the i^{th} priority level is found using:

$$L_{iq} = \frac{\rho_i \sum_{n=1}^i \rho_n}{\left(1 - \sum_{n=1}^{i-1} \rho_n\right) \left(1 - \sum_{n=i}^i \rho_n\right)}, \quad (30)$$

$$i = 1, 2, 3 \text{ and } \sum_{j=1}^i \rho_j < 1.$$

If L_q is the expected number of customers in the queue then:

$$L_q = \frac{1}{\lambda} (\lambda_1 L_{1q} + \lambda_2 L_{2q} + \lambda_3 L_{3q}) \quad (31)$$

and the average waiting times in the queue is

$$W_q = \frac{1}{\lambda} (\lambda_1 W_{1q} + \lambda_2 W_{2q} + \lambda_3 W_{3q}) \quad (32)$$

where the average waiting time for the i^{th} priority level is

$$W_{iq} = \frac{L_{iq}}{\lambda} \quad (33)$$

for $i = 1, 2, 3$.

The expected number of customers and the average waiting times for an M/M/1 without priorities are:

$$L_q = \frac{\rho^2}{1 - \rho}$$

and (34)

$$W_q = \frac{L_q}{\lambda}$$

where the arrival rate for the non-priority is $\lambda = \lambda_1 + \lambda_2 + \lambda_3$, and where λ_1 , λ_2 and λ_3 are the same as in the priority queue. In addition, $\mu = \mu_1 + \mu_2 + \mu_3$ and μ_1 , μ_2 and μ_3 are also the same as in the priority queue.

For the purpose of numerical comparisons between priority and non-priority customers, Table 1 shows different values for arrival and service rates for a priority model assuming $\lambda = \lambda_1 + \lambda_2 + \lambda_3$, and $\mu = \mu_1 + \mu_2 + \mu_3$ when customers are not prioritized.

Conclusion

Based on results shown in Table 1, the following conclusions are put forth:

1. The queue length in the non-priority systems always constitutes an upper bound for the queue length in the priority system.
2. The average waiting time for the non-priority customers is an upper bound for the priority system.
3. Priority queues are more efficient when customers are classified according to their importance or needs for service.
4. As the intensity factor approaches one, the expected number of customers and the average waiting times increase for the highest priority customers.

This study shows that the recursive formal based approach may be used to find exact values of steady state probabilities for a three priority

queuing system. Priority queues are more efficient than non-priority, particularly when customer arrivals are classified according to their importance or their service needs. In real

life applications the number of the highest priority customers is limited; therefore, imposing such a condition on queue length will make using the recursive technique much easier.

Table 1: Expected Queue length and Waiting times for different values of μ and λ

μ	λ	ρ_1	ρ_2	ρ_3	L_q		W_q	
					With	Without	With	Without
6	3	0.167	0.167	0.167	0.128	0.500	0.064	0.167
6	4	0.167	0.333	0.167	0.375	1.333	0.156	0.167
6	4	0.167	0.167	0.333	0.533	1.333	0.267	0.167
6	5	0.167	0.333	0.333	1.500	5.143	0.625	1.029
6	4	0.167	0.333	0.167	0.375	1.333	0.156	0.167
6	5	0.167	0.167	0.333	1.500	5.143	0.625	0.570
7	5	0.167	0.333	0.333	0.918	0.714	0.394	0.357
7	6	0.143	0.143	0.429	3.215	5.143	1.378	0.857
7	6	0.143	0.143	0.571	1.615	5.143	0.519	0.857
7	4	0.143	0.571	0.143	0.178	1.752	0.051	0.357
7	5	0.286	0.143	0.143	0.426	1.786	0.106	0.357
7	5	0.286	0.286	0.143	0.576	1.786	0.165	0.357
7	4	0.286	0.143	0.286	0.178	1.752	0.051	0.355
7	5	0.286	0.143	0.143	0.426	0.714	0.106	0.357
7	6	0.286	0.286	0.286	0.576	5.143	0.165	0.857
7	6	0.286	0.143	0.286	1.549	5.143	0.387	0.857
7	6	0.286	0.286	0.429	2.313	5.143	0.661	0.857
7	5	0.286	0.143	0.143	0.426	0.714	0.102	0.357
7	6	0.429	0.143	0.143	1.077	5.143	0.231	0.857
7	6	0.429	0.286	0.286	1.550	5.143	0.369	0.857
7	6	0.571	0.143	0.143	1.147	5.143	0.246	0.857

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Weight: Does It Really Matter?

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Differential weighting promises to improve the validity of a measure. This study examines whether similar results would be found using weighted, unweighted and standardized z scores from the *All Stars Core* survey. It was concluded that the weighted systems were developed to equate the questions within the scales and to ease the process for customers without access to data analysis programs; however, the standardized scores were the more appropriate method for equating the test items.

Key words: Differential weighting, standardized scores, z -scores.

Introduction

According to Russell and Hubley (2005), the multiplication model of weighting is typically used with subjective importance ratings. In studies, quality of life, self-esteem, job satisfaction and personality have been among the variables assessed (Streiner, Goldberg & Miller, 1993; Trauer & Mackinnon, 2001). With all methods of weighting, the most weight is given to the most desirable response, and the least weight is given to the least desirable response. In mathematical theory, differential weighting promises to substantially improve the validity of the measure; however, in practice, it does not prove to be worth the trouble, especially item weighting (Wang & Stanley, 1970). Standardizing raw item data has been shown (Peterson, Kolen & Hoover, 1989; Wang & Stanley) to have the closest representation to achieving equally effective weighting.

This question as to whether weight matters, and more specifically, to determine if similar results would be found using weighted, unweighted and standardized z scores from the *All Stars Core* survey (Hansen, 2004) in reliability analyses and in repeated measures multivariate analyses of variance.

Methodology

Data Source

The data source for this study was from 393 sixth-grade students in a rural county in the southeastern United States. The sample included 190 (48.3%) males and 203 (51.7%) females who responded to the *All Stars Core* survey (Hansen, 2004) as a pre/post measure in an evaluation of a drug prevention intervention.

Measures

The *All Stars Core* survey consists of 62 multiple-choice items used to measure knowledge, attitudes, and behaviors regarding substance abuse. Items on the core measure were rationally combined to form scales, which measured alcohol, tobacco and other drug (ATOD) use factors and mediator factors. For this study, only six mediator factor scales were used:

1. Commitment: eight items assessing one's commitment to abstain from the use of alcohol, cigarettes, marijuana, and other drugs.

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2. School Bonding: seven items assessing one's perception of his or her teachers' attitudes towards him or her, acceptance, quality of school and teachers and sense of belonging at school.
3. Lifestyle Incongruence of Alcohol, Tobacco, and Other Drugs: six items assessing one's quality of life and ability to accomplish goals by avoiding alcohol, tobacco, and other drugs.
4. Normative Beliefs about Peer Drug Use: eight items assessing one's perception of his or her peers' use of and attitudes towards tobacco, alcohol, and other drugs.
5. Parent/Child Communication: three items assessing one's communication with parents about drugs and other important issues.
6. Parental Monitoring: three items assessing one's perception of parental knowledge regarding his or her friends.

The response scale for the mediator factors progressed from a rating of 1, which represented the least desirable level of behaviors, attitudes, perceptions, and skills, to a rating of 4, which represented the most desirable level. For the Normative Beliefs scale, four of the eight items had a response scale of 1 (None) to 5 (All). With different response scales, the response weights were on a scale ranging from 0 to 10.

Data Analysis

For data analyses, three types of scores were created: unweighted, weighted and standardized. The unweighted items were left in raw form. The weighted items were weighted based on the curriculum developer's specifications. For the standardized items, the pre- and post- test responses were combined into a database and transformed into standardized z scores; after standardization, the pre- and post-test items were separated into different variables. Reliabilities, repeated measures multivariate analysis of variance (MANOVA), and repeated measures analyses of variance (ANOVA) were conducted.

Results

Reliabilities

The weighted item method rendered similar, but slightly higher, internal consistency reliabilities than the other two scaling methods. Table 1 presents the alpha reliability coefficients for the mediator factor scales using the unweighted, weighted, and standardized scores.

Analyses of Variance

Initially, scores on the mediator factor scales weighted according to Hansen's (2004) weighting method were entered as dependent variables into a MANOVA to determine the mean change or difference from pre- to post-test. The results of the multivariate test of group differences indicated that an optimally linear combination of the six mediator factor scales from pre- to post- test was statistically significant ($F(6, 386) = 474.17, p = 0.00; \eta^2 = 0.88$), and the eta square indicated an enormous effect size, which could be interpreted as the six mediator factor scales accounting for 88% of the variance of the linear composite; such results are very unusual in educational research. The follow-up analyses revealed a statistically significant difference for all six mediator factor scales (see Table 2) with inflated F ratio and eta square results.

Subsequently, using the unweighted item scores, the results of the repeated measure multivariate test indicated that an optimal linear combination of the six mediator factor scales from pre- to posttest was also statistically significant ($F(6, 386) = 172.37, p = 0.00; \eta^2 = 0.73$); in addition, the eta square indicated a very strong effect size. The follow-up analyses revealed a statistically significant difference for all six mediator factor scales (see Table 3). The results were similar to the repeated measures MANOVA with follow-up univariate procedure that used the weighted item scores, but, with the unweighted item scores, the F ratios and eta squares were slightly decreased.

Table 1: Alpha Reliability Coefficients for Mediator Factor Scales

Scale	Unweighted		Weighted		Standardized	
	Pretest	Posttest	Pretest	Posttest	Pretest	Posttest
Commitment	.69	.70	.75	.76	.69	.74
School Bonding	.66	.66	.74	.75	.66	.74
Lifestyle Incongruence of Alcohol, Tobacco, and Other Drugs	.44	.44	.46	.48	.44	.47
Normative Beliefs About Peer Drug Use	.72	.47	.63	.57	.72	.64
Parent/Child Communication	.63	.63	.64	.66	.64	.65
Parental Monitoring	.72	.72	.74	.74	.73	.74

Table 2: Weighted Items: Means, Standard Deviations, and Univariates for the Mediator Factor Scales by Group as a Follow-up to the MANOVA Procedure

Scale	Pretest		Posttest		<i>F</i>	<i>p</i>	η^2
	M	SD	M	SD			
Commitment	1.48	1.57	1.74	1.84	179.00	.00	.31
School Bonding	2.85	1.84	3.38	2.18	1710.49	.00	.81
Lifestyle Incongruence of Alcohol, Tobacco, and Other Drugs	1.09	1.30	1.25	1.46	156.19	.00	.29
Normative Beliefs About Peer Drug Use	4.51	1.31	4.32	1.48	182.65	.00	.32
Parent/Child Communication	1.54	1.97	1.53	2.00	1202.65	.00	.76
Parental Monitoring	3.26	2.82	3.95	2.99	280.12	.00	.42

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Next, with the standardized item scores, the results of the repeated measure multivariate test indicated that an optimally linear combination of the six mediator factor scales from pre- to posttest was also statistically significant ($F(6, 386) = 2.95, p = 0.01; \eta^2 = 0.04$); however, the eta square indicated a weak effect size. The follow-up analyses revealed a statistically significant difference for only two of the six mediator factor scales: Lifestyle Incongruence and Parental Monitoring (see Table 4).

An examination of the statistical results for the weighted and unweighted item scores revealed the F ratios, follow-up univariate F ratios, and eta squares for each dependent variable entered into the MANOVA procedure were drastically out of the expected range for educational research. Conversely, the

MANOVA, follow-up univariate and eta square results with the standardized item scores yielded different findings compared to the other two methods. The F ratios and eta squares were comprehensible, and the follow-up univariates yielded only two statistically significant changes from pretest to posttest. Further, a simple examination of the means and standard deviations calls the inflated F ratios and eta squares into question.

After the repeated measures MANOVA indicated statistically significant differences, a series of separate repeated measures ANOVAs were conducted using the three types of scores to determine group mean differences from pretest to pretest. Tables 5, 6 and 7 display the separate univariate results for the mediator factor scales using unweighted, weighted and standardized items.

Table 3: Unweighted Items: Means, Standard Deviations, and Univariates for the Mediator Factor Scales by Group as a Follow-up to the MANOVA Procedure

Scale	Pretest		Posttest		F	p	η^2
	M	SD	M	SD			
Commitment	1.45	0.47	1.53	0.56	177.65	.00	.31
School Bonding	1.86	0.55	2.03	0.66	359.71	.00	.48
Lifestyle Incongruence of Alcohol, Tobacco, and Other Drugs	1.33	0.39	1.38	0.44	156.15	.00	.29
Normative Beliefs About Peer Drug Use	1.89	0.55	2.03	0.53	186.75	.00	.32
Parent/Child Communication	1.46	0.59	1.48	0.61	524.62	.00	.57
Parental Monitoring	1.98	0.85	2.19	0.90	264.62	.00	.40

Table 4: Standardized Items: Means, Standard Deviations, and Univariates for the Mediator Factor Scales by Group as a Follow-up to the MANOVA Procedure

Scale	Pretest		Posttest		<i>F</i>	<i>p</i>	η^2
	M	SD	M	SD			
Commitment	-0.06	0.51	0.03	0.62	0.31	.58	.00
School Bonding	-0.08	0.53	0.09	0.64	0.75	.39	.00
Lifestyle Incongruence of Alcohol, Tobacco, and Other Drugs	-0.06	0.46	0.01	0.53	4.37	.04	.01
Normative Beliefs About Peer Drug Use	-0.08	0.55	0.06	0.54	2.50	.11	.01
Parent/Child Communication	-0.01	0.75	0.00	0.77	2.76	.10	.01
Parental Monitoring	-0.10	0.78	0.09	0.86	4.28	.04	.01

Table 5: Unweighted Items: Means, Standard Deviations, and Univariates for the Mediator Factor Scales by Group Using Separate Repeated Measures ANOVAs

Scale	Pretest		Posttest		<i>F</i>	<i>p</i>	η^2
	M	SD	M	SD			
Commitment	1.45	0.47	1.53	0.56	11.07	.00	.03
School Bonding	1.86	0.55	2.03	0.66	32.68	.00	.08
Lifestyle Incongruence of Alcohol, Tobacco, and Other Drugs	1.33	0.39	1.38	0.44	4.53	.03	.01
Normative Beliefs About Peer Drug Use	1.89	0.55	2.03	0.53	22.71	.00	.06
Parent/Child Communication	1.46	0.59	1.48	0.61	0.16	.69	.00
Parental Monitoring	1.98	0.85	2.19	0.90	29.55	.00	.07

WEIGHT: DOES IT REALLY MATTER?

Table 6: Weighted Items: Means, Standard Deviations, and Univariates for the Mediator Factor Scales by Group Using Separate Repeated Measures ANOVAs

Scale	Pretest		Posttest		<i>F</i>	<i>p</i>	η^2
	M	SD	M	SD			
Commitment	1.48	1.57	1.74	1.84	10.43	.00	.03
School Bonding	2.85	1.84	3.38	2.18	29.84	.00	.07
Lifestyle Incongruence of Alcohol, Tobacco, and Other Drugs	1.09	1.30	1.25	1.46	3.69	.06	.01
Normative Beliefs About Peer Drug Use	4.51	1.31	4.32	1.48	6.65	.01	.02
Parent/Child Communication	1.54	1.97	1.53	2.00	0.00	.96	.00
Parental Monitoring	3.26	2.82	3.95	2.99	29.05	.00	.07

Table 7: Standardized Items: Means, Standard Deviations, and Univariates for the Mediator Factor Scales by Group Using Separate Repeated Measures ANOVAs

Scale	Pretest		Posttest		<i>F</i>	<i>p</i>	η^2
	M	SD	M	SD			
Commitment	-0.06	0.51	0.03	0.62	11.61	.00	.03
School Bonding	-0.08	0.53	0.09	0.64	32.37	.00	.08
Lifestyle Incongruence of Alcohol, Tobacco, and Other Drugs	-0.06	0.46	0.01	0.53	5.03	.03	.01
Normative Beliefs About Peer Drug Use	-0.08	0.55	0.06	0.54	23.52	.00	.06
Parent/Child Communication	-0.01	0.75	0.00	0.77	0.13	.72	.00
Parental Monitoring	-0.10	0.78	0.09	0.83	30.14	.00	.07

Each ANOVA yielded similar results except for the Normative Beliefs scale. With unweighted items, the F ratio for the Normative Beliefs scale was 22.71 with a p value of 0.00 and eta square of 0.06. The weighted items yielded an F ratio of 6.65 with a p value of 0.01 and eta square of 0.02. With the standardized items, the F ratio was 23.52 with a p -value of 0.00 and eta square of 0.06. These analyses indicate that the results of the standardized items paralleled the results with the unweighted items; however, the ratio of mean square error was reduced with the weighted items.

Conclusion

The weighted systems were developed to equate the questions within the scales and to ease the process for customers without access to data analysis programs; however, the standardized scores were the more appropriate method of equating the test items. A word of caution should be given when analyzing weighted items using the MANOVA procedure with follow-up univariates regardless of the weighting method. The findings may yield results that are incomprehensible to the field of educational research despite internally consistent reliabilities.

In an effort to resolve this perplexing issue, Hansen (personal communication, November 2, 2007), the instrument developer, noted when the measure was constructed in the 1980s the items were standardized by combining the pre- and post- tests. The mean score was obtained for each scale. The average layman had difficulty interpreting a mean of 0. In the 1990s, all scales were stretched to a response scale from 0 to 10 so a layman could consider a 10 as the most desirable score and a 0 as the least desirable score. The formula for stretching is:

Stretched Value =

$$(OBS + @ ABS(\min)) \times \left(\frac{10}{((@ ABS(\min) + \max))} \right)$$

where OBS is observed value, min is minimum value, and max is maximum value. Using this formula, the developer found this method was always dependent on the actual distribution of

scores within a study. More recently, a simpler method for weighting was implemented. For each item, the lowest score is always 0 and the highest score is always 10. For a five-response item, scores are 0, 2.5, 5, 7.5 and 10. In a four-item response, scores are 0, 3.3, 6.7 and 10. When averaged across items within a scale, scores will always range from 0 to 10. This simpler method allows the results within the database to be compared longitudinally.

When conducting research with weighted items, using both data analysis procedures, MANOVA with follow-up univariates and separate repeated measures ANOVAs is recommended. The MANOVA offers a more comprehensive analysis, but the F ratios are determined based on estimated means and the procedure could yield inflated F ratios and eta squares. By comparing the data analysis output, a researcher can decide which of the obtained analyses is most appropriate for their research question(s).

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Regression Models for Mixed Over-Dispersed Poisson and Continuous Clustered Data: Modeling BMI and Number of Cigarettes Smoked Per Day

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Clustered data, multiple observations collected on the same experimental unit, is common in epidemiological studies. Bivariate outcome data is often the result of interest in two correlated response variables. An efficient method is presented for dealing with bivariate outcomes when one outcome is continuous and the other is a count using a simple transformation to handle over-dispersed Poisson data. A multilevel analysis was performed on data from the National Health Interview Survey (NHIS) with body mass index (BMI) and the number of cigarettes smoked per day (NCS) as responses. Results show that these random effects models yield misleading results in cases where the data is not transformed.

Key words: Joint bivariate model, random effect model, multilevel, mixed model, GLIMMIX.

Introduction

Modeling bivariate outcome using joint multivariate random effect models (JMRE) is a popular approach in the medical field. There are a number of conditions where a disease under study is well understood when two outcomes are considered. For example, in clinical trials the clinician may be interested in the joint evolution of HIV RNA and CD4+ lymphocytes in a cohort of HIV-1 infected patients treated with active antiretroviral drugs. Bellamy (1995) studied the study of the risk factors associated with the progression of osteoarthritis (OA) of the knee. In this study two outcomes were collected, the Western Ontario and McMaster Universities (WOMAC) disability score and the number of missed work days for the past three months due to knee pain. The JMRE model allows the modeling of mixed effects and bivariate outcomes.

There are several advantages of modeling bivariate outcomes (see Laird and Ware, 1982; Dempster, et al., 1984; Bagella, 2000; Pantazis & Touloumi, 2007; McCulloch, 2008; Atem, et al., 2010). First, this model allows exploration of variations at different levels of a hierarchy and modeling of a correlation structure serially and across two outcomes. Second, the bivariate JMRE model achieves greater bias reduction in all model parameters compared to the two independent JMRE models. Third, there is greater flexibility in dealing with exploratory variables; the JMRE model can conveniently test hypotheses on either end point individually or simultaneously. JMRE can also handle missing data as the parameter estimates are obtained by techniques of maximum likelihood; the variance and means of the outcomes are estimated, thus the choice of the variance must be taken into consideration.

Rao (1973) suggested that irrespective of the chosen variance, the fixed effect estimates are unbiased; however, the estimates can achieve maximum efficiency only when the appropriate variance is specified. Lastly, multiple testing can be avoided by forming joint models without resorting to ad hoc methods such as the Bonferroni adjustment or using advanced methods such as those as presented by Dmitrienko, et al. (2009). Moreover, because the bivariate model is a regression model,

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classification and continuous predictors can be incorporated; the predictors can either be time variant or invariant.

This study develops a straightforward and efficient method to handle bivariate outcome data where one outcome is continuous and the other is count with over-dispersion; a test is proposed to identify possible over-dispersion in the count outcome. For modeling, data from the National Health Interview Survey (NHIS) from 1997-2006 was used to establish the joint relationship between body mass index (BMI; continuous) and number of cigarettes smoked per day (NCS; count), adjusting for race, gender and age. The National Health Interview Survey (NHIS) was founded in 1957 as an annual nationwide survey of approximately 40,000 households in civilian, non-institutionalized populations. It is conducted by the National Center for Health Statistics (NCHS) and administered by the United States Census Bureau.

Regression Techniques

Regression techniques for hierarchical data have been referred to in the literature under different names, including random coefficient models (Rao, 1965) and hierarchical linear model (Bryk & Raudenbush, 1987). Song, et al. (2008) refers to bivariate and multivariate analyses as structural level equations.

Bivariate Model

For the case of two continuous markers with correlated random effect superscripts a and b are used to distinguish the two markers. Subscripts j and i are used to denote the information of the j^{th} measurement for the i^{th} individual. Assuming that the marker trends can be explained by two linear mixed models with correlated random-effects, a bivariate model for the multilevel marker measurements can be presented as follows (Thiebaut, et al., 2002):

$$\begin{aligned} y_{ij}^a &= x_{ij}^a \beta^a + z_{ij}^a \lambda_i^a + e_{ij}^a \\ \text{and} \\ y_{ij}^b &= x_{ij}^b \beta^b + z_{ij}^b \lambda_i^b + e_{ij}^b \end{aligned} \quad (1)$$

Vectors $\lambda_i^a (k^a \times 1)$ and $\lambda_i^b (k^b \times 1)$ contain random (subject-specific) regression coefficients for k^a and k^b predictor variables included in the corresponding design vectors $Z_{ij}^a (1 \times k)$ and $Z_{ij}^b (1 \times k)$ respectively. The joint distribution of λ_i^a and λ_i^b is assumed to be multivariate normal with zero means and variance-covariance matrix:

$$\Sigma = \begin{pmatrix} \Sigma^a & \Sigma^{ab} \\ \Sigma^{ab} & \Sigma^b \end{pmatrix} \quad (2)$$

Matrices $\Sigma^a (k^a \times k^a)$ and $\Sigma^b (k^b \times k^b)$ are variance and covariance of the random effects for both outcomes respectively, while $\Sigma^{ab} (k^b \times k^a)$ specifies the covariance structure of the random effects between outcomes.

Vectors $\beta^a (p^a \times 1)$ and $\beta^b (p^b \times 1)$ contain fixed regression coefficients for both markers respectively; $x_{ij}^a (1 \times p^a)$ and $x_{ij}^b (1 \times p^b)$ are their corresponding design vectors containing the values of p^a and p^b exploratory variables. The coefficients e_{ij}^a and e_{ij}^b represent the level-1 residual for the two outcomes. The bivariate model can be presented in the matrix form:

$$\begin{pmatrix} Y_i^a \\ Y_i^b \end{pmatrix} = \begin{pmatrix} X_i^a & 0 \\ 0 & X_i^b \end{pmatrix} \begin{pmatrix} \beta^a \\ \beta^b \end{pmatrix} + \begin{pmatrix} Z_i^a & 0 \\ 0 & Z_i^b \end{pmatrix} \begin{pmatrix} \lambda_i^a \\ \lambda_i^b \end{pmatrix} + \begin{pmatrix} e_{ij}^a \\ e_{ij}^b \end{pmatrix} \quad (3)$$

Bivariate Model: Random Effects Approach

The outcomes of interest, BMI and NCS are denoted by $Y_{1i}(t)$ and $Y_{2i}(t)$ respectively, for subject i at time t . Assume that the outcomes can be described by two linear mixed models with correlated random effects. A joint model can be constructed from the basic random effect model proposed by Laird and Ware (1982):

$$\begin{aligned} Y_{1i}(t) &= \beta_1(t) + a_{1i} + b_{1i}(t) + \varepsilon_{1i}(t) \\ Y_{2i}(t) &= \beta_2(t) + a_{2i} + b_{2i}(t) + \varepsilon_{2i}(t) \end{aligned} \quad (4)$$

where $\beta_1(t)$ and $\beta_2(t)$ refer to the average changes of the outcomes. The dependent variables (BMI and NCS) are linked together through the joint distribution of their random effects

$$\begin{pmatrix} a_{1i} \\ a_{2i} \\ b_{1i} \\ b_{2i} \end{pmatrix} \sim N(0, D)$$

where D is a matrix of the random effects with the following variance-covariance structure:

$$\begin{pmatrix} \sigma_{a1}^2 & \cdots & \sigma_{a1b2} \\ \vdots & \ddots & \vdots \\ \sigma_{b2a1} & \cdots & \sigma_{b2}^2 \end{pmatrix}$$

The variance-covariance matrix of the model parameter is often derived by maximum likelihood or restricted maximum likelihood method.

The residual components are uncorrelated and independent of the random effects

$$\begin{pmatrix} \varepsilon_{1i} \\ \varepsilon_{2i} \end{pmatrix} \sim N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}\right).$$

The variance-covariance structure implies that conditioning on the random effects, both responses are independent. Other cases can be obtained by making additional assumptions about the variance-covariance matrix D . Thiebaut, et al. (2002) outlined further procedures on a number of special cases of the D matrix. For these analyses, models were fitted using the SAS GLIMMIX procedure, while the random effects were introduced through the

shared random effects procedures as described by De Gruttola, et al. (1994).

A common objective for joint modeling is to investigate how outcomes are correlated. For example, a researcher might be interested in how the correlation of BMI and NCS are associated with age, while controlling for race and gender. The correlation between outcome variables BMI and NCS is derived from the variance- covariance matrix of the random effect and is given by:

$$r_e = \frac{\sigma_{b_1 b_2}}{\sqrt{\sigma_{b_1}^2} \sqrt{\sigma_{b_2}^2}}$$

The marginal correlation between BMI and NCS as a function of time t is given by:

$$r_m(t) = \frac{\sigma_{a_1 a_2} + t(\sigma_{a_1 b_2} + \sigma_{a_2 b_1}) + t^2 \sigma_{b_1 b_2}}{\sqrt{\sigma_{a_1}^2 + 2t\sigma_{a_1 b_1} + t^2 \sigma_{b_1}^2 + \sigma_1^2} \sqrt{\sigma_{a_2}^2 + 2t\sigma_{a_2 b_2} + t^2 \sigma_{b_2}^2 + \sigma_2^2}}.$$

When $t = 0$ the equation reduces to

$$r_m(t) = \frac{\sigma_{a_1 a_2}}{\sqrt{\sigma_{a_1}^2 + \sigma_1^2} \sqrt{\sigma_{a_2}^2 + \sigma_2^2}}$$

This formula implies that the marginal correlation cannot be higher than the correlation between random intercepts. If the measurement errors of BMI and NCS are smaller, the marginal correlation at $t = 0$ better approximates the correlation between the random intercepts. The covariance parameters of the random effects and the error components determine the shape of the marginal correlation function. Further, as t increases, the marginal correlation converges to the correlation between the random slopes.

Methodology

Simulation Study

Yang, et al. (2007, 2009, 2010) discussed methods to simulate and test for an over-dispersed Poisson distribution. A simple and efficient way to simulate a mixture of

bivariate continuous and over-dispersed Poisson distribution using the specified parameters is:

$$\begin{aligned}\beta^a &= (1, 0.2, -0.2, 1)' a = 1, 5 \\ \beta^b &= (1, 0.2, 0.1, 0.1)', \rho = 0.5, \sigma^2 = 1 \\ \lambda_i^a &= \lambda_i^b = 0.12, n = 100, T = 7\end{aligned}$$

Data were simulated using a negative binomial distribution for the case where $\alpha = 5$. A negative binomial may result from a mixture of Poisson distributions with a Gamma distribution of the mean and a specified shape and scale parameters (R – Documentation). The mean to variance ratio was about 1:5. See Table 1, Figure 1 for a table and plot of the mean and variance for a non-dispersed and see Table 2, Figure 2 for a dispersed Poisson distribution. Using equation 4, 5,000 samples were generated; each sample of size 100 represents a mixed Poisson and continuous longitudinal data with 7 time points. Both outcomes were generated as a linear function of 4 predictors (x_i); the predictors were specified as both binary and continuous. The bias of the estimates using different transformations and correlations were approximately equal.

Results

Tables 3 - 5 summarize the results of the simulated dataset; Log likelihood (-2 Log L), AIC, AICC and BIC together with the means estimates, standard errors and p-values of our estimates. The AIC, AICC and BIC as defined in Akaike (1973, 1985), Sakamoto, et al. (1986) and Bozdogan (1987) are specified as:

$$2(-\log g(x, \hat{\theta}) + d), \quad AIC + \frac{2(d+1)(d+2)}{n-d-2}$$

and $-2\log g(x, \hat{\theta}) + d(\log(n^*))$ respectively.

These definitions of AIC, AICC and BIC imply that smaller AIC, AICC and BIC estimates provide a better fit for the model. Gurka, et al. (2011) showed that the model with independent correlation structure offers a parsimonious model, but may not always be the best model. However, this study shows that – in the case of mixed Poisson and continuous longitudinal data – the independent and the unstructured correlation tend to perform best and have the lowest AIC, AICC and BIC (see Table 3). In the case of a mixed over-dispersed Poisson and continuous clustered data a number of transformations for the outcome variables were examined. First, the case with no transformation on the outcome was considered; this model

Table 1: Mean and Variance for a Non-Dispersed Poisson Distribution

Simulated Data Results (Non-Dispersed Poisson)		
Replicate	Mean of Poisson	Variance of Poisson
1	4.46	4.95
2	4.04	3.75
3	3.98	3.08
4	3.30	2.79
5	4.54	3.56
6	4.18	3.82
7	4.32	3.81

Figure 1: Mean and Variance Plots for a Non-Dispersed Poisson Distribution
Results Obtained from one Replicate (n = 100, q = 7)

Table 2: Mean and Variance for a Dispersed Poisson Distribution

Simulated Data Results (Dispersed Poisson)		
Replicate	Mean of Poisson	Variance of Poisson
1	15.94	89.24
2	16.56	90.62
3	16.40	88.49
4	16.12	83.94
5	14.10	64.01
6	16.72	102.21
7	14.82	93.62

Figure 2: Mean and Variance plots for a Dispersed Poisson Distribution
Results Obtained from one Replicate ($n = 100$, $q = 7$)

performed poorly with extremely high values for AIC, AICC and AICC (see Table 4). Next, a number of data transformations were performed and the best model was selected based on the AIC, AICC, BIC and the standard errors of the estimates. The transformation $\log(Y+1)$ performed best for both responses using the independent and the unstructured correlation structure for the data (see Table 5).

Using NHIS data, approximately 264,727 people were interviewed over the 10-year period 1997-2006. The sample size for this analysis was reduced to 42,138 after cleaning. First, BMI values were analyzed with a general linear mixed model. The fixed effects in the model were gender, race and age. The random

effects in this model were year (time) and residual (see Table 7). Next, NCS was analyzed with similar fixed effect and random effect variables. The univariate analysis assumed a Poisson error because NCS is count data (see Table 8); however, the resulting fitting algorithm did not converge. The Poisson error might not be a proper residual term for this analysis even though NCS is count data because the means are not equal to the variances (see Table 6). Overdispersion was verified using techniques proposed by Lindsey (1999). Assuming a normal error for NCS, the deviance is 323842.2 which is more than twice the degrees of freedom of 42139, hence the Poisson data is overdispersed.

MODELS FOR OVER-DISPERSED POISSON AND CONTINUOUS CLUSTERED DATA

Table 3: Means, Standard Errors and p-values of Fixed Effects Parameter Estimates

Simulated Data Results (No Overdispersion)					
Variable	Independent	Compound Symmetry	First Order Autoregressive	Toeplitz	Unstructured
-2 Log L	2500.50	2572.83	2572.83	2572.83	2485.63
AIC	2507.60	2580.83	2580.83	2580.83	2507.63
AICC	2507.65	2580.89	2580.89	2580.89	2508.02
BIC	2514.39	2588.48	2588.48	2588.48	2528.66
α	-4.8887	-4.7744	-4.7744	-4.7744	-4.8593
β_1	27.1193	27.1193	27.1193	27.1193	27.1193
β_2	0.0034	0.0034	0.0034	0.0034	0.0034
β_3	0.6846	0.6846	0.6846	0.6846	0.6846
β_4	-0.0063	-0.0092	-0.0092	-0.0092	-0.0070
Standard Error					
α	1.5987	1.0841	1.0841	1.0841	1.3286
β_1	0.3131	0.2424	0.2424	0.2424	0.3425
β_2	0.0274	0.0426	0.0426	0.0426	0.0283
β_3	0.0423	0.0547	0.0547	0.0547	0.0429
β_4	0.0394	0.0265	0.0265	0.0265	0.0324
p-value					
α	0.0150	0.0093	0.0093	0.0093	0.0053
β_1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
β_2	0.5084	0.6408	0.6408	0.6408	0.5179
β_3	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
β_4	0.5675	0.4547	0.4547	0.4547	0.5820

Table 4: Means, Standard Errors and p-values of Fixed Effects Parameter Estimates

Simulated Data Results (Overdispersed Poisson Without Transformation)					
Variable	Independent	Compound Symmetry	First Order Autoregressive	Toeplitz	Unstructured
-2 Log L	3626.17	3668.83	3668.83	3668.83	3540.68
AIC	3633.57	3676.83	3676.83	3676.83	3562.98
AICC	3633.62	3676.89	3676.89	3676.89	3563.38
BIC	3640.65	3684.48	3684.48	3684.48	3584.30
α	4.8104	5.9763	5.9763	5.9763	6.0410
β_1	15.7333	15.7333	15.7333	15.7333	15.7333
β_2	0.0114	0.0114	0.0114	0.0114	0.0114
β_3	2.8471	2.8471	2.8471	2.8471	2.8471
β_4	0.0354	0.0061	0.0061	0.0061	0.0045
Standard Error					
α	3.3361	1.7362	1.7362	1.7362	2.1000
β_1	1.0875	1.0691	1.0691	1.0691	1.1838
β_2	0.0278	0.0436	0.0436	0.0436	0.0284
β_3	0.2171	0.2403	0.2403	0.2403	0.1950
β_4	0.0786	0.0342	0.0342	0.0342	0.0434
p-value					
α	0.2181	0.0308	0.0308	0.0308	0.0357
β_1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
β_2	0.4715	0.6047	0.6047	0.6047	0.4783
β_3	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
β_4	0.4694	0.3689	0.3689	0.3689	0.4897

MODELS FOR OVER-DISPERSED POISSON AND CONTINUOUS CLUSTERED DATA

Table 5: Means, Standard Errors and p-values of Fixed Effects Parameter Estimates

Simulated Data Results (Overdispersed Log Transformed Poisson Outcome)					
Variable	Independent	Compound Symmetry	First Order Autoregressive	Toeplitz	Unstructured
-2 Log L	-373.94	-336.83	-336.83	-336.83	-466.84
AIC	-366.74	-330.53	-330.53	-330.53	-443.44
AICC	-366.69	-330.50	-330.50	-330.50	-443.00
BIC	-359.86	-324.51	-324.51	-324.51	-421.07
α	1.9758	1.9803	1.9803	1.9803	1.9286
β_1	1.1255	1.1242	1.1242	1.1242	1.1809
β_2	0.0005	0.0005	0.0005	0.0005	0.0005
β_3	0.1852	0.1850	0.1850	0.1850	0.1953
β_4	0.0008	0.0007	0.0007	0.0007	0.0005
Standard Error					
α	0.1177	0.1027	0.1027	0.1027	0.1513
β_1	0.0827	0.0831	0.0831	0.0831	0.1288
β_2	0.0012	0.0016	0.0016	0.0016	0.0013
β_3	0.0181	0.0183	0.0183	0.0183	0.0193
β_4	0.0021	0.0015	0.0015	0.0015	0.0020
p-value					
α	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
β_1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
β_2	0.6150	0.6922	0.6922	0.6922	0.6211
β_3	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
β_4	0.6090	0.4955	0.4955	0.4955	0.6082

BMI and NCS were analyzed using a joint bivariate model (see Table 8) with normal and Poisson residuals for the two outcome variables, respectively. The joint bivariate model appears to converge; however, the corresponding univariate analyses for the over-dispersed Poisson error did not converge. This bivariate model is inappropriate because this analysis requires proper consideration of the correlation of the outcomes, which might not be true. In this case, the result of the joint bivariate analysis is similar to the univariate analysis of BMI as the outcome. This may be attributed to the correlation between the outcome variables BMI and cigarettes smoked not being accurately taken into consideration. In order to be sure that the model properly accounts for the association between both outcomes, it is important to ensure that the model assumptions of the independent univariate models are satisfied. For example, if a Poisson error for the univariate analysis of NCS as a dependent variable is assumed, the resulting model might be subject to over-dispersion (see Tables 2 & 6). Yang, et al. (2009) discussed the method of testing and how to manage these types of situations. In order to deal with over-dispersion, NCS is transformed using $\log(Y+1)$, where Y is NCS. This model is very similar to the model in equation 1 with $y_{ij}^a = \log(y_{ij}^a + 1)$.

After transforming to the count variable, NCS, the joint bivariate random effects model is fit. Fixed effects were gender, race, age, age interaction with age and the distribution (normal). The random effects were year and residual (see Table 9); this result is different from the previous joint bivariate model. Furthermore, the analysis of residual from the joint model with normal error for BMI and Poisson error for NCS shows that the model is not performing well. The Poisson model plot of residual is expected to have a funnel shape, but as Figure 3 shows, this is not the case. The model with normal error for BMI and normal error for log-transformed NCS tend to have improved residual plots, based on the distribution of the residuals. This model is also more efficient (see Figure 4) with $-2\log Re = 579056.2$, compared to the model with untransformed NCS (see Figure 3) with $-2\log Re = 663787.1$.

Conclusion

A number of methods have been discussed to handle correlated data with bivariate outcomes (Song, et al., 2008), Yang, et al., (2006, 2007, 2009), but little work has been done in cases with mixed over-dispersed Poisson and clustered continuous outcomes. Yang, et al., (2006, 2009) discussed estimation procedures for bivariate models with both complete and incomplete cases. Yang, et al., (2007, 2009) introduced various methods to test for over-dispersion using a univariate repeated measure data. Fieuws and Verbeke (2004) compared the univariate to the bivariate model with and without correlated random effects using the Hearing Data collected in the Baltimore Longitudinal Study of Aging (BLSA); they concluded that the bivariate correlated model performed best.

The purpose of this study was not to develop a new estimation technique, but rather to show that a simple transformation together with the correct correlation will stabilize the model. Modeling bivariate outcomes is essential when there is an association between primary outcomes or when the question of interest focuses on the joint behavior of multiple outcomes. The extent to which the dependent structure would be considered, however, depends on the question at hand. If interest is primarily on the population response means and the impact of covariates on these means, then a detailed consideration of the transformation and correlation mechanism may not be of significant importance. However, loss of efficiency could result if the assumed working correlation is far from the true correlation (Gardiner, 2009). On the other hand, if there is interest in both marginal and subject-specific inferences (for example, in estimating the growth trajectories of individuals (Potthoff & Roy, 1964), a careful evaluation of the transformation mechanism and correlation structure is of tremendous importance.

The linear mixed model can be used for both marginal and subject specific inference. For example, on the subject-specific inference mean and the population mean, the significance test for this approach depends highly on the chosen covariance structure; therefore, careful consideration in choosing the right correlation structure is required.

Table 6: Number Cigarettes per Day

NHIS Data Results			
Survey Year	N	Mean	Variance
1997	5578	16.27	146.87
1998	4619	15.98	141.91
1999	4316	15.39	144.02
2000	4395	15.32	149.78
2001	4616	14.96	134.03
2002	4158	14.73	128.41
2003	3900	14.33	131.44
2004	3818	14.36	129.28
2005	3840	13.85	120.16
2006	2899	14.00	144.20

Table 7: Modeling BMI with Normal Error

NHIS Data Results					
Effect	Estimate	Standard Error	DF	T-value	P-Value
Intercept	20.75	0.2043	9	101.56	<.0001
Male vs. Female	0.63	0.0366	84263	17.30	<.0001
White vs. Others	-0.23	0.0825	84263	-2.73	0.0064
Black vs. Others	1.20	0.0944	84263	12.67	0.0013
Age	0.25	0.0068	84263	37.13	<.0001
Age*Age	>-0.01	0.0001	84263	-37.22	<.0001

*The estimate of the Age interaction is -0.003

Table 8: Bivariate Model with BMI and Number of Cigarette Smoked per Day

NHIS Data Results						
Effect	Distribution	Estimate	Standard Error	DF	T-value	p-Value
Distribution	Normal	24.62	0.0347	84262	709.21	<.0001
Distribution	Poisson	1.18	0.0229	84262	51.30	<.0001
Male vs. Female		0.17	0.0025	84262	68.05	<.0001
White vs. Others		0.39	0.0067	84262	58.72	<.0001
Black vs. Others		0.08	0.0076	84262	10.56	<.0001
Age		0.04	0.0005	84262	89.48	<.0001
Age*Age		> -0.01	0.0001	84262	-71.98	<.0001

*The estimate of the Age interaction is -0.004

Table 9: Transformed Bivariate Model BMI and Number of Cigarette Smoked Per Day

NHIS Data Results						
Effect	Distribution	Estimate	Standard Error	DF	T-value	p-Value
Distribution	Normal	10.86	0.3838	84263	28.28	<.0001
Male vs. Female		0.39	0.0857	84263	4.510	<.0001
White vs. Others		0.10	0.1933	84263	0.540	0.5903
Black vs. Others		0.68	0.2213	84263	3.050	0.0023
Age		0.15	0.0159	84263	9.25	<.0001
Age*Age*		> -0.01	0.0002	84263	-8.98	<.0001

*The estimate of the Age interaction is -0.0016

Figure 3: Analysis of Residuals: Number of Cigarettes Smoked and BMI

Figure 4: Analysis of Residuals; Transformed Number of Cigarettes Smoked and BMI

The fixed effects estimates with different covariance structures may yield the same values, even though the standard errors of these estimates can vary widely. One objective of data analysis using a linear mixed model is to define an adequate error covariance structure in order to obtain efficient estimates of regression parameters; however, to properly estimate the covariance structure, the normality assumption of the random effect must be met. After both conditions are met, multilevel models are most suitable for analysis of longitudinal data and data with hierarchical structure. (Bock, 1989; Bryk & Raudenbush, 1996; Goldstein, 2003; Hoeksma & Knol, 2001; Raudenbush, 1989; Snijders, 1996).

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A Poisson Regression Model for Female Radium Dial Workers

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A Poisson regression model with interaction terms was applied to study the dose response relationship for radium-induced skeletal cancers. The model showed that the expected frequency count of bone tumors depended not only on the logarithmic dose and the time since first exposure, but also on the interaction between the logarithmic dose and the time since first exposure, whereas the dose-response model for head tumors depended only on the logarithmic dose.

Key words: Bone sarcoma, confounding factor, head carcinoma, interaction, Poisson regression model, radium dial painters.

Introduction

The tragedy of female dial painters attributed to radiation poisoning was one of the first widely known incidents of occupational hazards. Because it was a well-paying job many young women were attracted to work in the dial-painting industry in the United States. Unaware of radium poisoning, a common practice adopted by dial painters was to tip their brushes with their lips in order to provide a fine point for painting. The luminous paint usually contained 10 microcurie (μCi) per gram; as a result, dial painters were exposed to the intake of radium into their bodies. Several years after leaving the plant, the former dial painters began developing a variety of mysterious medical problems; the most common symptoms experienced were teeth and jaw problems. For the story of this deadly glow tragedy see Mullner (1999).

A new dose-response model is proposed, specifically a Poisson regression model, for radium-induced skeletal cancers, bone sarcoma (osteogenic sarcoma or fibrosarcoma) and head carcinoma (carcinoma of paranasal sinuses or mastoid air cells), which occurred among the U.S. female radium-dial painters. The dose-response relationship for

radium-induced skeletal cancers is very important in the establishment of safety standards for the protection of the public health based on occupationally relevant exposure. Further, this study seeks to enhance understanding about the radiation effect of other α -emitting radio-nuclides (e.g., plutonium) for which there are no human data available. (To learn more about the effect of radium poisoning, see Evans (1966, 1967, 1980, 1981), Evans, et al. (1969) and Loutit (1970).)

Evans (1943) established the radiation protection standard of 0.1 μCi of radium in the adult human. In 1967, data from separate studies were consolidated into a newly created Center for Human Radiology (CHR) at Argonne National Laboratory (ANL). Based on a follow-up of this consolidated data by the end of 1976, Rowland, et al. (1978, 1983) established a quasi-log-linear model for the incidence rate of bone/head tumors as a function of the product between a quadratic function of exposure dose and an exponential function of exposure dose. They concluded that a model of dose-squared-exponential function provided the best fit for the bone sarcomas, and that an acceptable fit to the head carcinoma data was provided by the linear function of the dose. However, Rosenblatt, et al. (1971) showed that a plot of tumor incidence as a function of doses may potentially be erroneous and misleading. As a result, the theoretical support for Rowland, et al. chosen models might not be adequate.

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Based on this, a better dose-response model needs to be identified, and after reviewing literature on this topic, the author devised a different idea to model the dose-response curve. Because bone/head tumors are rare cancers, Poisson regression model was decided upon for use. The Poisson regression model has proven to be an effective statistical tool in the analysis of cancer death rates (Frome, 1983; Frome & Checkoway, 1985; Frome, et al., 1990). In 2006 Lee showed that the tumor frequency was supposed to be not only a function of exposure dose levels, but also potential confounding factors including the age at first exposure, the duration of exposure and the time since first exposure. However, the Poisson regression model proposed in that study did not consider the interaction between the exposure variable (dose) and potential confounding variables. This study incorporates all interaction terms into the Poisson regression model.

Methodology

Study Population

The study population was a cohort of 4,337 females employed in the U.S. radium-dial industry which was maintained by the CHR at ANL. This is exactly the same cohort as that used by Rowland, et al. (1978), except that the cohort was enlarged due to extra effort to collect additional subjects after 1976. After the data was first consolidated in the CHR at ANL in 1967, all located subjects were followed for vital status by the staff of the CHR. Death certificates were obtained as soon as staff at the CHR had knowledge of the death and was coded (8th International Classification of Diseases) by the national Center for Health Statistics.

An attempt was made to contact all living subjects annually by mail, and subjects would be contacted by telephone if they did not respond to the mail inquiry. Details of follow-up method, follow-up period, dose measurement and others were given in Argonne's internal report (Radiological and Environmental Research Annual Report, 1984). Excluding those with unknown birth dates or without the social security numbers, 3,688 cases were usable (see Table 1). The measured population contained

most of the known radium-induced skeletal cancers. About 973 living cases were still unmeasured despite efforts to obtain their cooperation. Most of these women refused because they did not wish to be reminded of their association with the radium industry or for other reasons not related to their current state of health. There were no known skeletal cancers in this group.

Exposure Data

Measurements of radium body burden were conducted by whole body counting and radon breath tests as subjects proceeded through a medical examination by a nurse and physician from the medical group of CHR at Argonne. At the time of radium body burden measurement all subjects also received a complete clinical examination, electrocardiography, blood chemistries and urine tests. Due to the interest in bone changes due to radium, extensive sets of x-rays emphasizing the skeleton were completed at each examination.

The complete measurement of radium in the body of a dial painter yielded two values, one for ^{226}Ra and one for ^{228}Ra . Because the ratio of ^{228}Ra to ^{226}Ra could vary with each batch of paint being used it was not possible to compare radium cases on the basis of the quantity of radium within the body. What was needed was a method of defining a radium equivalent, so that all measured cases could be expressed in the same units. Two ways to calculate the radium equivalent dose are available.

It was found that an effectiveness ratio (^{228}Ra to ^{226}Ra) was 1.5 when average skeletal doses were used and 2.5 when initial systemic intake was used as a measure of the risk. Because the initial systemic intake was used in Rowland, et al. (1978), the initial systemic intake is also used herein to define the risk of the induction of bone sarcoma in a given dial painter: it is the intake of radium until the end of follow-up in 1984. The average values for each class interval were calculated as the arithmetic mean of their respective individual subject's data in that interval (see Tables 2-3).

Table 1: Female Radium Dial Workers with Known Status at the End of 1984

	Number	Average Age of 1 st Exposure $\pm$ SD	Number Alive	Number Not Located	Cases Known to be Deceased	Malignancy	
						Bone Sarcoma	Head Carcinoma
Measured	1884	21.6 $\pm$ 6.2	1402	8	474	46	19
Unmeasured	1804	25.5 $\pm$ 9.3	973	175	656	18	5
Total	3688	23.5 $\pm$ 8.1	2375	183	1130	64	24

It is the sum of the activity of ^{226}Ra , in μCi , that entered the body plus two and a half times the activity of ^{228}Ra , in μCi , that entered the body. The head carcinoma was induced by radon (^{222}Rn) formed by decay of ^{228}Ra trapped within the air spaces in bone. Because the half-life of ^{222}Rn is only 55 seconds, it precludes its migration into these cavities; for this reason, ^{228}Ra was not considered and only ^{226}Ra activity was used for the systemic intake.

The panel data used for analysis of bone sarcomas and head carcinomas is summarized respectively in Tables 2 and 3. The interval sizes chosen were almost the same as that of Rowland, et al. (1978), except that the weighted average of systemic intake for the lowest dose < 0.5 and the highest dose $> 1,000$. The interval of the lowest dose < 0.5 is broken into two intervals, < 0.25 and $0.25-0.49$; in contrast to Rowland, et al. who ignored the measured dose of subjects in the lowest level. Similarly, the range of the highest dose $> 1,000$ is broken into three intervals for bone sarcomas, designated as B1 (1,000-2,499, $\geq 2,500$), and B2 (1,000-1,299, 1,300-1,599, 1,600-1,899, 1,900-2,199, 2,200-2,499, $\geq 2,500$), and two intervals for head carcinomas, H1 ($\geq 1,000$) and H2 (1,000-1,499, $\geq 1,500$). However, little difference in the estimated model parameters with respect to different interval sizes for doses greater than 1,000 μCi were concerned; thus, only B1 and H1 were used for the purpose of estimating regression coefficients.

Person-years were calculated from the year of first employment to the time of diagnosis of a bone sarcoma, of death, or to the end of 1984. Person-years were summed across cases within exposure levels to estimate the rate denominator. Although the estimated latent period of bone sarcomas followed a lognormal distribution with a median of 22.0 years (or 27.5 years) for all 64 cases (or 46 measured cases), it was decided not to subtract any fixed amount of time from the total person-years to obtain the person-years at risk. The inclusion of those first few years of experience could help establish more precisely the baseline risk (Thomas, 1987). The weighted average systemic intake for each class is the sum of person-year micro-curries for that class divided by the number of person years in the class. Similarly, the time required between first exposure to radium and diagnosis of head carcinoma follows a lognormal distribution with a median 37.5 years for all 24-head carcinomas; no assumed log time was subtracted from the calculated person-years to estimate person-years at risk.

Three possible potential confounding variables were considered: the age at first exposure (AFE) = age that a dial painter began to put the tip of the paint brush into her lips (years), the duration of exposure (DOE) = period of time that took between the start of putting the tip of the paint brush into her lips and stop such a practice (days), and the time since first exposure (TFE) = years since the first exposure

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Table 2: Case Distribution and Bone Sarcoma Experience as a Function of Dose Level and Potential Time-Related Confounding Factors

B1: DOSE (Systemic intake/ $^{226}\text{Ra} + 2.5 \times ^{228}\text{Ra}$)		Number of Subjects	Person- Years (Years)	N (Bone Sarcoma)	Average Age at 1 st Exposure (AFE, Years)	Average Duration of Exposure (DOE, Days)	Average Time Since 1 st Exposure (TFE, Years)
Range (μCi)	Weighted Average (μCi)						
<0.25	0.04	881	35054	0	21.2	159.1	39.8
0.25-0.49	0.36	190	8176	0	21.7	233.5	43.0
0.5-0.99	0.72	172	7784	0	21.7	233.2	45.3
1.0-2.49	1.52	193	9782	0	19.7	212.6	50.7
2.5-4.9	3.59	96	5100	0	19.0	195.6	53.1
5-9.9	6.99	78	4281	0	19.5	119.5	54.9
10-24	16.46	73	4144	0	19.5	156.0	56.8
25-49	26.12	52	2932	1	19.4	156.2	56.4
50-99	69.73	21	1188	0	18.3	301.1	56.6
100-249	160.5	28	1472	1	18.3	307.8	52.6
250-499	374.3	36	1639	12	19.3	251.6	45.5
500-999	683.1	21	835	10	19.5	268.1	39.8
1,000-2,499	1665.4	26	611	18	18.8	157.9	23.5
$\geq 2,500$	3576.6	17	310	4	18.5	185.8	18.2

Table3: Case Distribution and Head Carcinoma Experience as a Function of Dose Level and Potential Time Related Confounding Factors

H1: DOSE (Systemic Intake/ ²²⁶ Ra)		Number of Subjects	Person- Years (Years)	N (Head Carcinoma)	Average Age at 1 st Exposure (AFE, Years)	Average Duration of Exposure (DOE, Days)	Average Time Since 1 st Exposure (TFE, Years)
Range (μ Ci)	Weighted Average (μ Ci)						
< 0.25	0.04	884	36155	0	32.2	158.9	40.9
0.25-0.49	0.35	213	9801	0	21.2	210.5	46.0
0.5-0.99	0.71	198	9487	0	21.3	210.9	47.9
1.0-2.49	1.53	237	12489	0	20.1	191.0	52.7
2.5-4.9	3.50	85	4630	0	19.1	217.8	54.5
5-9.9	6.90	50	2826	0	19.1	155.0	56.5
10-24.9	16.0	59	3402	0	19.3	197.6	57.7
25-49	35.3	40	2148	1	18.6	217.4	53.7
50-99	68.6	23	1141	1	18.2	370.6	49.6
100-249	175.	33	1303	6	17.9	143.4	39.5
250-499	364.	33	1379	6	19.2	259.2	41.8
500-999	616.	16	444	2	21.9	238.9	27.8
$\geq 1,000$	1566	13	289	3	17.8	179.2	22.2

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Poisson Regression Model

Because bone sarcomas and head carcinomas are rare cancers, the frequency count (Y) of bone sarcomas (or head carcinomas) was assumed to follow a Poisson process, that is, the probability of N bone (or head) tumors is given by

$$P(Y = N) = e^{-\mu} \cdot \frac{\mu^N}{N!}, N = 0, 1, 2, \dots, (\mu > 0), \quad (1)$$

where μ denotes the expected count number of bone (or head) tumor. The tumor rate is Y/PYR, where PYR denotes the total exposure person years. Further, a Poisson regression model with interaction terms was applied to model the expected frequency counts of bone (or head) tumor as a function of logarithmic dose, temporal confounding factors together with their interaction with the logarithmic dose as follows:

$$\begin{aligned} \ln \mu = & \alpha_0 + \ln(PYR) + \alpha_1 LDOSE + \alpha_2 AFE \\ & + \alpha_3 DOE + \alpha_4 TFE + \alpha_5 LDOSE \cdot AFE \\ & + \alpha_6 LDOSE \cdot DOE + \alpha_7 LDOSE \cdot TFE \end{aligned} \quad (2)$$

where $\ln$, the natural logarithmic function, of the left-hand side of (2) denotes link function, $\ln(PYR)$ is the offset (McCullagh & Nelder, 1989), and LDOSE is the natural logarithm of the weighted average systemic intake.

The reason the logarithm of the dose level (LDOSE) was used as opposed to the dose level was that the ratio between the highest to the lowest dose level was greater than 1,000. The method of maximum likelihood estimation was employed in computing the unknown regression coefficients (α_i 's) of equation 2 by setting distribution = Poisson, link = log, and offset = $\ln(PYR)$ in the Proc GENMOD provided by the SAS package (SAS/STAT User's Guide, 1999). Based upon the well-formulated hierarchical principle, a backward elimination procedure was employed to retain the significant terms in equation 2 (Kleinbaum, et al., 1982). A criterion of the best fit is that the ratio of the scaled deviance divided by the degrees of freedom (d.f.) associated with the fitted model equals to one (Fleiss, et al., 2003).

Results

A total of 64 and 24 subjects were diagnosed with bone sarcomas and head carcinomas respectively. The prevalence for bone sarcoma (1.7% = 64/3,688) is 2.7 times as large as that (0.7% = 24/3,688) for head carcinoma (see Table 1). The reason for this significant difference in the incidence rate was that the head carcinoma seems to appear much later. The time of appearance for bone sarcoma was approximately 5 years, whereas 19 years for head carcinoma if the time of appearance was plotted against the initial systemic intake (Rowland, 1994). The highest systemic intake was the age at first exposure (AFE); values ranged from 16.0 to 21.7, which confirmed that the female radium dial workers were very young.

The average duration of exposure was shorter for low dose ranges than that for high dose ranges because the entire cohort in this study was comprised of two major sub-cohorts, pre-1930 and post-1930. A warning not put the tip of the paint brush into their mouth was issued by the government to workers in the dial painting industry in 1926; hence, workers in the post-1930 cohort received much less exposure. Similarly, the average time since first exposure (TFE) value for the class over 2,500 μCi was only 18.2 years which was far shorter than those in the range of less than 1,000 μCi . This was because most of 17 measured in that class were already diseased. Incidentally, the highest systemic intake was 6,331 μCi .

Table 4 shows the parameter estimate, standard error/p-value and scaled deviance/degrees of freedom associated with each of the risk factors used in (2) for the dataset B1. Using the p-value < 0.05 as a criterion for variable inclusion, the final models for the bone tumor that represent the dataset B1 is given respectively by

$$\ln \mu = 4.8 - 1.2 \cdot LDOSE - 0.4 \cdot TFE + 0.051 \cdot LDOSE \cdot TFE, \quad (3)$$

Table 4: Estimated Regression Coefficients (p-value) and Scaled Deviance (degrees of freedom) for Bone Sarcoma

Data Set	Intercept (p-value)	LDOSE (p-value)	TFE (p-value)	LDOSE*TFE (p-value)	Scaled Deviance (d.f.)
B1	4.78 (0.38)	-1.19 (0.09)	-0.36 (0.002)	0.051 (0.001)	6.12 (10)

for dataset B1, the interaction term $LDOSE \times TFE$ was significant. As a result, $LDOSE$ and TFE (the lower order term) were retained in the model, even though the p-value for the term of $LDOSE$ (p-value = 0.09) in equation was not significant.

Table 5 shows the parameter estimates, standard errors, p-value, model deviances and degrees of freedom after fitting Poisson model of (2) to dataset H1. According to Table 5, the Poisson models for H1 is given respectively by

$$\ln \mu = -11.29 + 0.978 \cdot LDOSE. \quad (4)$$

Discussion

Time since first exposure (TFE) (see eq. 3), shown as a confounding factor, had an effect on the occurrence of bone sarcomas in addition to the logarithmic dose. Worse, a significant interaction existed between the logarithmic dose and the time since first exposure: This implies that, for different time since first exposure, the effect of the logarithmic dose on the expected frequency of bone tumors is different. In other words, time since first exposure is an effect modifier (Kleinbaum, et al., 1982). By contrast, time since first exposure is neither a confounder nor an effect modifier for the expected frequency of head carcinomas. An advantage of using the logarithmic dose level is reflected in that it is not necessary to be concerned if the term of dose-squared or the term of power higher than two is included or not. From a Taylor's series expansion, $\ln(DOSE)$ contains all powers of $DOSE$ in the model.

The Environmental Protection Agency proposed the maximum level for radium in drinking water to be set at 5 pCi/liter, where pCi denotes picocurie and one picocurie, one-trillionth of a curie (Train, 1975). Using the generally accepted values of 2.2 liters of water consumed per day and a gut absorption rate of 21%, the systemic intake calculated by Rowland, et al. (1978) is 843 pCi of ^{226}Ra . Using the linear model for head carcinoma, the incidence rate after 1-year intake calculated by Rowland, et al. is 1.3×10^{-8} . However, by using equation 4, the incidence rate for head carcinomas is 1.2×10^{-5} . In a comparison with this estimate, the Rowland, et al. (1978) estimate seems too conservative. Rowland, et al. did not calculate the rate for bone sarcoma, however, using equation 3, the rates for bone sarcomas were 3.4, 0.09, 0.002, and 6.2×10^{-5} , respectively for $TFE = 10, 20, 30$, and 40 years.

Although the data for the frequency of bone/head tumors seemingly have excessive zeros over a wide range of logarithmic dose levels, the zero-inflated Poisson model (Lambert, 1992) was not able to be used for datasets B1 or H1 because it was not possible to model its frequency as a mixture of two models: one is a degenerated point mass function at zero count and the other is a Poisson model for count greater than one. When attempted using the SAS Proc GENMOD, the scaled deviance (36.7) was much larger than its degrees of freedom (11).

Baum (1973) claimed that the dose-response curve of radiation induced tumors was often represented by a power function of dose with exponents less than one. By using the atomic bomb of surviving population in

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Table 5: Estimated Regression Coefficients (p-value) and Scaled Deviances (degrees of freedom) for Head Carcinoma

Data Set	Intercept (p-value)	LDOSE (p-value)	Scaled Deviance (d.f.)
H1	-11.29 (< 0.0001)	0.978 (< 0.0001)	7.51 (11)

Hiroshima and Nagasaki, Japan, Baum found that for data on leukemia in Hiroshima and Nagasaki, the dose-response curve was adequately represented by power functions of dose with exponents between 0.65 and 1.0. However, in view of results from this study, the expected frequency was a function of not only the logarithmic dose, but also potential time-related confounding factors (time since first exposure) and the interaction between the logarithmic dose and time since first exposure. Hence, Baum's claim for the dose-response relationship is clearly invalid.

Recent studies have also addressed other aspects of radiation poisoning among U.S. radium dial workers. Carnes, et al. (1997) adopted Cox's (1972) hazard regression to build a dose response model. Although they incorporated AFE, a time-related confounding factor, into their model, the AFE was shown to be insignificant according the Poisson model used in this study. In addition, Carnes, et al. did not consider interaction in their study. An overview of studies of the U.S. radium dial workers was presented by Fry (1998). In addition, Renttzi (2004) addressed the case of radium dial workers as human experimentation with radiation harmful effect.

Conclusion

Using the Poisson regression model, data regarding radiation poisoning among female radium dial workers were re-analyzed. A dose-response model was obtained respectively for bone sarcoma and head carcinoma. The model showed that the expected frequency of bone sarcomas was not only a function of the logarithmic dose and the time since first exposure, but also the interaction between the

logarithmic dose and the time since first exposure, whereas the dose-response model for head carcinomas was a function of the logarithmic dose only. Among all dose-response models available in the literature, the Poisson regression model proposed in this article was deemed best because it is simple, precise and informative.

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Ordinal Regression Analysis: Using Generalized Ordinal Logistic Regression Models to Estimate Educational Data

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The proportional odds (PO) assumption for ordinal regression analysis is often violated because it is strongly affected by sample size and the number of covariate patterns. To address this issue, the partial proportional odds (PPO) model and the generalized ordinal logit model were developed. However, these models are not typically used in research. One likely reason for this is the restriction of current statistical software packages: SPSS cannot perform the generalized ordinal logit model analysis and SAS requires data restructuring. This article illustrates the use of generalized ordinal logistic regression models to predict mathematics proficiency levels using Stata and compares the results from fitting PO models and generalized ordinal logistic regression models.

Key words: Generalized ordinal logistic regression models, proportional odds models, partial proportional odds model, ordinal regression analysis, mathematics proficiency, stata, comparison.

Introduction

Ordinal data in education are substantive. Perhaps the most well-known model for estimating an ordinal outcome variable is the proportional odds (PO) model (Agresti, 1996, 2002, 2007; Anath & Kleinbaum, 1997; Armstrong & Sloan, 1989; Hardin & Hilbe, 2007; Long, 1997; Long & Freese, 2006; McCullagh, 1980; McCullagh & Nelder, 1989; O'Connell, 2000, 2006; Powers & Xie, 2000). Current general-purpose statistical software packages, such as SAS, SPSS and Stata, use this model as the default for ordinal regression analysis. The PO model is used to estimate the cumulative probability of being at or below a particular level of a response variable, or being beyond a particular level, which is the complementary direction. In this model, the effect of each predictor is assumed to be the

same across the categories of the ordinal dependent variable. This means that for each predictor, the effect on the odds of being at or below any category remains the same within the model. This restriction is referred to as the proportional odds, or the parallel lines, assumption.

The assumption of proportional odds is often violated, however, because it is strongly affected by sample size and the number of covariate patterns – for example, including continuous covariates or interactions as the predictors (Allison, 1999; Brant, 1990; O'Connell, 2006). It is misleading and invalid to interpret results if this assumption is not tenable. It has been suggested that the separate underlying binary logistic regression models are fitted and then are compared with the original PO model (Allison, 1999; Bender & Grouven, 1998; Brant, 1990; Clogg & Shihadeh, 1994; Long, 1997; O'Connell, 2000, 2006). Although this strategy would help researchers identify the reason why the overall PO assumption is violated, it is not clear how a well-fitting parsimonious model with a violated PO assumption is developed and interpreted.

To address this issue, the partial proportional odds (PPO) model (Peterson &

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Harrell, 1990) and the generalized ordinal logit model (Fu, 1998; Williams, 2006) were developed. The PPO model allows for interactions between a predictor variable that violates the PO assumption and different categories of the ordinal outcome variable. The analysis of a PPO model using SAS GENMOD procedure requires a restructured data set, which includes a new binary variable indicating whether an individual is at or beyond a particular level (O'Connell, 2006; Stokes, Davis & Koch, 2000).

The generalized ordinal logit model developed by Fu (1998) and William (2006) relaxes the PO assumption by allowing the effect of each explanatory variable to vary across different cut points of the ordinal outcome variable without data restructuring. In addition, this model estimates parameters differently from the PPO model using SAS. Williams' *gologit2* program (2006) for Stata is a more powerful extension of Fu's *gologit* (1998); it can estimate the generalized ordered logit model, the PPO model, the PO model and the logistic regression model within one program.

In educational research, the PO model is widely used. However, the use of the generalized ordinal logit model appears to be overlooked even in cases where the PO assumption is violated. One likely reason for this is the restriction of current statistical software packages: SPSS cannot perform the generalized ordinal logit model analysis and SAS requires data restructuring prior to data analysis, therefore, it is important to help educational researchers better understand this model and utilize it in practice.

The purpose of this study is to illustrate the use of generalized ordinal logistic regression models to predict mathematics proficiency levels using Stata and to compare the results of fitting PO and the generalized ordinal logistic regression models. This article is an extension of previous research focusing on the PO model (Liu, 2009), and the Continuation Ratio model with Stata (Liu, O'Connell, & Koirala, 2011). Ordinal regression analyses are based on data from the 2002 Educational Longitudinal Study (ELS) in which the ordinal outcome of students' mathematics proficiency was forecast from a set

of predictors, such as, using computers for fun, school work and to learn on their own.

Theoretical Framework

General Logistic Regression Model and the Proportional Odds Model

The binary logistic regression model estimates the odds of success or experiencing an event for the dichotomous response variable given a set of predictors. The logistic regression model can be defined as (Allison, 1999; Menard, 1995):

$$\begin{aligned}\ln(Y') &= \text{logit} [\pi(\underline{x})] \\ &= \ln \left(\frac{\pi(\underline{x})}{1 - \pi(\underline{x})} \right) \\ &= \alpha + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p\end{aligned}\quad (1)$$

In an ordinal logistic regression model, the outcome variable has more than two levels. It estimates the probability being at or below a specific outcome level given a collection of explanatory variables. The ordinal logistic regression model can be expressed in the logit form (Liu, 2009; Long, 1997; Long & Freese, 2006) as follows:

$$\begin{aligned}\ln(Y'_j) &= \text{logit} [\pi(x)] \\ &= \ln \left(\frac{\pi(x)}{1 - \pi(x)} \right) \\ &= \alpha_j + (-\beta_1 X_1 - \beta_2 X_2 - \dots - \beta_p X_p)\end{aligned}\quad (2)$$

where $\pi_j(\underline{x}) = \pi(Y \leq j \mid x_1, x_2, \dots, x_p)$ is the probability of being at or below category j , given a set of predictors, $j = 1, 2, \dots, J-1$, α_j are the cut points and $\beta_1, \beta_2, \dots, \beta_p$ are logit coefficients. When there are j categories, the PO model estimates $J-1$ cut points. This PO model assumes that the logit coefficient of any predictor is independent of categories, i.e., the coefficients for the underlying binary models are the same across all cutpoints. The equal logit slope or the proportional odds assumption can be assessed by the Brant test (Brant, 1990), which estimates logit coefficients for underlying binary logistic regressions, and provides the chi-square test

statistics for each predictor and the overall model in Stata.

To estimate the ln (odds) of being at or below the j^{th} category, the PO model can be rewritten as the following form:

$$\begin{aligned} \text{logit} [\pi(Y \leq j | x_1, x_2, \dots, x_p)] \\ = \ln \left(\frac{\pi(Y \leq j | x_1, x_2, \dots, x_p)}{\pi(Y > j | x_1, x_2, \dots, x_p)} \right) \\ = \alpha_j + (-\beta_1 X_1 - \beta_2 X_2 - \dots - \beta_p X_p). \end{aligned} \quad (3)$$

Thus, this model predicts cumulative logits across $J-1$ response categories. The cumulative logits can then be used to calculate the estimated cumulative odds and the cumulative probabilities being at or below the j^{th} category.

Different software packages may estimate parameters differently and the ordinal logistic regression model can be expressed in different forms (Liu, 2009). For example, Stata follows the above form with a negative sign before the logit coefficients. SAS, however, uses a different form when estimating the cumulative odds of being at or below a particular category using the ascending option.

The Generalized Ordinal Logistic Regression Model

The generalized ordinal logistic regression model extends the PO model by relaxing the PO assumption. In this model, if the assumption is violated by a certain predictor, then its effect can be estimated freely across different categories of the dependent variable. The model is expressed as:

$$\begin{aligned} \ln(Y_j') = \ln \left(\frac{\pi_j(\underline{x})}{1 - \pi_j(\underline{x})} \right) \\ = \alpha_j + (\beta_{1j} X_1 + \beta_{2j} X_2 + \dots + \beta_{pj} X_p). \end{aligned} \quad (4)$$

The above form can also be expressed as proposed by Fu (1998) and Williams (2006):

$$\begin{aligned} \text{logit} [\pi(Y > j | x_1, x_2, \dots, x_p)] \\ = \ln \left(\frac{\pi(Y > j | x_1, x_2, \dots, x_p)}{\pi(Y \leq j | x_1, x_2, \dots, x_p)} \right) \\ = \alpha_j + (\beta_{1j} X_1 + \beta_{2j} X_2 + \dots + \beta_{pj} X_p), \end{aligned} \quad (5)$$

where, in both equations, α_j are the intercepts or cutpoints, and $\beta_{1j}, \beta_{2j}, \dots, \beta_{pj}$ are logit coefficients. This model estimates the odds of being beyond a certain category relative to being at or below that category. A positive logit coefficient generally indicates that an individual is more likely to be in a higher category as opposed to a lower category of the outcome variable. To estimate the odds of being at or below a particular category, however, the signs before both the intercepts and logit coefficients in equation (5) must be reversed.

In this expression, all of the effects of the explanatory variables are allowed to vary across each of the cutpoints. If some of these effects are found to be stable, they can be constrained to be equal as in the PO model; thus, generalized ordinal logistic regression model refers to the case where at least one of the coefficients for a predictor varies across categories. Compared to SAS, neither data restructuring nor interactions between categories and predictor variables with non-proportional odds are required by Stata – this makes data analysis of the generalized ordinal logit model much easier.

Methodology

Sample

The data used in this study are from the Educational Longitudinal Study of 2002 (ELS: 2002). The ELS 2002 study, conducted by the National Center for Educational Statistics (NCES), was designed to provide longitudinal data regarding high school students' achievement, attitude and experiences, and their postsecondary school education and the labor market. In the 2002 base year of the study a cohort of more than 15,000 high school sophomores from a national sample of 752 public and private high schools participated in

the study by taking cognitive tests and responding to surveys.

The outcome variable was students' mathematics proficiency levels in high school, which was an ordinal variable with five levels (1 = students can do simple arithmetical operations on whole numbers; 2 = students can do simple operations with decimals, fractions, powers, and root; 3 = students can do simple problem solving; 4 = students can understand intermediate-level mathematical concepts and/or find multi-step solutions to word problems; and 5 = students can solve complex multiple-step word problems and/or understand advanced mathematical material) (Ingels, Pratt, Roger, Siegel, & Stutts, 2004, 2005). These five proficiency domains were hierarchically structured: mastery of higher proficiency level indicated mastery of all previous levels. Those students who failed to pass through level 1 were assigned to level 0. Table 1 provides the categories and frequencies of all mathematics proficiency levels.

Data Analysis.

After the PO model was fitted with a single explanatory variable using the Stata *ologit* command the full-model was then fitted with all three explanatory variables. The *brant* test command, one of the Stata *SPost* (Long & Freese, 2006) routines for the analysis of post-estimations, was used to examine the PO assumption and identify predictors that violated the assumption. Stata *gologit* (Fu, 1998) and *gologit2* (Williams, 2006) commands were then used to fit the generalized ordinal regression models and the results from both PO models and the generalized ordinal regression models were compared.

Results

Proportional Odds Model with a Single Explanatory Variable

A PO model with a single predictor, using computers for fun, was fitted first using the Stata *ologit* command with the logit function as default. Table 2 provides the results for the single-predictor PO model.

Table 1: Proficiency Categories and Frequencies (Proportions) for the Study Sample, ELS 2002 (N = 15,976)

Proficiency Category	Description	Frequency and Percent of Total Sample
0	Did not pass level 1	842 (5.27%)
1	Can do simple arithmetical operations on whole numbers	3,882 (24.30%)
2	Can do simple operations with decimals, fractions, powers, and root	3,422 (21.42%)
3	Can do simple problem solving	4,521 (28.30%)
4	Can understand intermediate-level mathematical concepts and/or find multi-step solutions to word problems	3,196 (20.01%)
5	Can solve complex multiple-step word problems and/or understand advanced mathematical material	113 (0.71%)

The log likelihood ratio Chi-Square test with 1 degree of freedom, $LR \chi^2_{(1)} = 992.52$, $p < 0.001$, indicated that the logit regression coefficient of the predictor (using computer for fun) was statistically different from 0, therefore, the model with one predictor provided a better fit than the null model with no independent variables. The Pseudo $R^2 = 0.023$, which is the likelihood ratio R^2_L , suggested that the relationship between the response variable, mathematics proficiency, and the predictor, using computer for fun, was small.

The estimated logit regression coefficient, $\beta = 0.384$, $z = 31.28$, $p < 0.001$, indicated that the predictor variable, using computers for fun, had a significant effect on mathematics proficiency. Substituting the value of the coefficient into formula (3), $\text{logit} [\pi(Y \leq j | X_1)] = \alpha_j + (-\beta_1 X_1)$, $\text{logit} [\pi(Y \leq j | \text{fun})] = \alpha_j - 0.384 (\text{fun})$. $OR = e^{(-0.384)} = 0.681$, indicated that the odds of being at or below a particular proficiency level relative to beyond that level decreased by a factor of 0.681 with one unit increase in the frequency of using computers for fun. In other words, a higher frequency of using computers for fun was related to the likelihood of being in a higher proficiency level. To estimate the probability of being beyond a category of mathematics proficiency, which is the complement of the probability of being at or below a category, it is only necessary to exponentiate 0.384; this results in $OR = 1.468$, indicating that the odds of being beyond a proficiency level was 1.468 time greater with one unit increase in the frequency of using computers for fun.

Full Proportional Odds Model with Three Predictor Variables

Next, the full PO model with all three predictor variables was fitted. Table 2 provides the results of the full model. The log likelihood ratio Chi-Square test, $LR \chi^2_{(3)} = 1391.45$, $p < 0.001$, indicated that the full model with three predictor provided a better fit than the null model with no independent variables. The likelihood ratio $R^2_L = 0.032$ was larger than that of the single-variable model, but was still small. Compared with the single-variable model (3.020), the AIC statistic indicated that the full-model fitted the data slightly better (2.992).

The logit effects of all three predictors on mathematics proficiency were significant. Similar to the single variable PO model, the estimated logit regression coefficient for using computers for fun (*fun*), $\beta = 0.314$, $z = 22.44$, $p < 0.001$; the logit coefficient for using computers for school work (*schoolwk*), $\beta = 0.307$, $z = 19.815$, $p < 0.001$; and finally, for using computers to learn on their own (*learn*), $\beta = -0.072$, $z = -5.295$, $p < 0.001$. The predictors, using computers for fun and using computers for school work, were positively associated with the odds of being beyond a proficiency level. In terms of odds ratio (OR), the odds of being beyond a proficiency level were 1.369 times greater with one unit increase in the frequency of using computers for fun, and 1.360 times greater with one unit increase in the frequency of using computers for school work. For every one unit increase in using computers to learn on their own, however, the odds of being beyond a particular category decreased by a factor of 0.931 ($OR = 0.931$).

The full model also estimated five cutpoints, which were used to differentiate adjacent categories of the mathematics proficiency. $\alpha_1 = -1.022$, which was the cutpoint for the cumulative logit model for $Y > 0$; α_2 was the cutpoint for the cumulative logit model for $Y > 1$; the final α_5 was used as the cutpoint for the logit model when $Y > 4$.

Brant Test of the Proportional Odds Assumption

The Brant test of the PO assumption was examined using the *brant* command of the Stata *SPost* (Long & Freese, 2006) routines. Stata Brant test provided results of a series of separate binary logistic regression across different category comparisons, univariate Brant test results for each predictor and the omnibus test for the overall model. Table 3 shows five ($j-1$) associated binary logistic regression models for the full PO model, where each split compares $Y > \text{cat. } j$ to $Y \leq \text{cat. } j$ because data were dichotomized according to probability comparisons. Examining the logit coefficient of all three variables across five logistic regression models, it is evident that the effect of using computers for fun was similar across these models. The effect of using computers for

school work was similar across the first three models but it increased from model 3 to 5. The logit coefficient in model 5 was almost double that observed in model 1. The effect of using computers to learn on their own was close among the first four logistic regression models, however, the direction of this effect changed in model 5. Visual examination provided only preliminary results of whether the parallel effects assumption was tenable.

To test the PO assumptions, the Brant test provided the results for the overall model and each predictor. Table 4 presents χ^2 tests and p values for the full PO model and separate variables. The omnibus Brant test for the full model, $\chi^2_{12} = 29.59$, $p = 0.003$, indicates that the proportional odds assumption for the full model was violated. To identify which predictor variables violated the assumption, separate Brant tests were examined for each predictor variable.

Table 2: Results of the Single-Variable PO Model and the Full PO Model

Variable	Single-Variable Model		Full Model	
	b (se(b))	OR	b (se(b))	OR
α_1	-1.488		-1.022	
α_2	.627		1.20	
α_3	1.571		2.082	
α_4	2.900		3.437	
α_5	6.475		7.033	
fun	.384**	1.468	.314**	1.369
schoolwk			.307**	1.360
learn			-.072**	.931
$LR R^2$	.023		.032	
Brant Test (Omnibus Test)	$\chi^2_4 = 5.14$		$\chi^2_{12} = 29.59$ **	
Model Fit	$\chi^2_1 = 992.52$ **		$\chi^2_3 = 1391.45$ **	

* $p < 0.05$; ** $p < 0.01$

Table 3: A Series (j-1) of Associated Binary Logistic Regression Models for the Full PO Model, Each Split Compares $Y > \text{cat. } j$ to $Y \leq \text{cat. } j$

	$Y > 0$	$Y > 1$	$Y > 2$	$Y > 3$	$Y > 4$	Brant Test p Value
Variable	Logit (b)	Logit (b)	Logit (b)	Logit (b)	Logit (b)	
Constant	1.00	-1.091	-2.014	-3.485	-8.523	
fun	.357	.327	.316	.285	.316	.328
schoolwk	.286	.278	.293	.351	.492	.02*
learn	-.094	-.067	-.081	-.068	.144	.094

* $p < 0.05$; ** $p < 0.01$

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Results revealed that the univariate Brant tests for the PO assumption were upheld for using computers for fun and using computers to learn on their own. Conversely, the Brant test was violated for using computers for school work.

Table 4: Brant Tests of the PO Assumption for Each Predictor and the Overall Model

Variable	Test	p Value
fun	$\chi^2_4 = 4.62$	.328
schoolwk	$\chi^2_4 = 11.55$	.021*
learn	$\chi^2_4 = 7.93$	.094
All (Full-Model)	$\chi^2_{12} = 29.59$	.003**

* $p < 0.05$; ** $p < 0.01$

Results of the Generalized Ordinal Logistic Regression Model Using Stata *gologit*

When the PO assumption is not satisfied, Stata *gologit* (Fu, 1998) relaxes the proportionality assumption by allowing the logits effects of predictor variables to vary across cutpoints, which dichotomize the underlying proficiency outcome. Similar to a series of underlying binary logistic regression models where the data were dichotomized across different categories, the effects of the predictor variables estimated by the generalized ordinal logistic regression model could vary freely.

Table 5 and Figure 1 show the results of the generalized ordinal model. The logit effects and corresponding odds ratios (OR) of all three variables were different across all five models comparing probabilities of being beyond category j versus at or below that category. For example, the odds ratios for using computers for fun across five comparisons were 1.428, 1.385, 1.368, 1.322 and 1.314, respectively. They were similar because the equal slopes assumption test was tenable for this predictor variable. After relaxing the PO assumption, Stata *gologit* estimated 12 more parameters in the generalized ordinal logistic regression model than the full PO model by Stata *ologit*.

Results of the Generalized Ordinal Logistic Regression Model Using *gologit2*

Stata *gologit2* (Williams, 2006) is an extension of *gologit* (Fu, 1998), and can estimate various types of generalized models, including the partial proportional odds model (PPO), the PO model and the binary logistic regression model. Although Stata *gologit2* allows the effects of all predictor variables to vary even when some violate the PO assumption, it can relax the PO assumption and put equal-slope constraints on those variables whose effects are constant across cutpoints: The model is then referred to as the PPO.

Table 6 and Figure 2 show the results of the generalized ordinal logistic regression model or the PPO model using *gologit2*. Because only one predictor variable, using computers for school work, violated the PO assumption, the other two variables, using computers for fun and using computers to learn on their own, were held constant in the PPO model. For example, the logit coefficients and odds ratios for using computers to learn on their own were the same across five comparisons (OR = 0.913). The OR for using computer for school work were different across each cutpoint, they were: 1.331, 1.329, 1.342, 1.436 and 1.906, respectively. The PPO model estimated by Stata *gologit2* was more parsimonious than the generalized ordinal logistic regression model by *gologit* because the former model estimated five fewer parameters than the latter.

In terms of odds ratio, using computers for fun was positively associated with the odds of being above a particular mathematics proficiency level as opposed to being at or below that level (OR = 1.372); however, using computers to learn on their own had a negative effect on the odds of being above a particular proficiency level (OR = 0.93). Because the effect of using computers for school work was not invariant across five comparisons, separate interpretations were required. Using computers for school work was associated with the likelihood of being in a higher mathematics proficiency level. The effects became much stronger when mathematics proficiency level moved from low to high, further, the largest effect was identified among the final comparison (proficiency level 5 versus from 0 to 4).

Conclusion

This article reviewed the proportional odds model and demonstrated the use of generalized ordinal regression models to estimate mathematics proficiency. The results of fitting the PO models and the generalized ordinal logistic regression models were interpreted. In addition, two different methods used to estimate the generalized ordinal models by Williams (2006) and Fu (1998) were illustrated and compared.

Compared to the PO model, the generalized ordinal logistic model provides a better solution when the proportional odds assumption is violated. The effects of the predictors which meet the PO assumption can be interpreted in the same way as that in the PO model. The effects of explanatory variables that violate the PO assumption must be interpreted separately at each comparison (i.e., being

beyond a particular category versus at or below that category), and need more attention.

When the proportional odds assumption is untenable, the generalized ordinal logistic model proposed by Fu (1998) may be used for preliminary analysis. Williams' model (2006) is a more powerful extension of that of Fu (1998) in that it incorporated and expanded Fu's procedure. Numerous different types of generalized ordinal models can be estimated by Williams' *gologit2* procedure, including the commonly used partial proportional odds model (PPO), which only relaxes the PO assumption when it is violated by one or a few predictors, but holds constant for those which have equal effects. Although not provided herein, methods of model diagnostics for ordinal logistic regression models were introduced by O'Connell and Liu (2011).

Table 5: Results of the Generalized Ordinal Logit Model Using Stata *gologit*
($Y > \text{cat. } j$ vs. $Y \leq \text{cat. } j$)

	Y > 0 vs. Y ≤ 0		Y > 1 vs. Y ≤ 1		Y > 2 vs. Y ≤ 2		Y > 3 vs. Y ≤ 3		Y > 4 vs. Y ≤ 4	
Variable	b (se(b))	OR	b (se(b))	OR	b (se(b))	OR	b (se(b))	OR	b (se(b))	OR
fun	.356 (.030)**	1.428	.326 (.016)**	1.385	.313 (.016)**	1.368	.279 (.022)**	1.322	.273 (.129)*	1.314
schoolwk	.276 (.037)**	1.318	.277 (.019)**	1.319	.299 (.018)**	1.348	.370 (.023)**	1.447	.540 (.116)**	1.716
learn	-.091 (.035)**	.913	-.067 (.017)**	.935	-.081 (.016)**	.922	-.066 (.019)**	.936	.180 (.093)	1.197
	α ₁ = 1.022		α ₂ = -1.083		α ₃ =-2.024		α ₄ =-3.520		α ₅ = -8.642	
LR R ²	0.033									
Model Fit	χ ² ₁₅ = 1429.62									

* $p < 0.05$; ** $p < 0.01$

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Figure 1: Generalized Ordinal Logistic Model Using Stata *gologit*

```
gologit Profmath BYS45A_REC BYS45B_REC BYS45C_REC
```

```
Iteration 0: Log Likelihood = -21943.368
```

```
Iteration 1: Log Likelihood = -21237.489
```

```
Iteration 2: Log Likelihood = -21228.561
```

```
Iteration 3: Log Likelihood = -21228.555
```

```
Iteration 4: Log Likelihood = -21228.555
```

Generalized Ordered Logit Estimates	Number of obs	=	14207
	Model chi2(15)	=	1429.62
	Prob > chi2	=	0.0000
Log Likelihood = -21228.5552037	Pseudo R2	=	0.0326

Profmath	Coef.	Std. Err.	z	P> z	[95% Conf. Interval]	
-----+-----						
mleq1						
BYS45A_REC	.356211	.0303759	11.73	0.000	.2966753	.4157468
BYS45B_REC	.2763788	.0372811	7.41	0.000	.2033091	.3494484
BYS45C_REC	-.0914208	.0350232	-2.61	0.009	-.1600651	-.0227765
_cons	1.021761	.1098978	9.30	0.000	.8063653	1.237157
-----+-----						
mleq2						
BYS45A_REC	.3257729	.01639	19.88	0.000	.2936492	.3578967
BYS45B_REC	.2768884	.0189779	14.59	0.000	.2396925	.3140843
BYS45C_REC	-.0673821	.0171035	-3.94	0.000	-.1009042	-.0338599
_cons	-1.082717	.0676152	-16.01	0.000	-1.21524	-.9501931
-----+-----						
mleq3						
BYS45A_REC	.3134542	.0163592	19.16	0.000	.2813907	.3455177
BYS45B_REC	.2989051	.0178569	16.74	0.000	.2639063	.333904
BYS45C_REC	-.081139	.0155428	-5.22	0.000	-.1116022	-.0506758
_cons	-2.02405	.0716248	-28.26	0.000	-2.164432	-1.883668
-----+-----						
mleq4						
BYS45A_REC	.2787754	.0223384	12.48	0.000	.234993	.3225578
BYS45B_REC	.3697106	.0227828	16.23	0.000	.3250571	.4143642
BYS45C_REC	-.0657926	.018757	-3.51	0.000	-.1025556	-.0290296
_cons	-3.530265	.1037457	-34.03	0.000	-3.733603	-3.326927
-----+-----						
mleq5						
BYS45A_REC	.27337	.1291764	2.12	0.034	.0201889	.5265512
BYS45B_REC	.5401159	.1155738	4.67	0.000	.3135954	.7666363
BYS45C_REC	.180175	.0928936	1.94	0.052	-.0018932	.3622431
_cons	-8.642421	.6316348	-13.68	0.000	-9.880403	-7.404439
-----+-----						

Compared to SAS, fitting generalized ordinal regression models using Stata is more straightforward because Stata does not require data restructuring and the results are easier to interpret (SAS needs an interaction term between the predictor with the violated effect and ordinal categories). The latest VGAM package (v. 0.8.3) for R (Yee, 2010, 2011) includes the functions of fitting the non-proportional odds and the partial proportional odds models, which is similar to Stata *gologit* and *gologit2*. Although different statistical packages may have advantages of fitting these models, the choice is left to researchers; this study does not imply an overall preference of one over another.

In educational research, the use of ordinal categorical data is common, thus, it is crucial for researchers to determine the most appropriate models to analyze ordinal

categorical dependent variables. It is hoped that this demonstration clarifies some of the issues that researchers must consider in selecting appropriate statistical models for analyzing ordinal data when the PO assumption is violated.

Notes

Previous versions of this article were presented at the Modern Modeling Methods Conference in Storrs, CT (May, 2011), the 76th Annual and the 17th International Meeting of Psychometric Society (IMPS) in Hong Kong (July, 2011), the Northeastern Educational Research Association Annual Conference in Rocky Hill, CT (October, 2011), and the Annual Meeting of American Educational Research Association (AERA), Vancouver, British Columbia, Canada (April, 2012).

Table 6: Results of the Generalized Ordinal Logit Model/Partial Proportional Odds Model Using Stata *gologit2* ($Y > \text{cat. } j$ vs. $Y \leq \text{cat. } j$)

	Y > 0 vs. Y ≤ 0		Y > 1 vs. Y ≤ 1		Y > 2 vs. Y ≤ 2		Y > 3 vs. Y ≤ 3		Y > 4 vs. Y ≤ 4	
Variable	b (se(b))	OR	b (se(b))	OR	b (se(b))	OR	b (se(b))	OR	b (se(b))	OR
fun	.317 (.014)**	1.373	.317 (.014)**	1.373	.317 (.014)**	1.373	.317 (.014)**	1.373	.317 (.014)**	1.373
schoolwk	.286 (.032)**	1.331	.284 (.018)**	1.329	.294 (.017)**	1.342	.362 (.022)**	1.436	.645 (.116)**	1.906
learn	-.072 (.014)**	.931	-.072 (.014)**	.931	-.072 (.014)**	.931	-.072 (.014)**	.931	-.072 (.014)**	.931
	α ₁ = 1.073		α ₂ = -1.060		α ₃ = -2.053		α ₄ = -3.650		α ₅ = -8.357	
LR R ²	.032									
Model Fit	χ ² ₇ = 1414.05									

* $p < 0.05$; ** $p < 0.01$

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Figure 2: Generalized Ordinal Logistic Model Using Stata *gologit2*

```
. gologit2 Profmath BYS45A_REC BYS45B_REC BYS45C_REC, pl(BYS45A_REC BYS45C_REC)
> lrforce
```

```
Generalized Ordered Logit Estimates          Number of obs   =       14207
                                             LR chi2(7)       =       1414.05
                                             Prob > chi2      =        0.0000
Log likelihood = -21236.343                 Pseudo R2        =        0.0322
```

```
( 1)  [0]BYS45A_REC - [1]BYS45A_REC = 0
( 2)  [0]BYS45C_REC - [1]BYS45C_REC = 0
( 3)  [1]BYS45A_REC - [2]BYS45A_REC = 0
( 4)  [1]BYS45C_REC - [2]BYS45C_REC = 0
( 5)  [2]BYS45A_REC - [3]BYS45A_REC = 0
( 6)  [2]BYS45C_REC - [3]BYS45C_REC = 0
( 7)  [3]BYS45A_REC - [4]BYS45A_REC = 0
( 8)  [3]BYS45C_REC - [4]BYS45C_REC = 0
```

	Profmath	Coef.	Std. Err.	z	P> z	[95% Conf. Interval]	
0							
	BYS45A_REC	.316712	.0140561	22.53	0.000	.2891625	.3442615
	BYS45B_REC	.2857963	.0322509	8.86	0.000	.2225857	.3490069
	BYS45C_REC	-.0718391	.0135787	-5.29	0.000	-.0984529	-.0452254
	_cons	1.073406	.0995634	10.78	0.000	.8782656	1.268547
1							
	BYS45A_REC	.316712	.0140561	22.53	0.000	.2891625	.3442615
	BYS45B_REC	.2841401	.0181596	15.65	0.000	.2485479	.3197323
	BYS45C_REC	-.0718391	.0135787	-5.29	0.000	-.0984529	-.0452254
	_cons	-1.060135	.0650042	-16.31	0.000	-1.187541	-.932729
2							
	BYS45A_REC	.316712	.0140561	22.53	0.000	.2891625	.3442615
	BYS45B_REC	.2938264	.0173751	16.91	0.000	.2597717	.327881
	BYS45C_REC	-.0718391	.0135787	-5.29	0.000	-.0984529	-.0452254
	_cons	-2.052606	.0673611	-30.47	0.000	-2.184631	-1.920581
3							
	BYS45A_REC	.316712	.0140561	22.53	0.000	.2891625	.3442615
	BYS45B_REC	.3620197	.0216704	16.71	0.000	.3195466	.4044928
	BYS45C_REC	-.0718391	.0135787	-5.29	0.000	-.0984529	-.0452254
	_cons	-3.650049	.0877478	-41.60	0.000	-3.822031	-3.478066
4							
	BYS45A_REC	.316712	.0140561	22.53	0.000	.2891625	.3442615
	BYS45B_REC	.6451267	.1084022	5.95	0.000	.4326623	.8575912
	BYS45C_REC	-.0718391	.0135787	-5.29	0.000	-.0984529	-.0452254
	_cons	-8.357108	.4475284	-18.67	0.000	-9.234247	-7.479968

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The Length-Biased Lognormal Distribution and Its Application in the Analysis of Data from Oil Field Exploration Studies

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The length-biased version of the lognormal distribution and related estimation problems are considered and sized-biased data arising in the exploration of oil fields is analyzed. The properties of the estimators are studied using simulations and the use of sample mode as an estimate of the lognormal parameter is discussed.

Key words: Length-biased lognormal distribution, estimation, simulations, sample mode, bootstrap.

Introduction

The term length-biased data refers to sample data where the probability of recording an observation depends on the magnitude, for example x , of the observation. In particular, the larger the observation, the higher the probability of observing the related event and, hence, including the corresponding observation in the sample. Length-biased data occur in many research areas and in fields of application, such as, medical science, ecology and geological sciences. Further, the term size-biased data is used to describe the situation where the probability of inclusion of an observation depends on a certain function: $w(x) > 0$ of x .

The length-biased version of the original probability density function (pdf.) that is of interest as a model is considered for modeling length-biased data. The lognormal distribution (LN) with parameters (μ, σ) is known to be a useful model in many applications. Therefore, it

is natural to expect the applications of length-biased lognormal distributions (LBLN) in some data analysis problems. For example, the lognormal distribution is commonly used in the analysis of data in geological studies, and Meisner and Demirmen (1981) observed that size-biased data occur in oil-field exploration studies. Yan (2004) considered the presence of length-biasedness in data on incubation periods arising in the SARS epidemic. Among many probability models that are considered for the analysis of these data, the length-biased lognormal distribution is one such model. Quin, et al. (2002) considered such a distribution for data on Breslow thickness in cancer research.

With respect to the properties of the length-biased lognormal distribution, in general, if $f(x; \theta)$ is the original pdf of a non-negative random variable X with $E(X) < \infty$, then its length-biased version is given by

$$g(x; \theta^*) = x f(x; \theta) / E(X), \quad x > 0,$$

where $\theta \in \Omega$ is a scalar or a vector of the parameters of the original distribution of X and $\theta^* \in \Omega^*$ denotes a scalar or a vector of the parameters of the corresponding length-biased version. In some cases θ^* is the same as θ . In practical situations, the interest is in estimating θ , the parameter(s) of the original distribution using length-biased data. However, due to the nature of the available data (length-biased data)

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the experimenter has no other choice but to use the length-biased version of the original distribution. Thus, there is a need to study the properties of the θ estimator with respect to $g(x; \theta^*)$, but such an estimation problem is not straightforward for the lognormal distribution.

Methodology

The random variable X is said to have a lognormal distribution with parameters (μ, σ) (denoted by LN (μ, σ)), if its pdf is

$$f(x; \mu, \sigma) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2\sigma^2}(\log x - \mu)^2\right], \quad (1)$$

where

$$x > 0, -\infty < \mu < \infty, \sigma > 0.$$

Length-Biased Lognormal Distribution-Definition and Properties

Using the definition of length-biased distribution, the pdf of the length-biased lognormal distribution (denoted by LBLN (μ, σ)) is given by

$$g(x; \mu, \sigma) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2\sigma^2}(\log x - (\mu + \sigma^2))^2\right] \quad (2)$$

where

$$x > 0, -\infty < \mu < \infty, \sigma > 0.$$

For convenience (2) will be expressed as

$$g(x; \mu, \sigma) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2\sigma^2}(\log x - \mu^*)^2\right], \quad (2a)$$

where

$$x > 0, \mu^* = \mu + \sigma^2, -\infty < \mu < \infty \text{ and } \sigma > 0.$$

The properties of the pdfs (1) and (2) are presented in Table 1. The mode of LBLN shown in Table 1 depends only on μ and not on σ^2 as for LN. From Table 2, it is clear that the

structure of the Fisher information for LBLN is not the same; hence the related results will not be the same when LBLN is used instead of LN in data analysis.

Parameter Spaces of LN (μ, σ) and LBLN (μ, σ)

In practical situations, for the analysis of length-biased data, the LN (μ, σ) is replaced by LBLN (μ, σ) . Further, examination of the pdfs for (1), (2) and (2a) shows that, although the listed pdfs seem to have the same form, there exists an in-built relationship between the parameters (μ, σ) of LBLN (μ, σ) . Thus, studying the implications of this relationship is necessary for the interpretation and estimation of parameters. A brief discussion related to the parameter spaces of (μ, σ) for these two distributions is useful for identifying the underlying problems in data analysis.

Let Ω_1 and Ω_2 denote the respective parameters of LN (μ, σ) and LBLN (μ, σ) . Then,

$$\Omega_1 = \{(\mu, \sigma) | -\infty < \mu < \infty, \sigma > 0\} \quad (3)$$

and

$$\Omega_2 = \{(\mu, \sigma) | -\infty < \mu^* = \mu + \sigma^2 < \infty, \sigma > 0\}. \quad (4)$$

From (3) and (4) it is clear that if the LBLN (μ, σ) is used as a model with $\mu^* = 0$, then it will represent only those members of the original LN (μ, σ) model for which $\mu^* = \mu + \sigma^2 = 0$, i.e. $\mu = -\sigma^2$. A similar restriction will arise for other values, $\mu^* = c$ for example, of μ^* , where c is some constant. Thus, there is a built-in restriction on the choice of the LBLN distribution with respect to the selection of the appropriate model for representing the original LN.

Maximum Likelihood Estimation (MLE)

Let $(X_1, X_2, \dots, X_n)$ be a random sample from a LBLN (μ, σ) distribution. The log-likelihood function $l(\mu, \sigma)$ is then given as

Table 1: Properties of LN (μ, σ) and LBLN (μ, σ)

Property	LN (μ, σ)	LBLN(μ, σ)
Mean	$\exp(\mu + \sigma^2 / 2)$	$\exp(\mu^* + \sigma^2 / 2)$
Median	$\exp(\mu)$	$\exp(\mu^*)$
Mode	$\exp(\mu - \sigma^2)$	$\exp(\mu^* - \sigma^2) = \exp(\mu)$
Variance	$\exp(2\mu + \sigma^2) \{ \exp(-\sigma^2) - 1 \}$	$\exp(2\mu^* + \sigma^2) \{ \exp(-\sigma^2) - 1 \}$

 Table 2: The Fisher Information Matrix of LN (μ, σ) and LBLN (μ, σ)

Fisher Information Matrix	LN(μ, σ)	LBLN(μ, σ)
	$I_1 = \begin{bmatrix} 1/\sigma^2 & 0 \\ 0 & 2/\sigma^2 \end{bmatrix}$	$I_2 = \begin{bmatrix} 1/\sigma^2 & 2/\sigma \\ 2/\sigma & 4 + 2/\sigma^2 \end{bmatrix}$

$$l(\mu, \sigma) = -n \sum \log x_i - n \log \sigma - \log \sqrt{2\pi} \frac{1}{\sigma^2} \sum (\log x_i - \mu - \sigma^2)^2. \quad (5)$$

The solutions to likelihood equations $\frac{\partial l}{\partial \mu} = 0$

and $\frac{\partial l}{\partial \sigma} = 0$ give the MLEs as:

$$\hat{\mu} = (\sum \log x_i / n) - \hat{\sigma}^2$$

and

$$\hat{\sigma}^2 = \frac{1}{n} \left[\sum (\log x_i)^2 - (\sum \log x_i)^2 / n \right]. \quad (6)$$

To study the properties of $(\hat{\mu}, \hat{\sigma}^2)$ the transformation $Y = \log X$ is considered in (2). It

is known that $Y \sim \text{Normal}(\mu + \sigma^2, \sigma)$. This leads to the following estimates corresponding to (6):

$$\hat{\mu} = \bar{Y} + cS^2,$$

where $c = -(n-1)/n$, $\hat{\sigma}^2 = \frac{(n-1)}{n} S^2$, and for the sample

$$Y_i = \log X_i, i = 1, 2, \dots, n, \bar{Y} = \sum \frac{Y_i}{n}$$

and

$$S^2 = \sum \frac{(Y_i - \bar{Y})^2}{(n-1)}. \quad (7)$$

From (7), it is clear that $\hat{\mu}$ is a biased estimator of μ . Further, the distribution of $\hat{\mu}$ cannot be expressed in closed form. Thus, the distributional properties of $\hat{\mu}$, unlike in the case of the original LN distribution, are not readily

available for statistical inference. Therefore, simulations are considered in order to understand the properties of the above defined estimator of μ . In particular, finding the confidence interval (C.I.) for μ is not straightforward. Hence, the bootstrap method for constructing the confidence interval for μ was considered to obtain the results.

Results

To illustrate the use of the methodology introduced above, data from oil field explorations (Meisner & Demirmen, 1981) was analyzed.

Table 3: Sizes of Oil Fields Data
(X = Field Size, Oil (10^6 BBLS), $n = 58$)

28	26	775	114	31
337	41	113	1328	21
13	455	89	482	70
215	62	58	6.9	154
177	43	33	178	15
22	11	8.1	35	25
170	19	56	42	335
21	50	181	93	75
8.8	29	450	5.9	8.8
49	100	10	8.8	17
12	125	20	8.8	8.8
6.9	25	100		

MLE of the Parameters (μ , σ) of LBLN

The MLE's of μ and σ were obtained (see Table 4) using the formulas in (7). The amount of bias in the estimate of μ can also be estimated using (7).

Table 4: Estimates of μ and σ

Parameter	Estimate	Standard Error
μ	2.0748	0.3729
σ	1.3317	0.1236

Simulations for Studying the Properties of $\hat{\mu}$

As noted, the distribution of $\hat{\mu}$ is not available in closed form (see equation (7)); therefore, to understand the properties of $\hat{\mu}$ simulations were conducted. In particular, the amount of bias in the estimates of values of μ is of interest. For these simulations, different values of n and (μ , σ) were used. The simulation results for $n = 20$ and certain values of (μ , σ) are shown in Table 5. Results obtained were expected from (7), and show that the absolute value of the bias in the estimate $\hat{\mu}$ of μ increases as σ increases. Results from the simulations for other values of n were not different from those recorded above and therefore for brevity are not included.

Estimation of μ Based on the Mode of LBLN (μ , σ)

The mode M of the LBLN (μ , σ) distribution from Table 1 is given by $M = \exp(\mu)$ which is free of σ^2 and, hence, leads to the formula $\mu = \ln(M)$. This expression can be employed to estimate μ using the sample mode. Note that such estimate of μ , unlike the MLE of μ , does not depend on the estimate of σ^2 .

For data presented in Table 3, the estimate of μ using the sample mode is 2.1747. This estimate is comparable with the MLE estimate of 2.0748 (see Table 4); however, because the sample mode is not known to be an efficient estimator of the location parameter it is not considered further.

Bootstrap Estimation of μ

As noted previously, because the distribution of $\hat{\mu}$ is not available in closed form, the nonparametric bootstrap method was used to estimate μ and its related confidence interval; results are shown in Table 6. Based on these results, the 95% and 90% C.I.s can be constructed.

The purpose of the above computations is for illustration, not for comparison of the results obtained herein with those obtained by Meisner and Demirmen (1981). However, the definition of the size-biased (also known as the weighted distribution) version of the LN (μ , σ)

Table 5: Simulation Results for the Properties of $\hat{\mu}$ (# of simulations = 5,000)

μ	σ	Mean of $\hat{\mu}$	MSE	μ	σ	Mean of $\hat{\mu}$	MSE	μ	σ	Mean of $\hat{\mu}$	MSE
-2	0.5	-1.98	0.0186	0	0.5	0.0122	0.0186	1	0.5	1.0111	0.0189
-2	1.0	-1.94	0.1416	0	1.0	0.0548	0.1486	1	1.0	1.0559	0.1417
-2	1.5	-1.89	0.6199	0	1.5	0.1187	0.6086	1	1.5	1.1146	0.5893
-2	2.0	-1.79	1.7518	0	2.0	0.2132	1.7597	1	2.0	1.2008	1.7003

Table 6: Bootstrap Estimate of μ for the Oil Fields Data
(Number of Replications: 3,000)

Summary Statistics	Observed	Bias	Mean	SE
Parameters	2.075	0.03512	2.11	0.265
BCa Percentiles	2.5%	5%	95%	97.5%
Parameters	1.5028	1.5857	2.4702	2.5518

given, and also considered by Meisner and Demirmen, may be useful to some readers.

Let $X \sim f(x; \theta)$. If $w(x) > 0$ is a function of x such that $E[w(X)] < \infty$, then the weighted distribution of X is defined by the pdf

$$g(x; \theta) = w(x)f(x; \theta) / E[w(X)], \quad (8)$$

where $w(x)$ is referred to as the weight function and θ is a scalar or a vector of parameters.

Meisner and Demirmen (1981) assumed that the original distribution of the size of the oil field, denoted by X , is LN (μ, σ) . Further, in the exploration of the oil field, the probability of discovering an oil field depends on the size of the oil field. Therefore, for modeling the collected sample data of the oil fields Meisner and Demirmen considered the weighted lognormal (WLN) with weight function $w(x) = x^\beta$. Using (8), the distribution of interest, the WLN (μ, σ) with the pdf is given by

$$g_2(x; \mu, \sigma) = \frac{1}{x\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2\sigma^2}(\log x - (\mu + \beta\sigma^2))^2\right], \quad (9)$$

where

$$x > 0, -\infty < \mu < \infty, \sigma > 0$$

and β may have a known or unknown value.

Meisner and Demirmen (1981) discussed the possible values of β . In particular, they noted that, because the sizes of oil fields change with the exploration period, the values of β could be in a two-sided neighborhood of the value 1. Therefore, this illustration, considering $\beta = 1$, that is assuming the sizes of the oil fields have the LBLN (μ, σ) distribution given by (2.2), is justified. Table 7 shows the estimates of μ for the other values of β ; Meisner and Demirmen considered β as a random variable and developed a Bayesian approach for the analysis of these data. To construct the estimates

in Table 7, the modified version of (7) for accommodating β was used.

Table 7: Changes in the Estimate of μ for Values of β

β	0.9	1.0	1.1
μ Estimate	2.25	2.07	1.89

If the estimate 2.1747 of μ is acceptable, then considering that the mode of LBLN (μ, σ) is a function of μ alone, it can be used for finding a value of β (a sort of ad hoc estimate of β) by extending Table 5 to include more values of β than may be necessary. In particular, using such a table it can be shown that if $\beta = 0.94$ then $\hat{\mu} = 2.17$ (approximately), which is close to the above estimate 2.1747.

Note that, in view of the unstable behavior of the sample mode, such an estimate should be carefully considered. However, in this analysis, observations show that the assumption of $\beta = 1$ (which is close to the value of $\beta = 0.94$) used for modeling the data from Table 4 has some relevance. Further, it should be noted that other more robust methods exist for locating the sample mode (Bickel & Fruthworth, 2006). The traditional method was used in this study for demonstration purposes.

Conclusion

The length-biased lognormal distribution was introduced along with an application in the analysis of data from oil field explorations. The maximum likelihood estimation of the parameters of the length-biased lognormal was discussed briefly. In particular, the properties of the estimator of μ are not tractable. Therefore, the related properties were studied using simulations. Results presented regarding the modal value of the length-biased lognormal show that the estimation of μ using the sample mode is straightforward, but the efficiency of such an estimator is doubtful. The concepts of weighted lognormal distribution as a generalization of the length-biased lognormal and related modeling problems were also briefly mentioned.

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A Study on Underwriting Cycle of Property Insurance Industry of China

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Methods in underwriting cycle research are compared. A second-order autoregressive model, which includes structural transition and Christiano-Fitzgerald (CF) Filter method, is used to analyze China's underwriting cycle with annual property insurance loss ratio data from 1982 to 2008. Results show that the underwriting cycle is 11-12 years and, from the phase of underwriting cycle, management suggestions about underwriting cycle phenomenon are provided.

Key words: Underwriting cycle, property insurance, second-order autoregressive model, CF filter, structural transition.

Introduction

An underwriting cycle refers to a period phenomenon of underwriting profit that fluctuates over time. A comprehensive underwriting cycle moves through four stages: mature hard market, immature soft market, mature soft market and immature hard market. As a specific phenomenon of the property insurance industry, the underwriting cycle has a significant impact. The phenomenon of underwriting cycles penetrates into all aspects of business of insurance companies and influences product pricing, claims payments, marketing strategy decisions and reserve calculations. Ernst & Young (2009) lists the future top ten risks of the Chinese insurance industry in their *Annual Report of Insurance Industry Operating Risk in China Market*. They state that regulatory intervention, underwriting cycle management and climate change – among others – will

become major risk factors for the Chinese insurance industry in the future, and that the underwriting cycle is the most important among the various risk factors. For this reason, research into property insurance underwriting cycles is particularly important. Although some professionals have studied underwriting cycles of property insurance, there is not a generally accepted empirical result regarding underwriting cycles.

Underwriting cycles were proposed by a broker company in the United States. Venezian (1985) proofed the existence of underwriting cycles for the property insurance industry, and Cummins and Outreville (1987) confirmed their existence in insurance markets outside of the U.S.A. Chen (1997) found the underwriting cycle existed in Asian emerging markets (including Japan, Singapore and Malaysia); he also notes that, even if there no underwriting cycle of whole non-life insurance industry exists in an individual country, there is an underwriting cycle phenomenon for some business lines, such as property insurance in Korea and motor insurance in Chinese Taipei.

In China, there have been a few studies on the underwriting cycle. Cai (2005) introduced the principle of an underwriting cycle in the world, his research focuses on insurance supply and demand. Wang and Shi (2006) used a second order autoregressive model with simple loss ratio data and concluded that there was no underwriting cycle in the Chinese property

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insurance industry. However, they recognized there was an underwriting cycle in the motor insurance business line that is about 6 years. A similar study was conducted by Zhang and Zhu (2007). Li and Li (2010) used a filter method and simple loss ratio data and reported that the underwriting cycle for non-life insurance industries of China was 4-5 years. Ji and Zheng (2009) used a second order autoregressive model and spectral analysis with gross ratio; they identified both long underwriting cycles of 12.5-16.7 years, and medium underwriting cycles of 5.6 years.

Wang and Shi (2006) and Ji and Zheng (2009) used same method, but came to opposite conclusions. This raised the question if the difference is due to the difference between a simple loss ratio and a gross ratio. If so, the cycle phenomenon on simple loss ratio and gross ratio will be consistent after excluding abnormal data. Differences between findings of Li and Li (2010) and Wang and Shi (2006) also raises the question if it was abnormal data in the underwriting cycle, invisible in second order autoregressive model, that led to their conclusions.

A second order autoregressive model with a structural transition is used here to analyze whether simple loss ratio time-series data exhibits a structural transition. It determines the reason for structural transition and introduces dummy variables at points in the structural transition to analyze the underwriting cycle of the property insurance industry in China. Taking into account that the lack of an underwriting cycle is caused by abnormal data in a simple loss ratio time-series, a Christiano-Fitzgerald Filter was used to separate the trend and periodic components of simple loss ratio time-series one by one, and then to identify the existence of underwriting cycle of property insurance in China by use of a second order autoregressive model.

Measure Methods on Underwriting Cycle

Four methods are typically used to measure an underwriting cycle:

- (1) Direct Observation. Direct observation uses some simple chart to express loss ratio data and operating profit data, the direction of

chart or peak can be observed and used to judge the existence of an underwriting cycle and to estimate the length of the cycle. This method is most intuitive, but is also the most rough; thus, very few of applications rely on it because it is not possible to obtain an exact length of an underwriting cycle.

- (2) Autoregressive Model. This method is applied widely and results in an exact length of an underwriting cycle by using a second order autoregressive model. Some researchers have identified the existence of structural transitions that caused the underwriting cycle to disappear and have shown that the structural transition, or presence of a transition, affects the test of an underwriting cycle and its length measurement (see Venezian, 1985; Cummins and Outreville, 1987; Chen, 1997; Leng, 2006). However, if dummy variables are introduced at a transition point, the length of the underwriting cycle can be obtained. This method can calculate the length of underwriting cycle and find the transition and its causes so that the phenomenon of the underwriting cycle can be understood. The downsides of this method are that data for analysis cannot be too short a time span and it cannot explain either the start or end points.
- (3) Spectral Analysis. Spectral analyses were first used in physics, but have recently been employed to study economic cycles. These analyses can estimate economic cycles with shorter time series. Ji and Zheng (2009) used this approach to study underwriting cycles. This method has no requirement for data time-series and all data involved in the equation without losing the sample point. Because all data is placed into equations and there are clear calculation and process criteria, this approach can avoid subjectivity in analysis. However, this method results in different lengths of underwriting cycles for different data time-series even if the data comes from the same business line: Sometimes the difference is huge and the model cannot explain the difference.

- (4) Christiano-Fitzgerald (CF) Filter Analysis. Filter analysis starts from time series volatility. It removes white noise from a time series and then obtains the regularity of its implied. This approach mainly used to study economic cycles and was used by Li and Li (2010) to study underwriting cycles. The method provides different results under different hypotheses for different filters. Generally, the CF filter is used to study economic cycles. CF filters can isolate trend and periodic components in time series data. Studying a periodic component can result in identifying an underwriting cycle with high credibility, but the chart cycle from this method has no higher credibility.

Each method has its own advantages and disadvantages. As an objective phenomenon, an underwriting cycle will have almost same length regardless of what method is used. This article uses a CF filter and second order autoregressive model with a structural transition to study the underwriting cycle of the property insurance industry in China.

Methodology

The Existence of an Underwriting Cycle: Indicators Selected and Data Resource

The best indicator is gross ratio or underwriting profit margin. Venezian (1985) used underwriting profit margin as the variable to test the existence of underwriting cycles in the property insurance industry in the United States. Gross loss ratio, or underwriting profit margin, arose in many references as an indicator of testing. Because there is no consistency of expense ratio in China, this study used a simple loss ratio, which is equal to ratio of losses and premiums. The gross loss ratio is equal to the simple loss ratio plus gross expenses ratio; because the expenses ratio is typically stable, a simple loss ratio can be substituted for the gross loss ratio. Data in this study is 1982-2008 property insurance collected from the China Insurance Yearbook and China Statistical Yearbook.

The Existence of an Underwriting Cycle: Stationary Test

It is first necessary to judge whether a time series is stationary both in the second order autoregressive model and the CF filter. A common test used for time series data is the Augmented Dickey-Fuller (ADF) test statistic; ADF analyzes the stationary of data and tests whether the data has unit root. Results of this test are shown in Table 1.

Table 1 shows a t-statistic equal to -1.110974 ; this result indicates that the null hypothesis cannot be rejected, thus, the time-series data has unit root, which is not smooth. From this, it may be determined that outliers are present in the simple loss rate time series; for this reason, a dummy variable was introduced into the second order autoregressive model and analyzed by CF filter after treatment of abnormal values to conduct empirical analysis about the existence of underwriting cycle.

Empirical Analysis: Second Order Autoregressive Method

Next, the stability of loss rate time-series is tested. The loss rate time-series is stability when autocorrelation and partial autocorrelation tests are used. Structural transition exists in loss rate time-series (Leng, 2002), but the exact point of transition is unknown, so the Chow Square Test is used to judge that point. Table 2 shows that the F-value is 5.023, which is higher than the 1% level, and the LLR = 14.598 in 1991. These are the largest in all results and they indicated the presence of an abnormal phenomenon in 1991; this is the structural transition.

Compared with the situation of the property insurance industry development in China in 1991, it is postulated that there may be two reasons for the structural transition in that year. First, with increased competition in domestic market the loss rate increased. The insurance industry carried out an open policy in all of China in 1991, so more companies entered the insurance industry and competition increased. Insurance companies competed for market share and lower underwriting levels led to a surge of loss rate so that the loss rate after 1991 is significantly higher than before. Second, the American insurance market is a very

important market in the world; it has huge premiums, especially liability premiums. Chinese insurance companies possibly did not understand the coverage of American liabilities or the legislation associated with those liabilities, so Chinese companies may have assumed a large insurance liability blindly in world market in 1980s. In addition, Chinese insurance companies assumed a lot of claims of liability insurance in 1991 and ignored the characteristics of reinsurance claims lags at that same time.

Due to this, a dummy variable is introduced in a second order autoregressive model as:

$$CR(t) = c + aCR(t-1) + bCR(t-2) + dD + eDCR(t-1) + fDCR(t-2) + u \quad (1)$$

Using Eviews 6.0 (statistical software) for analysis results in the regression shown in Table 3.

After introducing the dummy variable (Table 3), $a > 0$ and $b < 0$ can be found; a and b are then used to calculate the underwriting cycle of the property insurance industry, which is 11.938.

$$\begin{aligned} T &= \frac{2\pi}{\cos^{-1}\left(a/2\sqrt{-b}\right)} \\ &= \frac{2\pi}{\cos^{-1}\left(0.862382/2\sqrt{-(-0.340534)}\right)} \\ &= 11.938 \end{aligned}$$

Empirical Analysis: CF Filter

Economic variables include trend, periodic and random components. If the trend and random components can be separated from the periodic component, the periodic component can be used to measure the cycle of an economic variable. Normally, the random component is ignored because it has little effect and the CF filter is used to separate the trend and periodic components and to analyze the periodic component (Table 4).

Use of a second order autoregressive model to test the periodic component results in

Variable	c	a	b
Coefficient	-0.00127	1.73261	-0.96809
Standard Deviation	6.80E-05	0.008428	0.008202
t-Value	-1.86578	205.5874	-118.076
R ²	0.999643		

$$\begin{aligned} T &= \frac{2\pi}{\cos^{-1}\left(a/2\sqrt{-b}\right)} \\ &= \frac{2\pi}{\cos^{-1}\left(1.732610/2\sqrt{-(-0.968092)}\right)} \\ &= 11.720 \end{aligned}$$

Table 1: ADF Test Output

	t-Statistic	Prob.*
Augmented Dickey-Fuller test statistic	-1.110974	0.6950
Test critical values:		
1% level	-3.724070	
5% level	-2.986225	
10% level	-2.632604	

*Mackinnon (1996) one-sided p-values.

Table 2: Chow Square Test – Structural Transition

Year	F-value	Probability	LLR	Probability
1987	1.286	0.308	4.621	0.202
1988	1.633	0.215	5.735	0.125
1989	2.446*	0.095	8.164**	0.043
1990	2.901*	0.062	9.427**	0.024
1991	5.023***	0.010	14.598***	0.002
1992	2.524*	0.088	8.386**	0.039
1993	2.981*	0.057	9.643**	0.022
1994	3.329**	0.042	10.56**	0.014
1995	1.599	0.223	5.627	0.131
1996	1.954	0.155	6.723*	0.081
1997	0.986	0.420	3.619	0.306
1998	0.352	0.788	1.351	0.717
1999	0.541	0.660	2.049	0.562
2000	0.508	0.681	1.930	0.587
2001	0.424	0.738	1.618	0.655
2002	0.729	0.547	2.723	0.436
2003	1.177	0.345	4.262	0.235
2004	1.370	0.282	4.895	0.180
2005	1.361	0.285	4.867	0.182
2006	1.282	0.309	4.609	0.203

*Means 10% level, **Means 5% level, ***Means 1% level. Structure transition is in 1991.

Table 3: Regression Analysis Table - Introduced Dummy Variable

Variable	Coefficient	Standard Deviation	t-Value	R ²
c	0.155	0.165	0.935	0.669
a	0.862	0.487	1.771	
b	-0.249	0.497	-0.500	
d	0.278	0.209	1.330	
e	-0.968	0.534	-1.814	
f	0.540	0.534	1.012	

Conclusion

The existence of a structural transition in 1991 in the Chinese property insurance industry is verified by using simple loss rate data. A second order autoregressive model and CF filter were also used to calculate the underwriting cycle of the P&C insurance industry in China; the cycles are approximately 12 years in length. At the end of the paper, we give two suggestions to underwriting cycle management. Because the phenomenon of underwriting cycles is a risk factor, it is necessary to strengthen the management of underwriting cycles to lower their influence of volatility on the insurance business. Two strategies are suggested.

Recommendations for Underwriting Cycle Management

- (1) **Procyclical Policy:** This policy's target is to maintain the market shares of insurance companies. At the very stage, the underwriting strategy will be maintained, regardless of changes in prices. The internal management of insurance companies may lead to increased cycle phenomenon and also to increased procyclical leverage effects. Insurance companies need to analyze all kinds of risks in operating procedures and allow a limit fluctuation.
- (2) **Countercycle Policy:** This policy's target is to maintain the profitability of insurance companies. Insurance companies need to reduce their business line in soft market and only keep some profitable businesses so that they will have sufficient capital and surplus to expand in hard market.

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Table 4 Trend and Periodic Component Filter Table

Year	Trend Component	Periodic Component	Year	Trend Component	Periodic Component
1982	0.43178	0.023206	1996	0.55212	0.025064
1983	0.46395	0.026539	1997	0.53744	0.019601
1984	0.4877	0.023344	1998	0.56252	0.009925
1985	0.4252	0.014245	1999	0.53197	-0.00145
1986	0.41764	0.001426	2000	0.51837	-0.01179
1987	0.39252	-0.01192	2001	0.50494	-0.01881
1988	0.40884	-0.02244	2002	0.53785	-0.02118
1989	0.43324	-0.02749	2003	0.56653	-0.01878
1990	0.41533	-0.02584	2004	0.52721	-0.01254
1991	0.51941	-0.01797	2005	0.54965	-0.0042
1992	0.46525	-0.00592	2006	0.52357	0.004285
1993	0.48249	0.007262	2007	0.49964	0.011113
1994	0.55175	0.018337	2008	0.6019	0.015071
1995	0.41103	0.024713			

The Weighted Hellinger Distance for Kernel Distribution Estimator of Function of Observations

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The asymptotic mean weighted Hellinger distance (AMWHD) is derived for the kernel distribution estimator of a function of observations. In addition, the AMWHD is compared with the asymptotic mean integrated square error (AMISE) of the estimator. A completely data based method is proposed to select the bandwidth in the estimator using the mean weighted Hellinger distance (MWHD).

Key words: Kernel estimation, distribution function estimation, bandwidth, Hellinger distance, mean square error, function of random variables.

Introduction

Given a random sample $X_1, X_2, \dots, X_n$ from a distribution $F(x)$ with unknown density function $f(x)$, the kernel density estimator (Rosenblatt, 1956) of $f(x)$ is given by

$$\hat{f}(x) = \frac{1}{nb} \sum_{i=1}^n k\left(\frac{x - X_i}{b}\right),$$

where b is the smoothing bandwidth and k is a symmetric function satisfying $\int k(x)dx = 1$. The kernel distribution function estimator (Nadaraya, 1964) of $F(x)$ is given by

$$\hat{F}(x) = \frac{1}{n} \sum_{i=1}^n \left(\frac{x - X_i}{b} \right),$$

where K is the distribution function of the kernel k , $K(x) = \int_{-\infty}^x k(u)(du)$, and b is the bandwidth.

Consider the function $g(X_1, X_2, \dots, X_m)$ that depends on $m \geq 1$ observations. Assume that g is a real value and is symmetric in its m arguments. Frees (1994) proposed an estimate for the density function $h(t)$ of random variable $g(X_1, X_2, \dots, X_m)$ which is given by

$$\hat{h}(t) = \frac{1}{b \binom{n}{m}} \sum_{(n,m)} w \left(\frac{t - g(X_{i_1}, \dots, X_{i_m})}{b} \right),$$

where b is the bandwidth, the sum extends over all $1 \leq i_1 < i_2 < \dots < i_m \leq n$, and $w(\cdot)$ is a kernel function. If $m = 1$ and $g(x) = x$, then the estimator $\hat{h}(t)$ reduces to the estimator $\hat{f}(x)$.

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The estimator $\hat{h}(t)$ has many applications in real life. For example, in spatial statistics g can be the inter point distance between pairs of objects and in insurance g can be the sum of m claims (Frees, 1994; Ahmad & Fan, 2001; Mugdadi & Ahmad, 2004).

Nadaraya (1964) and Mugdadi and Ghebregiorgis (2005) proposed a kernel distribution estimator of the distribution function of function of observations $H(t)$ as:

$$\hat{H}(t) = \frac{1}{\binom{n}{m}} \sum_{(n,m)} W\left(\frac{t - g(X_{i_1}, \dots, X_{i_m})}{b}\right),$$

where $W(x) = \int_{-\infty}^x w(t)dt$, b is the bandwidth and the sum extends over all $1 \leq i_1 < i_2 < \dots < i_m \leq n$. Theoretical and simulation analyses show that choice of kernel is not crucial for distribution function estimation in the case of independent and identically (i.i.d) random variables; the most important choice is that of bandwidth. A typical way to select the bandwidth is to minimize one error measure, and the most commonly used is the mean integrated square error (MISE) and its asymptotic (AMISE), where

$$MISE(\hat{H}(t)) = E \int [\hat{H}(t) - H(t)]^2 dt.$$

Another criterion is the mean Hellinger distance (MHD), where

$$MHD(\hat{H}(t)) = E \int [\hat{H}^{\frac{1}{2}}(t) - H^{\frac{1}{2}}(t)]^2 dt.$$

Kanzawaa (1993) discussed the relationship between the asymptotic mean Hellinger distance (AMHD) and the AMISE for $\hat{f}(x)$, Ahmad and Mugdadi (2006) examined the relationship between asymptotic mean weighted Hellinger distance (AMWHD) and the AMISE for both $\hat{f}(x)$ and $\hat{F}(x)$, and Mugdadi (2004) studied the AMWHD for $\hat{h}(t)$. This investigation

examines the relationship between the AMWHD and the AMISE for $\hat{H}(t)$ and proposes a data method to select the bandwidth for $\hat{H}(t)$ based on the AMWHD ($\hat{H}(t)$).

The Asymptotic Mean Weighted Hellinger Distance

One error criterion used to evaluate the estimator is the mean weighted Hellinger distance (MWHD) and its asymptotic (AMWHD), where $MWHD(\hat{H}(t))$ is defined by:

$$MWHD(\hat{H}(t)) = E \int [\hat{H}^{\frac{1}{2}}(t) - H^{\frac{1}{2}}(t)]^2 H(t) dt.$$

It can be argued that

$$MWHD(\hat{H}(t)) = \frac{1}{4} MISE(\hat{H}(t)),$$

assuming that $\hat{H}(t) \approx H(t)$ results in:

$$\begin{aligned} MISE(\hat{H}(t)) &= \int E[\hat{H}(t) - H(t)]^2 dt \\ &= \int E[\hat{H}^{\frac{1}{2}}(t) - H^{\frac{1}{2}}(t)]^2 [\hat{H}^{\frac{1}{2}}(t) + H^{\frac{1}{2}}(t)]^2 dt \\ &\approx 4E \int [\hat{H}^{\frac{1}{2}}(t) - H^{\frac{1}{2}}(t)]^2 H(t) dt \\ &= 4MWHD(\hat{H}(t)) \end{aligned}$$

Next, the $AMWHD(\hat{H}(t))$ is derived and compared with the $AMISE(\hat{H}(t))$. Mugdadi and Ghebregiorgis (2005) derived $AMISE(\hat{H}(t))$ as:

$$AMISE(\hat{H}(t)) = \frac{T(H)}{\binom{n}{m}} - \frac{b}{\binom{n}{m}} \rho(w) + \frac{b^4}{4} \mu_2(w)^2 R(H''),$$

where

$$\rho(w) = 2 \int u W(u) w(u) du,$$

$$T(H) = \int H(t)[1 - H(t)]dt$$

and

$$R(h) = \int h^2(t)dt.$$

Theorem

If the fourth derivative of $H(t)$ exists, then

$$AMISE(\hat{H}(t)) =$$

$$\frac{T(H)}{4 \binom{n}{m}} - \frac{b}{4 \binom{n}{m}} \rho(w) + \frac{b^4}{16} \mu_2(w)^2 R(H'').$$

Proof

$$MWHd(\hat{H}(t)) =$$

$$\int E\hat{H}(t)H(t)dt - 2 \int E\hat{H}^{\frac{1}{2}}(t)H^{\frac{3}{2}}(t)dt + \int H^2(t)dt.$$

Using integration by parts and expanding $H(t - bu)$ in a 2nd order Taylor's series about t results in:

$$\begin{aligned} E(\hat{H}(t)) &= E \left(\frac{1}{\binom{n}{m}} \sum_{(n,m)} W \left(\frac{t - g(X_1, X_2, \dots, X_m)}{b} \right) \right) \\ &= \int w(u) \left(\frac{H(t) - buH'(t) + \frac{b^2 u^2 H''(t)}{2}}{1} \right. \\ &\quad \left. - \frac{b^3 u^3 H^{(3)}(t)}{6} + \frac{b^4 u^4 H^{(4)}(t)}{24} + o(b^4) \right) du \\ &\approx H(t) + \frac{b^2 H''(t)}{2} \mu_2(w) + \frac{b^4}{24} \mu_4(w) H^{(4)}(t) \end{aligned}$$

therefore,

$$\int E[\hat{H}(t)H(t)]dt \approx$$

$$\left[\int H^2(t)dt + \frac{b^2 \mu_2(w)}{2} \int H''(t)H(t)dt \right. \\ \left. + \frac{b^4 \mu_4(w)}{24} \int H^{(4)}(t)H(t)dt \right]$$

If Z is a random variable with a standard normal distribution, then

$$\hat{H}(t) \approx E(\hat{H}(t)) + Z \sqrt{\text{Var}(\hat{H}(t))}.$$

Mugdadi and Ghebregiorgis (2005) derived $\text{Var}(\hat{H}(t))$, this is given by:

$$\text{Var}(\hat{H}(t)) =$$

$$\left[O\left(\frac{1}{n}\right) + O\left(\frac{b^2}{n}\right) + \binom{n}{m}^{-1} H(t)(1-H(t)) \right. \\ \left. + \binom{n}{m}^{-1} o(b) - \binom{n}{m}^{-1} bH'(t)\rho(w) \right].$$

Thus,

$$\hat{H}(t)$$

$$\approx H(t) + \frac{b^2 H''(t)}{2} \mu_2(w) + \frac{b^4 H^{(4)}(t)}{24} \mu_4(w)$$

$$\begin{aligned} &+ Z \left[\left[O\left(\frac{1}{n}\right) + O\left(\frac{b^2}{n}\right) + \binom{n}{m}^{-1} H(t)(1-H(t)) \right. \right. \\ &\quad \left. \left. + \binom{n}{m}^{-1} o(b) - \binom{n}{m}^{-1} bH'(t)\rho(w) \right] \right]^{\frac{1}{2}} \\ &\approx H(t) \left[1 + \frac{b^2 H''(t)\mu_2(w)}{2H(t)} + \frac{b^4 \mu_4(w)H^{(4)}(t)}{24H(t)} \right. \\ &\quad \left. + Z \left(\frac{1-H(t)}{\binom{n}{m} H(t)} - \frac{bH'(t)\rho(w)}{\binom{n}{m} H^2(t)} + O\left(\frac{1}{n}\right) + O(b^2) \right) \right]^{\frac{1}{2}} \end{aligned}$$

therefore,

$$\hat{H}^{\frac{1}{2}}(t) \approx \left[1 + \frac{b^2 H''(t) \mu_2(w)}{4H(t)} + \frac{b^4 \mu_4(w) H^{(4)}(t)}{48H(t)} + \frac{Z}{2} \left[\frac{1-H(t)}{\binom{n}{m} H(t)} - \frac{bH'(t)\rho(w)}{\binom{n}{m} H^2(t)} \right]^{\frac{1}{2}} + O\left(\frac{1}{n}\right) + O(b^2) - \frac{b^4}{32} \left(\frac{H''(t)}{H(t)} \right)^2 (\mu_2(w))^2 - \frac{Z^2}{8} \left[\frac{1-H(t)}{\binom{n}{m} H(t)} - \frac{bH'(t)\rho(w)}{\binom{n}{m} H^2(t)} \right] + O\left(\frac{1}{n}\right) + O(b^2) \right]$$

and

$$E(\hat{H}^{\frac{1}{2}}(t)) \approx \left[1 + \frac{b^2 H''(t) \mu_2(w)}{4H(t)} + \frac{b^4 \mu_4(w) H^{(4)}(t)}{48H(t)} - \frac{b^4}{32} \left(\frac{H''(t)}{H(t)} \right)^2 (\mu_2(w))^2 - \frac{1}{8} \left[\frac{1-H(t)}{\binom{n}{m} H(t)} - \frac{bH'(t)\rho(w)}{\binom{n}{m} H^2(t)} \right] + O\left(\frac{1}{n}\right) + O(b^2) \right]$$

thus

$$\int [E\hat{H}^{\frac{1}{2}}(t)H^{\frac{3}{2}}(t)]dt \approx$$

$$\left[\int H^2(t)dt + \frac{b^2}{4} \mu_2(w) \int H''(t)H(t)dt + \frac{b^4}{48} \mu_4(w) \int H^{(4)}(t)H(t)dt - \frac{b^4}{32} \mu_2^2(w) \int (H''(t))^2 dt - \frac{1}{8} \int H(t)(1-H(t))dt + \frac{b}{8} \rho(w) + O\left(\frac{1}{n}\right) + O(b^2) \right]$$

therefore,

$$AMWHD(\hat{H}(t)) \approx$$

$$\left[\frac{b^4}{16} \mu_2^2(w) R(H'') + \frac{1}{4\binom{n}{m}} \int (H(t)) \times [1-H(t)]dt - \frac{b}{4\binom{n}{m}} \rho(w) \right]$$

Under these conditions, the following corollaries can be proven.

Corollary 1

$$AMWHD(\hat{H}(t)) \approx \frac{AMISE(\hat{H}(t))}{4}.$$

Similar to Powell and Stocker (1996), the optimal bandwidth to minimize the $AMWHD(\hat{H}(t))$ is shown in corollary 2.

Corollary 2

$$b_{opt} = \left[\frac{\rho(w)}{\mu_2^2(w)R(h')} \right]^{\frac{1}{3}} \left(\frac{n}{m} \right)^{-\frac{1}{3}}$$

Bandwidth Selection

The choice of bandwidth is very important in the Kernal density estimator as well as in the Kernal distribution estimator. One of the simplest methods to select bandwidth is based on equation (2.8). Assume that the data is from a normal distribution with mean equal to zero and variance σ_1^2 . If s^2 is the variance of the data $g(X_{i_1}, \dots, X_{i_m})$ for all

$1 \leq i_1 < \dots < i_m \leq n$, then $R(h') = \frac{1}{4\pi s^3}$, thus

$$b_{opt} = \left[\frac{\rho(w)4\pi}{\pi_2^2(w)} \right]^{\frac{1}{3}} \left(\frac{n}{m} \right)^{-\frac{1}{3}} s \quad (3.1)$$

This shows that b_{opt} depends only on the standard deviation and on the Kernel function.

A completely different data based method is proposed to select the bandwidth for a Kernal distribution estimator of the function of observations. The method is based on minimizing the $MWHD(\hat{H}(t))$. The $MWHD(\hat{H}(t))$ is defined as:

$$\begin{aligned} MWHD(\hat{H}(t)) &= E \int [\hat{H}^{\frac{1}{2}}(t) - H^{\frac{1}{2}}(t)]^2 H(t) dt \\ &= \left[E \int \hat{H}(t) H(t) dt + E \int H^2(t) dt \right. \\ &\quad \left. - 2E \int \hat{H}^{\frac{1}{2}}(t) H^{\frac{1}{2}}(t) dt \right] \\ &= \left[E \int \hat{H}(t) H(t) dt + E \int H^2(t) dt \right. \\ &\quad \left. - 2 \int (E \hat{H}^{\frac{1}{2}}(t)) H^{\frac{1}{2}}(t) dt \right]. \end{aligned}$$

Minimizing $MWHD(\hat{H}(t))$ is therefore equivalent to minimizing $MWHD1(\hat{H}(t))$, where,

$$MWHD1(\hat{H}(t)) =$$

$$\int (E \hat{H}(t)) H(t) dt - 2 \int (E \hat{H}^{\frac{1}{2}}(t)) H(t)^{\frac{2}{3}} dt$$

Thus, $MWHD1(\hat{H}(t))$ can be estimated as follows. Let $m_{(1)}$ be a fixed choice of m variables and let $I(A)$ be the indicator function. Also, define

$$H_{n, m_{(1)}}(t) = \frac{1}{\binom{n}{m} - 1} \sum_{(n, m), m \neq m_{(1)}} I(t - g(X_{i_1}, \dots, X_{i_m}))$$

and

$$\hat{H}_{-m_{(1)}}(t) = \frac{1}{\binom{n}{m} - 1} \sum_{(n, m), m \neq m_{(1)}} W\left(\frac{t - g(X_{i_1}, \dots, X_{i_m})}{b}\right)$$

which is the distribution estimated based on a sample with $m_{(1)}$ deleted. Thus,

$MWHD1(\hat{H}(t))$ is estimated by

$$MWHD. EST =$$

$$\frac{1}{\binom{n}{m}} \sum_{1 \leq i_1 < \dots < i_m < n} \left[\hat{H}_{-m_{(1)}}(g(X_{i_1}, \dots, X_{i_m})) \right. \\ \left. \times H_{n, m_{(1)}}(g(X_{i_1}, \dots, X_{i_m})) \right]$$

As noted, there are many applications for $\hat{H}(t)$. One example, introduced by Free (1993), regards an insurance claims problem. Table 1 shows total hospital charges (in dollars) in one Wisconsin (USA) hospital for females aged 30-49 in the year 1989.

Consider the case $m = 2$ and the function $g(X_1, X_2) = X_1 + X_2$. By minimizing $MWHD. EST$, the bandwidth is determined to be 0.437. Figure 1 shows the kernel distribution function for $g(X_1, X_2)$ using data in Table 1. It is clear that the kernel

estimate is smooth and $\hat{H}(t)$ is 0 when $t \leq 0$ because the sum of the charges should be positive; also, $\lim_{t \rightarrow \infty} \hat{H}(t) = 1$.

Table 1: Total 1989 Hospital Charges (USD) for Females Aged 30-49

2337	1765	1802
2179	2467	2011
2348	3609	2270
4765	2141	3425
3041	1850	3558
2088	3191	2315
2872	3020	1642
1924	2473	5878
2294	1898	2101
2182	7787	2242
2138	6169	5746

Figure 1: Kernel Distribution Function for $g(X_1, X_2)$

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Brief Reports Four Period Crossover Designs

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In higher-order four period crossover designs with two treatments, sixteen possible treatment sequences can result: AAAA, AAAB, AABA, AABB, ABAA, ABAB, ABBA, ABBA and their duals. Higher-order crossover designs are useful for several reasons: they allow estimation of a treatment effect even in the presence of a carry-over effect, they provide estimates of intra-subject variability and they draw inference on the carry-over effect. The real question related to a two-treatment four-period crossover design is the real world application of these designs. This article considers four designs: Design I: ABBA and its dual; Design II: ABBA, AABB and their duals, Design III: ABBA, ABAA and their duals, Design IV: ABBA, ABAB and their duals. A traditional model that specifies a first-order carryover effect is assumed and methods for estimating treatment and first-order carryover effects in the set of four period trials are outlined.

Key words: Four period crossover design, carryover effect, bioequivalence.

Introduction

The crossover design, which compares two treatments over two periods, has held a dominant position in the application of crossover designs to the extent that – in the majority of articles and texts – it is referred to as *the crossover design*. Crossover designs are popular for comparing several non-curative treatments for their efficacy. For convenience, a crossover design with t treatments, p periods and s sequences is denoted as a $C(t, p, s)$.

Critiques of the $C(2, 2, 2)$ with sequences AB and BA are well known; the most serious of these is that the carryover effect is confounded with sequence by period effects leading to erroneous analyses. To overcome the disadvantages of the $C(2, 2, 2)$, a higher-order crossover design may be used. Two strategies can be employed to overcome the problems

inherent in the $C(2, 2, 2)$ design. The first strategy is to extend the number of sequences, such as Balaam's $C(2, 2, 4)$ design (Balaam, 1968); this design has four sequences, AA|AB|BA|BB. In addition, unbiased estimates of treatment and carryover effect can be formulated using a strategy outlined by Matthews (Matthews, 1994; Laska, Meisner & Kushner, 1983; Reed, 2010). The second strategy is to extend the classic design by adding a third period and/or a fourth period and repeating one of the two treatments.

Higher-order four period crossover designs with two treatments can result in sixteen possible treatment sequences: AAAA, AAAB, AABA, AABB, ABAA, ABAB, ABBA, ABBA and their duals. This article considers four designs: Design I: ABBA and its dual; Design II: ABBA, AABB and their duals, Design III: ABBA, ABAA and their duals, Design IV: ABBA, ABAB and their duals. This article presents methods for estimating treatment and first-order carryover effects in the set of four period trials, assuming a traditional model that specifies a first-order carryover effect.

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Crossover Design Model with Continuous Data

Assume that the primary goal is to compare two treatments A and B used in a study by estimating the treatment contrast $\tau_A - \tau_B$ and period effects π_1 and π_2 ; first order carryover effects λ_A , λ_B and μ are regarded as nuisance parameters. Also assume that the response variable is continuous and that there is one response from each subject in each period. Finally, it is assumed that each treatment has a simple first-order carryover effect that does not interact with the direct effect of the treatment in the subsequent period. This model then assumes the following for the response of patient y_{ij} .

If y_{ijk} denotes the observed response of subject j ($j = 1, \dots, n$) in period i ($i = 1, \dots, p$), then

$$y_{ijk} = \mu + \pi_i + \tau_{d(i,j)} + \lambda_{d(i-1,j)} + \beta_j + \varepsilon_{ij},$$

where π_i is the effect of period i , $\tau_{d(i,j)}$ is the direct effect of treatment D , $\lambda_{d(i-1,j)}$ is the simple first-order carryover effect of treatment D , and $d(i,j)$ is the treatment allocated to patient j in period i . $\lambda_{d(0,j)} = 0$ for all j . It is assumed that all effects are fixed effects. β_j is the effect of patient j and ε_{ij} is the error term. The random subject effect, β_j , and the experimental error, ε_{ij} , are assumed to be mutually independently distributed as $N(0, \sigma_\beta^2)$ and $N(0, \sigma_\varepsilon^2)$.

Design I: ABBA and Its Dual

An optimal two-sequence three period crossover design is the ABB/BAA design (Laska & Meisner, 1985; Hedayat & Stufken, 2003). This design is sometimes referred to as the two-sequence dual design because it allows an estimate of both treatment and carryover effect. The first design considered extends this by adding a fourth period and considering the sequence ABBA and its dual (see Table 1).

In sequence ABBA, the contrast, $c_1 = y_{11} + 2y_{12} + y_{13} + y_{14}$ has expectation $5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (2\tau_A + 3\tau_B) + (2\lambda_A + 2\lambda_B)$. In sequence BAAB, the contrast $c_2 = y_{21} + 2y_{22} + y_{23} - y_{24}$ has expectation $5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (2\tau_B + 3\tau_A) + (2\lambda_A + 2\lambda_B)$. The difference between contrast c_1 and c_2 forms an unbiased estimator of $\tau_A - \tau_B$. For the construction of an unbiased estimator of any carryover effect, $\lambda_A -$

λ_B , consider $c_3 = y_{11} - y_{12} + y_{13} - y_{14}$ and $c_4 = y_{21} - y_{22} + y_{23} - y_{24}$. The difference between c_3 and c_4 forms an unbiased estimate of $\lambda_A - \lambda_B$. Note that if the last period is omitted, this design reduces to an optimal two-sequence dual design. If the last two periods are eliminated, the design becomes the standard AB/BA crossover design.

Design II: ABBA, AABBB and Their Duals

This four-sequence, four-period design is a combination of two Balaam designs. The first two periods are the same as Balaam's design, while periods 3 and 4 are copies of Balaam's design reversed (see Table 2).

In sequence ABBA, the contrast $c_1 = y_{11} + y_{12} - y_{13} + y_{14}$ has expectation $2\mu + (\pi_1 + \pi_2 - \pi_3 + \pi_4) + (2\tau_A + \lambda_A)$. In AABBB, the contrast $c_2 = y_{21} + y_{22} - y_{23} - y_{24}$ has expectation $2\mu + (\pi_1 + 2\pi_2 - \pi_3 + \pi_4) + (2\tau_A + \lambda_B)$. In sequence BAAB, the contrast $c_3 = y_{31} + y_{32} - y_{33} - y_{34}$ has expectation $2\mu + (\pi_1 + 2\pi_2 - \pi_3 + \pi_4) + (2\tau_B + \lambda_B)$, and in BBAA the contrast $c_4 = y_{41} + y_{42} - y_{43} - y_{44}$ has expectation $2\mu + (\pi_1 + 2\pi_2 - \pi_3 + \pi_4) + (2\tau_B + \lambda_A)$. A combination of $(c_1 - c_4) + (c_2 - c_3)$ forms an unbiased estimate of treatment effect $(\tau_A - \tau_B)$.

In sequence ABBA, the expected value of $E[c_5] = E[y_{11} + 2y_{12} + y_{13} + y_{14}] = 5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (2\tau_A + 3\tau_B) + (2\lambda_A + 2\lambda_B)$; in AABBB, the expected value of $E[c_6] = E[y_{21} + 2y_{22} + y_{23} - y_{24}] = 5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (3\tau_A + 2\tau_B) + (3\lambda_A + \lambda_B)$; in BAAB, the expected value of $E[c_7] = E[y_{31} + 2y_{32} + y_{33} - y_{34}] = 5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (2\tau_B + 3\tau_A) + (2\lambda_A + 2\lambda_B)$; and in BBAA, the expected value of $E[c_8] = E[y_{41} + 2y_{42} + y_{43} - y_{44}] = 5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (3\tau_B + 2\tau_A) + (\lambda_A + 3\lambda_B)$. A combination of $(c_1 - c_3) + (c_2 - c_4)$ forms an unbiased estimate of treatment effect $(\lambda_A - \lambda_B)$.

Design III: ABBA, ABAA and Their Duals

In sequences ABBA, ABAA, BAAB, and BABB the expected values of $E[c_1]$, $E[c_2]$, $E[c_3]$ and $E[c_4]$ are: $E[y_{11} + y_{12} + y_{13} - y_{14}] = 2\mu + (\pi_1 + \pi_2 + \pi_3 - \pi_4) + (2\tau_B + \lambda_A)$, $E[y_{21} + y_{22} + y_{23} - y_{24}] = 2\mu + (\pi_1 + \pi_2 + \pi_3 - \pi_4) + (\tau_A + \tau_B - \lambda_A + \lambda_B)$, $E[y_{31} + y_{32} + y_{33} - y_{34}] = 2\mu + (\pi_1 + \pi_2 + \pi_3 - \pi_4) + (2\tau_A + \lambda_B)$ and $E[y_{41} + y_{42} + y_{43} - y_{44}] = 2\mu + (\pi_1 + \pi_2 + \pi_3 - \pi_4) + (\tau_A + \tau_B + \lambda_A -$

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λ_B), respectively (see Table 3). The linear combination of $(c_1 - c_4) - (c_2 - c_3)$ forms an unbiased estimate of treatment effect $(\lambda_A - \lambda_B)$, while the linear combination of $2(c_1 - c_3) + (c_2 - c_4)$ forms an unbiased estimate of treatment effect $(\tau_A - \tau_B)$.

Design V: ABBA, ABAB and Their Duals

In sequence ABBA, the expected value of $E[c_1] = E[y_{11} - y_{12} + y_{13} + y_{14}] = 2\mu + (\pi_1 - \pi_2 + \pi_3 + \pi_4) + (2\tau_A + \lambda_B - \lambda_A)$; in ABAA, the expected value of $E[c_2] = E[y_{21} - y_{22} + y_{23} + y_{24}] = 2\mu + (\pi_1 - \pi_2 + \pi_3 + \pi_4) + (2\tau_A + \lambda_B)$. For sequence BAAB, the expected value of $E[c_3] = E[y_{31} - y_{32} + y_{33} + y_{34}] = 2\mu + (\pi_1 - \pi_2 + \pi_3 + \pi_4) + (2\tau_B + \lambda_A - \lambda_B)$, and in BABB, the expected value of $E[c_4] = E[y_{41} - y_{42} + y_{43} + y_{44}] = 2\mu + (\pi_1 - \pi_2 + \pi_3 + \pi_4) + (2\tau_B + \lambda_A)$ (see Table 4). The linear combination of $(c_1 - c_2) - (c_3 - c_4)$ forms an unbiased estimate of treatment effect $(\lambda_A - \lambda_B)$, while the linear combination of $2(c_2 - c_4) + (c_1 - c_3)$ forms an unbiased estimate of treatment effect $(\tau_A - \tau_B)$.

Discussion

This article considered four two-treatment in four-period crossover designs. For a simple one period carryover effect model, the four designs presented are ideal because the design

efficiencies are optimal. The designs with the highest efficiency (100%) are the AABB, ABBA and their duals (Table 2). The other designs considered weigh in at 91% (Hedayat & Stufken, 2003). All designs are robust, simple and easily implemented.

Higher-order crossover designs are useful because they allow a treatment effect to be estimated even in the presence of a carry-over effect, they provide estimates of intra-subject variability and they draw inference on the carry-over effect (Chow & Lu, 1992). Are these four-period crossover designs useful? Perhaps. The true question relates to the application of these designs.

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Table 1: Expected Values for Design I

Sequence	Period 1 (k = 1)	Period 2 (k = 2)	Period 3 (k = 3)	Period 4 (k = 4)
ABBA (i = 1)	$y_{11} = \mu + \pi_1 + \tau_A$	$y_{21} = \mu + \pi_2 + \tau_B + \lambda_A$	$y_{31} = \mu + \pi_3 + \tau_B + \lambda_B$	$y_{14} = \mu + \pi_4 + \tau_A + \lambda_B$
BAAB (i = 2)	$y_{21} = \mu + \pi_1 + \tau_B$	$y_{22} = \mu + \pi_2 + \tau_A + \lambda_B$	$Y_{23} = \mu + \pi_3 + \tau_A + \lambda_A$	$Y_{24} = \mu + \pi_4 + \tau_B + \lambda_A$

Expected values for sequences:

- ABBA, $E[c_1] = E[y_{11} + 2y_{12} + y_{13} + y_{14}] = 5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (2\tau_A + 3\tau_B) + (2\lambda_A + 2\lambda_B)$
- BAAB, $E[c_2] = E[y_{21} + 2y_{22} + y_{32} - y_{42}] = 5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (2\tau_B + 3\tau_A) + (2\lambda_A + 2\lambda_B)$
- ABBA, $E[c_3] = E(y_{11} - y_{12} + y_{13} - y_{14}) = (\pi_1 - \pi_2 + \pi_3 - \pi_4) - \lambda_A$
- BAAB, $E[c_4] = E(y_{21} - y_{22} + y_{32} - y_{42}) = (\pi_1 - \pi_2 + \pi_3 - \pi_4) - \lambda_B$

Table 2: Expected Values for Design II: ABBA, AABB and Their Duals

Sequence	Period 1 (k = 1)	Period 2 (k = 2)	Period 3 (k = 3)	Period 4 (k = 4)
ABBA (i = 1)	$\mu + \pi_1 + \tau_A$	$\mu + \pi_2 + \tau_B + \lambda_A$	$\mu + \pi_3 + \tau_B + \lambda_B$	$\mu + \pi_4 + \tau_A + \lambda_B$
AABB (i = 2)	$\mu + \pi_1 + \tau_A$	$\mu + \pi_2 + \tau_A + \lambda_A$	$\mu + \pi_3 + \tau_B + \lambda_A$	$\mu + \pi_4 + \tau_B + \lambda_B$
BAAB (i = 3)	$\mu + \pi_1 + \tau_B$	$\mu + \pi_2 + \tau_A + \lambda_B$	$\mu + \pi_3 + \tau_A + \lambda_A$	$\mu + \pi_4 + \tau_B + \lambda_A$
BBAA (i = 4)	$\mu + \pi_1 + \tau_B$	$\mu + \pi_2 + \tau_B + \lambda_B$	$\mu + \pi_3 + \tau_A + \lambda_B$	$\mu + \pi_4 + \tau_A + \lambda_A$

Expected values for sequences:

- ABBA, $E[c_1] = E[y_{11} + y_{12} - y_{13} + y_{14}] = 2\mu + (\pi_1 + \pi_2 - \pi_3 + \pi_4) + (2\tau_A + \lambda_A)$
- AABB, $E[c_2] = E[y_{21} + y_{22} - y_{23} + y_{24}] = 2\mu + (\pi_1 + \pi_2 - \pi_3 + \pi_4) + (2\tau_A + \lambda_B)$
- BAAB, $E[c_3] = E[y_{31} + y_{32} - y_{33} + y_{34}] = 2\mu + (\pi_1 + \pi_2 - \pi_3 + \pi_4) + (2\tau_B + \lambda_B)$
- BBAA, $E[c_4] = E[y_{41} + y_{42} - y_{43} + y_{44}] = 2\mu + (\pi_1 + \pi_2 - \pi_3 + \pi_4) + (2\tau_B + \lambda_A)$
- ABBA, $E[c_5] = E[y_{11} + 2y_{12} + y_{13} + y_{14}] = 5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (2\tau_A + 3\tau_B) + (2\lambda_A + 2\lambda_B)$
- AABB, $E[c_6] = E[y_{21} + 2y_{22} + y_{23} - y_{24}] = 5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (3\tau_A + 2\tau_B) + (3\lambda_A + \lambda_B)$
- BAAB, $E[c_7] = E[y_{31} + 2y_{32} + y_{33} - y_{34}] = 5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (2\tau_B + 3\tau_A) + (2\lambda_A + 2\lambda_B)$
- BBAA, $E[c_8] = E[y_{41} + 2y_{42} + y_{43} - y_{44}] = 5\mu + (\pi_1 + 2\pi_2 + \pi_3 + \pi_4) + (3\tau_B + 2\tau_A) + (\lambda_A + 3\lambda_B)$

Table 3: Expected Values for Design III: ABBA, ABAA and Their Duals

Sequence	Period 1 (k = 1)	Period 2 (k = 2)	Period 3 (k = 3)	Period 4 (k=4)
ABBA (i = 1)	$\mu + \pi_1 + \tau_A$	$\mu + \pi_2 + \tau_B + \lambda_A$	$\mu + \pi_3 + \tau_B + \lambda_B$	$\mu + \pi_4 + \tau_A + \lambda_B$
ABAA (i = 2)	$\mu + \pi_1 + \tau_A$	$\mu + \pi_2 + \tau_B + \lambda_A$	$\mu + \pi_3 + \tau_A + \lambda_B$	$\mu + \pi_4 + \tau_A + \lambda_A$
BAAB (i = 3)	$\mu + \pi_1 + \tau_B$	$\mu + \pi_2 + \tau_A + \lambda_B$	$\mu + \pi_3 + \tau_A + \lambda_A$	$\mu + \pi_4 + \tau_B + \lambda_A$
BABB (i = 4)	$\mu + \pi_1 + \tau_B$	$\mu + \pi_2 + \tau_A + \lambda_B$	$\mu + \pi_3 + \tau_B + \lambda_A$	$\mu + \pi_4 + \tau_B + \lambda_B$

Expected values for sequences:

- ABBA, $E[c_1] = E[y_{11} + y_{12} + y_{13} - y_{14}] = 2\mu + (\pi_1 + \pi_2 + \pi_3 - \pi_4) + (2\tau_B + \lambda_A)$
- ABAA, $E[c_2] = E[y_{21} + y_{22} + y_{23} - y_{24}] = 2\mu + (\pi_1 + \pi_2 + \pi_3 - \pi_4) + (\tau_A + \tau_B - \lambda_A + \lambda_B)$
- BAAB, $E[c_3] = E[y_{31} + y_{32} + y_{33} - y_{34}] = 2\mu + (\pi_1 + \pi_2 + \pi_3 - \pi_4) + (2\tau_A + \lambda_B)$
- BABB, $E[c_4] = E[y_{41} + y_{42} + y_{43} - y_{44}] = 2\mu + (\pi_1 + \pi_2 + \pi_3 - \pi_4) + (\tau_A + \tau_B + \lambda_A - \lambda_B)$

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Table 4: Expected Values for Design IV: ABBA, ABAB and Their Duals

Sequence	Period 1 (k = 1)	Period 2 (k = 2)	Period 3 (k = 3)	Period 4 (k=4)
ABBA (i = 1)	$\mu + \pi_1 + \tau_A$	$\mu + \pi_2 + \tau_B + \lambda_A$	$\mu + \pi_3 + \tau_B + \lambda_B$	$\mu + \pi_4 + \tau_A + \lambda_B$
ABAB (i = 2)	$\mu + \pi_1 + \tau_A$	$\mu + \pi_2 + \tau_B + \lambda_A$	$\mu + \pi_3 + \tau_A + \lambda_B$	$\mu + \pi_4 + \tau_B + \lambda_A$
BAAB (i = 3)	$\mu + \pi_1 + \tau_B$	$\mu + \pi_2 + \tau_A + \lambda_B$	$\mu + \pi_3 + \tau_A + \lambda_A$	$\mu + \pi_4 + \tau_B + \lambda_A$
BABA (i = 4)	$\mu + \pi_1 + \tau_B$	$\mu + \pi_2 + \tau_A + \lambda_B$	$\mu + \pi_3 + \tau_B + \lambda_A$	$\mu + \pi_4 + \tau_A + \lambda_B$

Expected values for sequences:

- ABBA, $E[c_1] = E[y_{11} - y_{12} + y_{13} + y_{14}] = 2\mu + (\pi_1 - \pi_2 + \pi_3 + \pi_4) + (2\tau_A + \lambda_B - \lambda_A)$
- ABAA, $E[c_2] = E[y_{21} - y_{22} + y_{23} + y_{24}] = 2\mu + (\pi_1 - \pi_2 + \pi_3 + \pi_4) + (2\tau_A + \lambda_B)$
- BAAB, $E[c_3] = E[y_{31} - y_{32} + y_{33} + y_{34}] = 2\mu + (\pi_1 - \pi_2 + \pi_3 + \pi_4) + (2\tau_B + \lambda_A - \lambda_B)$
- BABB, $E[c_4] = E[y_{41} - y_{42} + y_{43} + y_{44}] = 2\mu + (\pi_1 - \pi_2 + \pi_3 + \pi_4) + (2\tau_B + \lambda_A)$

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Ratio Type Estimator of Ratio of Two Population Means in Stratified Random Sampling

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A ratio estimator is proposed for the ratio of two population means using auxiliary information in stratified random sampling. Bias and mean squared error expressions are obtained under large sample approximation, and the proposed estimator is compared both theoretically and empirically with the conventional estimator of ratio for two population means in stratified random sampling.

Key words: Ratio of two population means, auxiliary information, stratified random sampling, bias, mean squared error.

Introduction

The problem of estimating population means is considered in a wide range of applications in many areas of human activities. A ratio of two population means is also applicable in many situations, such as per hectare production of crops, per capita income and per kilometer population density. Many researchers have studied the estimation of the ratio of two population means in simple random sampling (Singh, 1965; Rao&Pareira, 1968; Shah & Shah, 1978; Ray & Singh, 1985; Upadhyaya& Singh, 1985; Upadhyaya, et al., 1985; Singh & Rani, 2005, 2006; Sindhu, et al., 2009). Other sampling designs have not attracted much attention; in many situations, it has been observed that stratified random sampling provides efficient estimators compared to those of simple random sampling. Thus, this article estimates the ratio of two population means under stratified random sampling.

Consider a finite population $U = U_1, U_2, \dots, U_N$ of size N . This population U is divided into L strata each of size N_h and sample of size n_h is drawn from each stratum such that $n = \sum_{h=1}^L n_h$ ($h=1,2,\dots,L$). If y_0 and y_1 are the study variates, x is an auxiliary variate, and y_{0hi} , y_{1hi} and x_{hi} ($h=1,2,\dots,L$; $i=1,2,\dots,N_h$) are the observations taken from the i^{th} unit of the h^{th} stratum on study variates y_0 , y_1 and auxiliary variate x respectively, then the following are defined:

h^{th} stratum mean for study variate y_0 :

$$\bar{Y}_{0h} = \frac{1}{N_h} \sum_{i=1}^{N_h} y_{0hi}$$

h^{th} stratum mean for study variate y_1 :

$$\bar{Y}_{1h} = \frac{1}{N_h} \sum_{i=1}^{N_h} y_{1hi}$$

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h^{th} stratum mean for auxiliary variate x :

$$\bar{X}_h = \frac{1}{N_h} \sum_{i=1}^{N_h} y_{1hi}$$

Population mean of study variate y_0 :

$$\bar{Y}_0 = \frac{1}{N} \sum_{h=1}^L \sum_{i=1}^{N_h} y_{0hi} = \frac{1}{N} \sum_{h=1}^L N_h \bar{Y}_{0h} = \sum_{h=1}^L W_h \bar{Y}_{0h}$$

Population mean of study variate y_1 :

$$\bar{Y}_1 = \frac{1}{N} \sum_{h=1}^L \sum_{i=1}^{N_h} y_{1hi} = \frac{1}{N} \sum_{h=1}^L N_h \bar{Y}_{1h} = \sum_{h=1}^L W_h \bar{Y}_{1h}$$

Population mean of auxiliary variate x :

$$\bar{X} = \frac{1}{N} \sum_{h=1}^L \sum_{i=1}^{N_h} x_{hi} = \frac{1}{N} \sum_{h=1}^L W_h \bar{X}_h$$

Sample mean of study variate y_0 for h^{th} stratum:

$$\bar{y}_{0h} = \frac{1}{n_h} \sum_{i=1}^{n_h} \bar{y}_{0hi}$$

Sample mean of study variate y_1 for h^{th} stratum:

$$\bar{y}_{1h} = \frac{1}{n_h} \sum_{i=1}^{n_h} \bar{y}_{1hi}$$

Sample mean of auxiliary variate x for h^{th} stratum:

$$\bar{x}_h = \frac{1}{n_h} \sum_{i=1}^{n_h} \bar{x}_{hi}$$

Stratum weight of h^{th} stratum:

$$W_h = \frac{N_h}{N}$$

Ratio of two population means:

$$R = \frac{\bar{Y}_0}{\bar{Y}_1}$$

The usual unbiased estimators of population means $\bar{Y}_0$, $\bar{Y}_1$ and $\bar{X}$ are

$$\bar{y}_{0st} = \sum_{h=1}^L W_h \bar{y}_{0h} \quad (1.1)$$

$$\bar{y}_{1st} = \sum_{h=1}^L W_h \bar{y}_{1h} \quad (1.2)$$

$$\bar{x}_{st} = \sum_{h=1}^L W_h \bar{x}_h \quad (1.3)$$

and the estimator of the ratio of two population means R in stratified random sampling is:

$$\hat{R}_{st} = \left(\frac{\bar{y}_{0st}}{\bar{y}_{1st}} \right).$$

Suggested Ratio Estimator

When the population mean $\bar{X}$ of auxiliary variate x is known, Singh (1965) suggested an estimator for R in simple random sampling as

$$T_1 = \left(\frac{\bar{y}_0}{\bar{y}_1} \right) \left(\frac{\bar{X}}{\bar{x}} \right) = R \left(\frac{\bar{X}}{\bar{x}} \right).$$

In stratified random sampling T_1 is defined as

$$T_{1st} = \left(\frac{\bar{y}_{0st}}{\bar{y}_{1st}} \right) \left(\frac{\bar{X}}{\bar{x}_{st}} \right)$$

In order to derive the bias and mean squared error expressions of estimators $\hat{R}_{st}$ and T_{1st} it is assumed that $\bar{y}_{0h} = \bar{Y}_{0h}(1 + e_{0h})$, $\bar{y}_{1h} = \bar{Y}_{1h}(1 + e_{1h})$, and $\bar{x}_h = \bar{X}_h(1 + e_{2h})$, such that, $E(e_{0h}) = E(e_{1h}) = E(e_{2h}) = 0$.

To the first degree of approximation the bias and mean squared error are

$$B(\hat{R}_{st}) = R \sum_{h=1}^L W_h^2 \gamma_h \left(\frac{S_{1h}^2}{\bar{Y}_1^2} - \frac{S_{01h}}{\bar{Y}_0 \bar{Y}_1} \right) \quad (2.1)$$

$$B(T_{1st}) = R \sum_{h=1}^L W_h^2 \gamma_h \left(\frac{S_{1h}^2}{\bar{Y}_1^2} + \frac{S_{xh}^2}{\bar{X}^2} - \frac{S_{01h}}{\bar{Y}_0 \bar{Y}_1} - \frac{S_{0xh}}{\bar{Y}_0 \bar{X}} + \frac{S_{1xh}}{\bar{Y}_1 \bar{X}} \right) \quad (2.2)$$

$$MSE(\hat{R}_{st}) = R^2 \sum_{h=1}^L W_h^2 \gamma_h \left(\frac{S_{0h}^2}{\bar{Y}_0^2} + \frac{S_{1h}^2}{\bar{Y}_1^2} - 2 \frac{S_{01h}}{\bar{Y}_0 \bar{Y}_1} \right) \quad (2.3)$$

$$MSE(T_{1st}) = R^2 \sum_{h=1}^L W_h^2 \gamma_h \left\{ \frac{S_{0h}^2}{\bar{Y}_0^2} + \frac{S_{1h}^2}{\bar{Y}_1^2} + \frac{S_{xh}^2}{\bar{X}^2} - 2 \left(\frac{S_{01h}}{\bar{Y}_0 \bar{Y}_1} + \frac{S_{0xh}}{\bar{Y}_0 \bar{X}} - \frac{S_{1xh}}{\bar{Y}_1 \bar{X}} \right) \right\} \quad (2.4)$$

where

$$S_{0h}^2 = \frac{1}{N_h - 1} \sum_{i=1}^{N_h} (y_{0hi} - \bar{y}_{0h})^2,$$

$$S_{1h}^2 = \frac{1}{N_h - 1} \sum_{i=1}^{N_h} (y_{1hi} - \bar{y}_{1h})^2,$$

$$S_{xh}^2 = \frac{1}{N_h - 1} \sum_{i=1}^{N_h} (x_{hi} - \bar{x}_h)^2,$$

$$S_{01h} = \frac{1}{N_h - 1} \sum_{i=1}^{N_h} (y_{0hi} - \bar{y}_{0h})(y_{1hi} - \bar{y}_{1h}),$$

$$S_{0xh} = \frac{1}{N_h - 1} \sum_{i=1}^{N_h} (y_{0hi} - \bar{y}_{0h})(x_{hi} - \bar{x}_h)$$

and

$$S_{1xh} = \frac{1}{N_h - 1} \sum_{i=1}^{N_h} (y_{1hi} - \bar{y}_{1h})(x_{hi} - \bar{x}_h).$$

Efficiency Comparison of Estimators

A comparison of equations (2.3) and (2.4) shows that the suggested estimator T_{1st} will be more efficient than conventional estimator $\hat{R}_{st}$ if

$$MSE(T_{1st}) - MSE(\hat{R}_{st}) < 0$$

that is, if

$$\sum_{h=1}^L W_h^2 \gamma_h \left\{ \frac{S_{xh}^2}{\bar{X}^2} - 2 \left(\frac{S_{0xh}}{\bar{Y}_0 \bar{X}} - \frac{S_{1xh}}{\bar{Y}_1 \bar{X}} \right) \right\} < 0 \quad (3.1)$$

If condition (3.1) is satisfied, the suggested estimator would be more efficient than the conventional estimator.

Empirical Study

Two natural datasets were used to compare the proposed estimator numerically (See Tables 1 and 2).

Conclusion

The theoretical comparison provides the condition under which the suggested estimator is more efficient than the conventional estimator $\hat{R}_{st}$. Table 3 shows that there is a considerable gain in efficiency by using the proposed ratio estimator T_{1ST} in comparison to the conventional estimator $\hat{R}_{st}$. Thus, if information regarding population mean $\bar{X}$ is available, the suggested estimator T_{1ST} is recommended for use in practice.

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Table 1: Population 1 (y_0 : Number of Workers, y_1 : Fixed Capital, x : Output)

N = 10 n = 4	$n_1 = 2$	$n_2 = 2$	$N_1 = 5$	$N_2 = 5$
	$\bar{Y}_{01} = 51.80$	$\bar{Y}_{02} = 60.60$	$\bar{Y}_{11} = 214.4$	$\bar{Y}_{12} = 333.8$
	$\bar{X}_1 = 1925.8$	$\bar{X}_2 = 315.6$	$S_{y_{01}} = 0.75$	$S_{y_{02}} = 4.84$
	$S_{y_{11}} = 74.87$	$S_{y_{12}} = 66.35$	$S_{x_1} = 615.92$	$S_{x_2} = 340.38$
	$S_{01_1} = 38.08$	$S_{01_2} = 287.92$	$S_{0x_1} = 411.16$	$S_{0x_2} = 1536.24$
	$S_{1x_1} = 39360.68$	$S_{1x_2} = 22356.52$		

Source: Murthy, 1967

Table 2: Population 2 (y_0 : Area (in 000 Hectare), y_1 : Production (in 000 MT), x : Productivity (MT/Hectare))

N = 20 n = 8	$n_1 = 4$	$n_2 = 4$	$N_1 = 10$	$N_2 = 10$
	$\bar{Y}_{01} = 6.2$	$\bar{Y}_{02} = 80.67$	$\bar{Y}_{11} = 3.53$	$\bar{Y}_{12} = 111.61$
	$\bar{X}_1 = 0.5$	$\bar{X}_2 = 1.41$	$S_{y_{01}} = 1.2$	$S_{y_{02}} = 10.82$
	$S_{y_{11}} = 74.87$	$S_{y_{12}} = 66.35$	$S_{x_1} = 615.92$	$S_{x_2} = 340.38$
	$S_{01_1} = 1.75$	$S_{01_2} = -92.02$	$S_{0x_1} = -0.02$	$S_{0x_2} = -7.04$
	$S_{1x_1} = 1.60$	$S_{1x_2} = 144.87$		

Source: National Horticulture Board of India, Official Web Site, <http://nhb.gov.in/statistics/area-production-statistics.html>

Table 3: Percent Relative Efficiencies of $\hat{R}_{st}$ and T_{1st} with respect to $\hat{R}_{st}$

Estimator	$\hat{R}_{st}$	T_{1st}
Population 1	100	9274.573
Population 2	100	400747.3

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JMASM Algorithms and Code *JMASM32: SAS Template for Single-Subject Experimental Designs*

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Meta-analysis has been used to synthesize research findings and to evaluate the effectiveness of treatments or the accuracy of diagnostic tools. Although meta-analytic techniques were developed to synthesize the results of several studies, controversy exists as to how to quantify the results from single-subject experimental designs (SSEDs). The most commonly used metrics are reviewed, including non-regression and regression based methods. The application of the SAS template is demonstrated through simulated data sets. The SAS templates can be modified to accommodate a more complex data structure.

Key words: Single-subject experimental designs (SSED), SAS template.

Introduction

Meta-analysis is a “statistical analysis of a large collection of results from individual studies for the purpose of integrating the findings” (Glass, 1976, p. 3). Meta-analyses have been adapted in a variety of settings, such as, special education (Swanson & Sachse-Lee, 2000), counseling (Hagen & Nordahl, 2008) and behavioral intervention research (Filter & Horner, 2009).

The majority of literature on meta-analyses focuses on group comparison experimental studies; single-subject experimental designs (SSEDs) studies are frequently excluded. Although these meta-analytic techniques effectively summarize and evaluate the results of studies with relatively large sample sizes, on-going controversy exists as to synthesizing results from SSEDs (Faith, Allison & Gorman, 1996). SSED research has grown in popularity in educational and psychological research designed to assess a treatment’s effect and different approaches for analyzing single-subject data have been considered over the past decades.

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SSEDs have been traditionally evaluated by visual analysis. Bulté and Onghena (2011) suggested that an investigation of treatment effects starts with a visual exploration of the single-case data as opposed to subjective interpretation based on visual analysis; however, evidence-based practice (EBP) emphasizes the importance of more objective outcome measures, especially magnitude of effect indices or effect sizes (Horner, et al., 2005). Methodologists have developed a number of quantitative descriptors as options to describe a treatment’s effect in SSEDs. Two main types of statistical summary approaches have been proposed: non-regression based and regression based approaches (Wendt, 2009). Although several metrics have been developed and used

for SSEDs, a question remains regarding what effect size metrics are most appropriate to measure effect size for SSEDs. Thus, this study was designed to develop a SAS procedure to test several metrics to compare their performance.

Regression Based Approaches: Four-Parameter Model

Huitema and McKean (2000) modified the piece-wise regression model by Center, Skiba and Casey (1985-1986) and introduced further regression coefficients that describe change in intercepts as well as in slope from the baseline (A) to treatment (B) phase:

$$Y_t = \beta_0 + \beta_1 T_t + \beta_2 D_t + \beta_3 [T_t - (n_1 + 1)] D_t + e_t \quad (1)$$

Y_t represents outcome score at time t , T_t is the time/session point, D indicates phase either A or B, n_1 is the number of time points in baseline, β_0 represents baseline intercept (i.e., Y at time = 0), β_1 expresses baseline linear trend, β_2 indicates difference in intercept predicted from treatment phase data and that predicted for time = $n_1 + 1$ from baseline phase data, and β_3 represents difference in slope between baseline and treatment, $e_t \sim N(0, \sigma^2)$. Thus, β_2 and β_3 provide estimates of a treatment's effect on intercept and on slope, respectively (Wendt, 2009).

The four parameter model interprets the results using ΔR^2 approaches, which can be converted to Cohen's d , and uses all data in both baseline and treatment phases (Wendt, 2009). The regression based approaches assume normality, equal variance and serial independence. Because these are not usually met by SSED data, careful interpretation is required depending on whether the data met these assumptions.

Regression Based Approaches: Multilevel Modeling

Researchers have proposed a multilevel modeling approach as an option for combining SSED data (Ferron, et al., 2009; Ferron, Farmer & Owens, 2010; Shadish & Rindskopf, 2007; Van den Noortgate & Onghena, 2003a, 2003b). Repeated measures are nested within subjects; lowest level measures within subject effect

change from baseline to intervention. The multilevel modeling approaches can explain why some subjects show more change than others; the variability among individuals in the size of treatment effects can be explained by including study and/or characteristics such as an individual's gender or study intervention type in the model. The multilevel modeling approach can resolve many of the limitations of traditional ordinary least square regression approaches (e.g., independent error assumption).

Non-Regression Based Approaches: Percentage of Non-Overlapping Data (PND)

Percentage of Non-Overlapping Data (PND) computes non-overlap between baseline and treatment phases (Scruggs, Mastropieri & Casto, 1987). PND identifies the highest data point in the baseline and calculates the percentage of data points during treatment exceeding this level. If a study includes several experiments, PND scores are aggregated by taking the median rather than mean because scores are usually not distributed normally (Wendt, 2009). The typical interpretation of PND is: The higher the percentage, the more effective the treatment. Readers can find specific criteria for interpreting PND scores in Scruggs, Mastropieri, Cook and Escobar (1986). Although PND is easy to interpret, it ignores all baseline data except one data point and PND cannot detect slope changes (Wendt, 2009).

Non-Regression Based Approaches: Percentage of All Non-Overlapping Data (PAND)

Percentage of All Non-Overlapping Data (PAND) computes the total number of data points that do not overlap between baseline and treatment phases (Parker, Hagan-Burke & Vannest, 2007). PAND determines overlapping data points: the minimum number that would have to be transferred across phases for complete data separation. It calculates % overlap by dividing the number of overlapping points by the total number of points and then subtracts this percent from 100 to obtain PAND (Wendt, 2009). Unlike PND, PAND uses all data points across both phases. It may be translated to Φ and Φ^2 to determine an effect size such as Cohen's d (Wendt, 2009).

Non-Regression Based Approaches: Percentage of Data Points Exceeding the Median (PEM)

Percentage of Data Points Exceeding the Median (PEM) computes the percentage of data points exceeding the median of baseline phase (Ma, 2006). It first locates the median point in baseline data and then draws a horizontal middle line passing through the median of the baseline into the treatment phase. PEM calculates the percentage of treatment phase data points above the middle line if behavior increase is anticipated, and below the middle line if behavior decrease is anticipated (Wendt, 2009). It is assumed that – if treatment is ineffective – data points will continually fluctuate around the middle line. The interpretation of PEM is: Values higher than 0.9 reflect highly effective treatment; values between 0.7 and 0.9 indicate moderately effective treatment; values less than 0.7 reflect questionable or ineffective treatment. In the presence of floor or ceiling data points, PEM reflects effect size while PND fails to reflect effect size. However, PEM is insensitive to magnitude of data points above the median, thus, it does not consider trend and variability in data points of treatment phase. It might reflect only partial improvement if an orthogonal slope exists in a baseline treatment pair after the first treatment phase (Wendt, 2009).

Non-Regression Based Approaches: Pairwise Data Overlap (PDO)

Pairwise Data Overlap (PDO) computes the overlap of all possible paired data comparisons between baseline and treatment phases (Parker & Vannest, in press). PDO first compares the baseline data points with all treatment data points, and then it determines the number of overlapping and non-overlapping points. PDO calculates the total number of non-overlapping points divided by the total number of comparison (Wendt, 2009). Compared to other indices, PDO takes slightly longer to calculate and requires that individual data point results be written down and added. The calculation is time consuming for long and crossed data series (Wendt, 2009).

Non-Regression Based Approaches: Percentage Reduction Data (PRD)

Percentage Reduction Data (PRD) computes the reduction of targeted behavior due to treatment (O'Brien & Repp, 1990). PRD is also termed Mean Baseline Reduction (MBR, Campbell, 2003, 2004). PRD determines the mean of the last three data points from the baseline (μA) and of the last three data points from the treatment (μB). It computes the amount of change between the baseline and treatment:

$$[(\mu A - \mu B) \div \mu A] \times 100 \quad (2)$$

Non-Regression Based Approaches: Percentage of Zero Data (PZD)

Percentage of Zero Data (PZD) computes the degree to which treatment completely suppresses targeted behavior (Scotti, et al., 1991). PZD identifies the first data point to reach zero in the treatment phase. It computes the percentage of data points that remain at zero from the first zero point onwards (Wendt, 2009). Interpretation of PZD scores are: PZD lower than 18% reflects ineffectiveness; PZD between 18% - 54% reflects questionable effectiveness; PZD between 55% - 80% reflects fair effectiveness; PZD higher than 80% reflects high effectiveness.

Methodology

SAS Template for SSEDs

The majority of literature on single case data noted that research on SSED effect size metrics requires the use of multiple metrics and the metrics are compared against each other. The comparisons must compare the metrics within the family of non-overlap as well as across regression versus non-regression based approaches. Although researchers are aware of the methodological issues regarding several SSED tools discussed, difficulties are frequently encountered in running and comparing the metrics due to the complexity of each metric involved. This study develops a SAS procedure consisting of several SAS macros to test a number of metrics for SSEDs. Four sets of single case data were generated using SAS macros written by Fan, Felsovalyi, Sivo and Keenan (2002). Table 1 shows one of the four

simulated AB datasets (condition 1). The total number of observations (T_t) is 18, Phase (D_t) is coded with a value of 0 for baseline (A) and 1 for treatment (B). In this dataset, the number of observations (n_1) for A phase is 8 and the number of observations (n_2) for B phase is 10.

Table 1: Simulated AB Dataset

Outcome (Y)	T_t	D_t	$T_t - (n_1 + 1)]D_t$
1.7	1	0	0
1.9	2	0	0
1.6	3	0	0
1.6	4	0	0
2.4	5	0	0
3.9	6	0	0
4.9	7	0	0
4.4	8	0	0
6.5	9	1	0
8.1	10	1	1
9.2	11	1	2
10.1	12	1	3
10.4	13	1	4
10.1	14	1	5
11.1	15	1	6
12.6	16	1	7
13.8	17	1	8
15.4	18	1	10

The SAS procedure in this article provides standardized parameter estimates for Huitema and McKean's model (2000): standardized slope estimates for phase A and standardized intercept and slope estimates for phase B. It also calculates the following non-regression metrics described above: PND, PAND, PEM, PZD and PRD (see Appendix).

Conclusion

It is not surprising that single-case designs are becoming increasingly more popular in diverse fields given the emphasis on establishing an evidence base for practice. This is due to the difficulties encountered in conducting large group experimental studies. Recently, a single case design standard was released by *What Works Clearinghouse* (Kratochwill, Hitchcock, Horner, Levin, Odom, Rindskopf & Shadish, 2010). Methodologists have developed several SSED metrics to assess and compare the efficiency of the design standards. Several methodological concerns have been expressed; controversy exists as to how to quantify the results of SSEDs. In addition, a few studies resulted in user friendly software capable of performing SSED metrics including both non-regression and regression based methods. The use of a SAS template developed in this study will assist researchers to calculate and compare most the commonly used SSED metrics and to synthesize the results from single-case datasets more efficiently.

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Appendix: SAS Procedure

The SAS procedure provides standardized regression parameter estimates as well as PND, PAND, PEM, PZD and PRD.

```

OPTIONS LINESIZE=100 NOSOURCE NOSOURCE2 NONOTES;

LIBNAME AUTOREG 'C:\Users\Desktop\Single Case';
%MACRO AUTOREG_N (ITER,N1,N2,N,RES,AR,ERR,BETA1,BETA2,BETA3,CONDIT) ;

/* Generate Dataset */;
DATA TEMP1;

    ARRAY SERIEA{&N} SERIEA1-SERIEA&N;

    SERIEA(1) = RANNOR(-1);

    DO J=2 TO &N;
        SERIEA(J) = RANNOR(-11) * SQRT(&RES) + SERIEA(J-
1) * SQRT(&AR);
    END;

    KEEP SERIEA1-SERIEA&N;
    OUTPUT;

PROC TRANSPOSE DATA=TEMP1 OUT=TEMP1;
DATA TEMP1;
    SET TEMP1;
    ID=_N_;
    SERIESA=COL1;
    OUTPUT;
    DROP COL1 _NAME_;

DATA TEMP2;
    TIME=1;
DO ID=1 TO &N;
    TIME = ID;
    IF ID <= &N1 THEN D = 0;
    ELSE D = 1;
    TIMED = (TIME - (&N1 + 1)) * D;
    Y = TIME * SQRT(&BETA1) + D * SQRT(&BETA2) +
TIMED * SQRT(&BETA3);
    OUTPUT;
END;

DATA INPUT1;
MERGE TEMP1 TEMP2;
BY ID;

```

SAS TEMPLATE SSED

Appendix: SAS Procedure (Continued)

```
TIMEAR=TIME; DAR=D; TIMEDAR=TIMED;
      Y = Y + SERIESA*SQRT(&ERR);
ITERATION = &ITER;
      CONDITION = &CONDIT;

RUN;
PROC APPEND BASE = INPUT DATA = INPUT1 FORCE; RUN;

/* Four Parameter Regression */

PROC REG DATA=INPUT1 OUTEST=RES_REG;
      MODEL Y = TIME D TIMED/OUTSTB OUTSEB NOPRINT;
      RUN;

/* outstb (1st line in data generate) shows standardized parameter
estimates*/
data REG_EST; set RES_REG;if _n_=1; keep time d timed;
output;
/* outseb (2nd line in data generate) shows standardized error of
parameter estimates*/
data REG_SE; set RES_REG; if _n_=2; keep time d timed SE_time SE_d
SE_timed;
      SE_time = time;
      SE_d = d;
      SE_timed =timed;
      output;
data REG_SE;set REG_SE; drop time d timed;

data RESULTS;
      merge REG_EST REG_SE ;

      BETA1=&BETA1;
      BETA2=&BETA2;
      BETA3=&BETA3;
      AR=&AR;
      ITERATION=&ITER;
      CONDITION=&CONDIT;

      KEEP TIME D TIMED SE_time SE_d SE_timed
      BETA1 BETA2 BETA3 AR ITERATION CONDITION;
RUN;

PROC APPEND BASE=Four_Par_RESULT (CNTLLEV=MEMBER) DATA=RESULTS FORCE;
/* Four-Paremeter_Regression result*/
RUN;
```

Appendix: SAS Procedure (Continued)

```

/*PND*/
DATA BASE;
    SET INPUT1;          IF D=0;
    KEEP ID D Y ITERATION CONDITION;

RUN;

DATA TTT;
    SET INPUT1;
    IF D=1;
    KEEP ID D Y ITERATION CONDITION;

RUN;

PROC MEANS NOPRINT DATA=BASE;
    VAR Y;
    OUTPUT OUT=RES MAX=MAXIMUM;

RUN;

DATA RES1;
    SET RES;
    ARRAY MAX{&N2} MAX1-MAX&N2;
    DO J=1 TO &N2;
        MAX(J)=MAXIMUM;
    END;
    DROP MAXIMUM _FREQ_ _TYPE_ J;

RUN;

PROC TRANSPOSE DATA=RES1 OUT=RES2;

RUN;

DATA BASE_TTT;
    MERGE TTT RES2;
    IF Y-COL1>0 THEN CHECK=1; ELSE CHECK=0;
    RUN;

PROC MEANS DATA=BASE_TTT NOPRINT;
    CLASS CONDITION;
    VAR CHECK;
    OUTPUT OUT=BASEPND ;
    RUN;

DATA PND; SET BASEPND;
    IF _STAT_='MEAN' AND _TYPE_=1;
    KEEP CHECK PND ITERATION CONDITION;
    PND=CHECK*100;
    ITERATION=&ITER;
    OUTPUT;
    FORMAT PND 10.3;

RUN;

```

SAS TEMPLATE SSED

Appendix: SAS Procedure (Continued)

```

/*PAND*/
proc means data = input1 noprint;
    var y;
    by d;
    output out = out1 min=min_y;
run;

data out2;
    set out1;
    keep min_y;
    if d=1;
run;

DATA out3;
    SET out2;
    ARRAY MIN{&N1} MIN1-MIN&N1;
DO J=1 TO &N1;
    MIN(J)=min_y;
    END;
    drop min_y J;
RUN;

data base;
    set input1;
    if D=0;
    KEEP ID D Y ITERATION CONDITION;
run;

PROC TRANSPOSE DATA=OUT3 OUT=RES;
RUN;

DATA BASE_TTT;
    MERGE BASE RES;
    IF Y-COL1>=0 THEN CHECK=1; ELSE CHECK=0;
    RUN;

PROC MEANS DATA=BASE_TTT NOPRINT;
    CLASS CONDITION;
    VAR CHECK;
    OUTPUT OUT=BASE_PAND ;
    RUN;

data PAND; set BASE_PAND;
    IF _STAT_='MEAN' AND _TYPE_=1;
    PAND=(1-CHECK)*100;
    output;
    keep CHECK PAND ITERATION CONDITION;
    FORMAT PAND 10.3;
RUN;

```


Appendix: SAS Procedure (Continued)

```

PROC APPEND BASE=PAND_RESULT (CNTLLEV=MEMBER) DATA=PAND; /* PAND
result*/
RUN;

/*PEM*/
proc means data = input1 noprint;
    var y;
    by d;
    output out = out1 median=med_y;
run;

data out2;
    set out1;
    keep med_y;
    if d=0;
run;

DATA out3;
    SET out2;
    ARRAY med{&N1} med1-med&N1;
DO J=1 TO &N1;
    med(J)=med_y;
    END;
    drop med_y J;
RUN;

PROC TRANSPOSE DATA=OUT3 OUT=RES;
RUN;

data ttt;
    set input1;
    if D=1;
    KEEP ID D Y ITERATION CONDITION;
run;

DATA BASE_TTT;
    MERGE ttt res;
    IF Y-COL1>=0 THEN CHECK=1; ELSE CHECK=0;
    RUN;

PROC MEANS DATA=BASE_TTT NOPRINT;
    CLASS CONDITION;
    VAR CHECK;
    OUTPUT OUT=BASE_pem ;
    RUN;

```

SAS TEMPLATE SSED

Appendix: SAS Procedure (Continued)

```
data pem; set BASE_pem;
  IF _STAT_='MEAN' AND _TYPE_=1;
  pem=CHECK*100;
  ITERATION=&ITER;      output;
  keep CHECK pem ITERATION CONDITION;
  FORMAT pem 10.3;
RUN;

PROC APPEND BASE=PEM_RESULT (CNTLLEV=MEMBER) DATA=PEM; /* PEM result*/
RUN;

/*PZD*/
DATA TTT;
  SET INPUT1;
  IF D = 1;
  IF Y = 0;
RUN;

DATA TTT2;
  SET TTT;
  IF _N_ = 1;
RUN;

DATA TTT3;
  SET TTT2;
  DO I = 1 TO &N1;
    OUTPUT;
  END;
  KEEP ID;
  RENAME ID=START;
RUN;

DATA TTT4;
  SET INPUT1;
  IF D = 1;
RUN;

DATA RES;
  MERGE TTT3 TTT4;
  IF TIME >= START;
  IF Y = 0 THEN CHECK_Z = 1; ELSE CHECK_Z = 0;
  KEEP CHECK_Z;
RUN;

PROC MEANS DATA = RES NOPRINT;
  OUTPUT OUT = RES2
    MEAN(CHECK_Z) = PZD;
RUN;
```

Appendix: SAS Procedure (Continued)

```

DATA PZD;
    SET RES2;
    PZD = PZD * 100;
    KEEP PZD;
RUN;

PROC APPEND BASE=PZD_RESULT (CNTLLEV=MEMBER) DATA=PZD; /* PZD result*/
RUN;

/*PRD*/
DATA BASE;
    SET INPUT1;
    IF D = 0;
    CNT = &N1;
    IF _N_ > CNT - 3;
    KEEP Y;
    RENAME Y = BASE_Y;
RUN;

DATA TTT;
    SET INPUT1;
    IF D = 1;
RUN;

DATA TTT; SET TTT;
    CNT = &N1;
    IF _N_ > CNT - 3;
    KEEP Y;
    RENAME Y = TTT_Y;
RUN;

DATA BASE_TTT;
    MERGE BASE TTT;
RUN;

PROC MEANS DATA = BASE_TTT NOPRINT;
    OUTPUT OUT = RES (KEEP=MEAN_B MEAN_T)
        MEAN(BASE_Y) = MEAN_B MEAN(TTT_Y) = MEAN_T;
RUN;

DATA PRD;
    SET RES;
    PRD = (MEAN_B - MEAN_T) / MEAN_B * 100;
RUN;

PROC APPEND BASE=PRD_RESULT (CNTLLEV=MEMBER) DATA=PRD; /* PRD result*/
RUN;

%MEND AUTOREG_N;
%AUTOREG_N (1, 8, 10, 18, 0.5, 0.5, 0.4, 0.2, 1, 0.4, 1);
%AUTOREG_N (1, 10, 20, 30, 0.2, 0.8, 0.1, 0.3, 0.3, 0.3, 2);
%AUTOREG_N (1, 16, 16, 32, 1, 0, 0.1, 0.6, 0.3, 0, 3);
%AUTOREG_N (1, 8, 24, 32, 0.8, 0.2, 0.4, 0.0, 0.0, 0.6, 4);

```

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