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Maximum Likelihood Solution for the Linear Structural Relationship With Three Parameters Known

Androulla Michaeloudis
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A maximum likelihood solution is obtained for the simple linear structural relation model where the underlying incidental distribution and one error variance are assumed known. Expressions for the asymptotic standard errors of the maximum likelihood estimates are obtained and these are verified using a simulation study.

Key words: Maximum likelihood estimates, linear structural relation, errors-in-variables model, asymptotic standard errors, simulation.

Introduction
A biochemical assay is a procedure used to measure an unknown quantity ($\eta$) of a specified substance (analyte) present in a biological material, such as blood, obtained in the form of a test specimen. Biochemists are often faced with the problem of assessing the comparative performance of a new assay method with a well established reference assay method (method comparison study). An important aspect of this assessment is an examination of the degree of agreement between the results produced. Inaccuracy is unavoidable due to the complexities surrounding the measurement process. The so-called true value of the quantity of analyte can never be known in any absolute sense as the result of the test sample’s composition. For example, non-analyte components present in a biological material can either enhance or inhibit the response of the analyte. These lead to what is referred to as interference biases (Strike, 1981). Different models and statistical methods have been employed as well as criticized in assessing method comparison studies (Bland & Altman, 1986; Stockl, Dewitte, & Thienpont, 1998; Linnet, 1999). This article proposes a method comparison study for the linear structural relation of an errors-in-variables model which takes into account the presence of random errors in assays and in the recalibration effect, as well as interference effects in the biological test material. The model is complicated, but in simplified form is given by the simple errors-in-variables model as:

$$X = U + \delta$$
$$Y = V + \epsilon$$
$$V = \alpha + \beta U,$$

where $\alpha$ and $\beta$ are constants defining a linear structural relation between the unobserved variables $U$ and $V$. The latter are known functions of the unknown quantity of analyte of interest, that is $U = f(\eta)$ and $V = g(\eta)$, $\delta$ and $\epsilon$ are the errors associated with the reference ($X$) and new ($Y$) assay methods respectively. It is assumed that $\delta$ and $\epsilon$ are normally and independently distributed $N(0, \sigma^2_\delta)$ and $N(0, \sigma^2_\epsilon)$ respectively, and are independent of $U$. The random variable $U$ is normally distributed with mean $\mu$ and variance $\sigma^2$, that

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is $N(\mu, \sigma^2)$. Thus, $(x_i, y_i), \ldots, (x_n, y_n)$ are $n$ independent observations of a bivariate normal variable $(X, Y)$, $N(\mu, \sigma^2 + \sigma^2, \beta^2 \sigma^2 + \sigma^2, \rho)$, where

$\rho = \beta \sigma^2 \left( (\beta^2 \sigma^2 + \sigma^2) \left( \sigma^2 + \sigma^2 \right)^{-1} \right) \frac{1}{2}$.

Birch (1964) and Barnett (1967) have obtained maximum likelihood solutions to model (1) for the cases where one $(\sigma^2)$ and both error variances $(\sigma^2, \sigma^2)$ are known. Note that in both cases the likelihood function has never been provided; this is provided in this article. The strengths and weaknesses of the reference method should be well-known to the analysts from their own direct experience and from nationally organized quality control schemes (Strike, 1981): thus, the distribution of $U$ in the population under study should be known from extensive data for the reference method when this is used on the same population.

Under these conditions a maximum likelihood solution for the linear structural relation of the simple errors-in-variables model (1) with three parameters known, namely $\mu$, $\sigma^2$ and $\sigma^2$, is considered herein. The information matrix for this case will be derived and, upon inverting this, expressions for the asymptotic standard errors of the derived maximum likelihood estimates will be obtained. These derived expressions will be verified by a simulation study. The effect, if any, of the knowledge of $\mu$ and $\sigma^2$ on the estimates, in particular the estimate of the slope of the linear structural relation, will be examined and will be compared with the derived maximum likelihood solution where only $\sigma^2$ is known.

The Problem

Assuming knowledge of $\mu$, $\sigma^2$, and $\sigma^2$ the structural errors-in-variables model (1) has three unknown parameters and a set of minimal sufficient statistics of dimension five and as such the model is expected to be identifiable. For a given set of real observations $X = (X, Y)$, the likelihood function for all real $\alpha, \beta$, and $\sigma^2 \geq 0$, where the set of unknown parameters is $\Psi = (\alpha, \beta, \sigma^2)$. The likelihood function is a continuous function; it tends to zero as $|\beta|$ or $\sigma^2$ become infinite and is

Figure 1: Formulas (2), (3) and (4)

Formula 2:

$I(X, \Psi) = \frac{\text{constant}}{\sigma^2 \left( \beta^2 \sigma^2 + \sigma^2 \right) + \sigma^2 \sigma^2} \times \exp \left[ -1 \left( \frac{1}{2} \sigma^2 + \sigma^2 \right) \frac{1}{\sigma^2 + \sigma^2} \right] \times \left\{ \beta^2 \sigma^2 + \sigma^2 \right\} \frac{nS_{xx} + (\bar{Y} - \alpha - \beta \mu) \sum (X - \mu)}{nS_{xx} + (\bar{Y} - \alpha - \beta \mu)^2} \right\} \left\{ S_{yy} + (\bar{Y} - \alpha - \beta \mu)^2 \right\}$

Formula 3:

$\hat{\alpha} = \bar{Y} - \beta \left( \frac{\sigma^2 \bar{X} + \mu \sigma^2}{\sigma^2 + \sigma^2} \right)$

Formula 4:

$\hat{\beta}^3 + \left( \frac{S_{yy}}{\sigma^2} \right) \hat{\beta}^2 + \left( \frac{\sigma^2 S_{xx} - \lambda \left( S_{yy} - \sigma^2 \right)}{\sigma^2} \right) \hat{\beta} - \frac{\lambda \sigma^2 S_{yy}}{\sigma^2} = 0$
differentiable everywhere (see formula (2) in Figure 1). By partially differentiating the log-likelihood function with respect to the three unknown parameters and equating to zero, three equations are obtained which can be rearranged to give formulas (3) and (4) (also shown in Figure 1).

$$\hat{\sigma}_e^2 = S_{yy} + \frac{\hat{\beta}^2 S_{xx}}{\lambda^2} - \frac{2\hat{\beta} S_{xy}}{\lambda} - \frac{\hat{\beta}^2 \sigma_\delta^2}{\lambda}, \quad (5)$$

where $S_{xx}, S_{yy}, S_{xy}$ are the sample statistics and $\lambda = \frac{(\sigma^2 + \sigma_\delta^2)}{\sigma^2}$.

The monotonocity of the likelihood function (2), and the fact that the likelihood tends to zero as $\sigma^2_e$ tends to $\pm\infty$, implies that there is only one value for $\hat{\sigma}_e^2$ for which the likelihood function is a maximum. Therefore, the log-likelihood is maximized either when $\hat{\sigma}_e^2 > 0$ or when $\hat{\sigma}_e^2 = 0$; these cases are considered next, but the case $\hat{\sigma}_e^2 = 0$ is not a practical case in a method comparison study.

Case 1: $\hat{\sigma}_e^2 > 0$

In this case the maximum likelihood estimates of $\alpha$, $\beta$ and $\sigma_e^2$ are given by the solutions of likelihood equations (3) – (5). By substituting for $\hat{\sigma}_e^2$ in (4), the following cubic equation for $\hat{\beta}$ is obtained

$$\hat{\beta}^3 - 3\lambda b_1 \hat{\beta}^2 + \lambda^2 \left(\frac{b_1}{b_2} + 2b_1^2\right) \hat{\beta} - \lambda^2 \frac{b_1^2}{b_2} = 0, \quad (6)$$

which factorizes to

$$\left(\hat{\beta} - \frac{\lambda b_1}{1}\right)\left(\hat{\beta}^2 - 2\lambda b_1 \hat{\beta} + \lambda^2 \frac{b_1^2}{b_2}\right) = 0, \quad (7)$$

where $b_1$ and $b_2$ are the two sample regression coefficients, that is $b_1 = \frac{S_{xy}}{S_{xx}}$ and $b_2 = \frac{S_{xy}}{S_{yy}}$. The cubic equation (6) yields one real root

$$\hat{\beta} = \lambda b_1, \quad (8)$$

and two complex roots

$$\hat{\beta} = \lambda \left[ b_1 \pm \frac{b_1}{b_2} \left( r^2 - 1 \right)^{\frac{1}{2}} \right], \quad (9)$$

where $r$ is the sample correlation coefficient $(b_1 b_2)^{\frac{1}{2}}$. Substituting the real root for $\hat{\beta}$ in (5) yields the following equation

$$\hat{\sigma}_e^2 = S_{yy} - b_1^2 S_{xx} \left(1 + \frac{\lambda \sigma_\delta^2}{S_{xx}}\right). \quad (10)$$

Case 2: $\hat{\sigma}_e^2 = 0$

Placing $\hat{\sigma}_e^2 = 0$ in cubic equation (4) leads to

$$\hat{\beta} \left(\hat{\beta}^2 + \frac{S_{xy}}{\sigma_\delta^2} - \frac{\lambda S_{yy}}{\sigma_\delta^2}\right) = 0; \quad (11)$$

this implies that either $\hat{\beta} = 0$ or

$$\hat{\beta}^2 + \frac{S_{xy}}{\sigma_\delta^2} \left(\hat{\beta} - \frac{\lambda S_{yy}}{\sigma_\delta^2}\right) = 0. \quad (12)$$

The case $\hat{\beta} = 0$ is excluded because, at this point, the likelihood function is undefined. Equation (12) factorizes to yield two real roots

$$\hat{\beta} = \frac{1}{2\sigma_\delta^2} \left[-S_{xy} \pm \left(S_{xy}^2 + 4\lambda^2 \sigma_\delta^2 \frac{S_{yy}}{S_{xx}}\right)^{\frac{1}{2}} \right], \quad (13)$$

where the one with same sign as $S_{xy}$ is the maximum likelihood estimator of $\beta$. 

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Maximum Likelihood Solution

The complete maximum likelihood solution of the linear structural errors-in-variables model for \( \mu, \sigma^2 \), and \( \sigma^2_\delta \) known is as follows. If

1. \[
S_{yy} > \frac{S_{yy}^2}{S_{xx}} \left\{ 1 + \frac{\sigma^2_\delta (\sigma^2 + \sigma^2)}{\sigma^2 S_{xx}} \right\}
\]
then

\[
\hat{\beta} = \left( \frac{\sigma^2 + \sigma^2_\delta}{\sigma^2 S_{xx}} \right) S_{xy},
\]

\[
\hat{\alpha} = \bar{y} - \hat{\beta} \left( \frac{\sigma^2 \bar{X} + \mu \sigma^2_\delta}{\sigma^2 + \sigma^2_\delta} \right),
\]

and

\[
\hat{\sigma}^2 = S_{yy} - \frac{S_{yy}^2}{S_{xx}} \left\{ 1 + \frac{\sigma^2_\delta (\sigma^2 + \sigma^2_\delta)}{\sigma^2 S_{xx}} \right\};
\]

otherwise

2. \[
\hat{\beta} = \frac{1}{2 \sigma^2_\delta} \left[ (S_{yy}) \pm \left\{ S_{xy}^2 + \frac{4 \sigma^2_\delta (\sigma^2 + \sigma^2_\delta) S_{yy}}{\sigma^2} \right\} \right],
\]

\[
\hat{\alpha} = \bar{y} - \hat{\beta} \left( \frac{\sigma^2 \bar{X} + \mu \sigma^2_\delta}{\sigma^2 + \sigma^2_\delta} \right),
\]

and

\[
\hat{\sigma}^2 = 0.
\]

Because the sample statistics \( S_{xy}, S_{xx}, \) and \( S_{yy} \) converge in probability to \( \beta \sigma^2, (\sigma^2 + \sigma^2_\delta) \) and \( (\beta^2 \sigma^2 + \sigma^2_\delta) \) respectively, the derived maximum likelihood estimates (14) are consistent estimates of \( \alpha, \beta \) and \( \sigma^2 \). If \( \sigma^2_\delta \) is set equal to zero \( (\sigma^2_\delta = 0) \) so that the errors-in-variables model (1) reduces to the simple linear regression model, the derived results are in agreement with the established results applicable to the latter model (that is, \( \hat{\alpha}_{OLS} \) and \( \hat{\beta}_{OLS} \)).

It is also noted that further knowledge of the specific values of \( \mu \) and \( \sigma^2 \) are relevant to the estimation of the scale parameter \( \alpha \). This is in contrast to all other solutions obtained where \( \mu \) and \( \sigma^2 \) were unknown, that is, in all previous solutions with \( \mu \) and \( \sigma^2 \) unknown, \( \hat{\alpha} = f(\hat{\beta}, \mu) \) (Birch, 1964 & Barnett, 1967), while with \( \mu \) and \( \sigma^2 \) known, \( \hat{\alpha} = f(\hat{\beta}, \mu, \sigma^2, \sigma^2_\delta) \) where \( f \) denotes a function.

It is worth noting that the derived solution can lead to the maximum likelihood solution when only \( \sigma^2_\delta \) is known, and when \( \mu \) and \( \sigma^2 \) are substituted by their corresponding estimates. This establishes the compatibility of the derived solution with the maximum likelihood solution where only one error variance is known.

Note that condition (1) of (14) forces the estimate for \( \hat{\sigma}^2 \) to be positive, that is, the first expression for \( \hat{\beta} \) applies if the likelihood does not reach its maximum in a boundary point owing to a positivity constraint of \( \sigma^2_\delta \). Because the probability of this to be true tends to one as the number of observations increases, it follows that \( \hat{\beta} \) is asymptotically equivalent to

\[
\hat{\beta}_\Delta = \left( \frac{\sigma^2 + \sigma^2_\delta}{\sigma^2_\delta} \right) S_{xy}.
\]

Hence, the maximum likelihood estimates of \( \beta \) and \( \hat{\beta}_\Delta \) have the same limiting distribution and their asymptotic standard errors are identical.

Asymptotic Variances

Expressions for the asymptotic variances of the maximum likelihood estimates of \( \psi = (\alpha, \beta, \sigma^2) \) can be obtained directly from the inverse information matrix, \( \left[ I(\psi) \right]^{-1} \). The information matrix is derived by calculating the
expected values of the second order derivatives of the log-likelihood function.

\[
I(\psi) = \begin{pmatrix}
\sigma^2 + \sigma^2_{\delta} & \mu (\sigma^2 + \sigma^2_{\delta}) & 0 \\
n \frac{T}{2} & \mu (\sigma^2 + \sigma^2_{\delta}) & 2 \beta \sigma^2 \sigma^2_{\delta} (\sigma^2 + \sigma^2_{\delta}) \\
0 & \frac{\beta \sigma^2 \sigma^2_{\delta} (\sigma^2 + \sigma^2_{\delta})}{T} & 2T \\
\end{pmatrix}
\]

where

\[
T = \sigma^2 (\beta^2 \sigma^2_{\delta} + \sigma^2_{e}) + \sigma^2_{\delta} \sigma^2_{e}
\]

and

\[
M = \frac{\sigma^4}{T^2} \left[ \sigma^2 (\beta^2 \sigma^2_{\delta} + \sigma^2_{e})^2 (\sigma^2 + 2 \sigma^2_{\delta}) + \sigma^4 \sigma^2_{e} (\sigma^2 + 2 \beta^2 \sigma^2_{\delta}) \right].
\]

The inverse of this \((3 \times 3)\) asymptotic covariance matrix of the maximum likelihood estimates \(\hat{\alpha}, \hat{\beta}\) and \(\hat{\sigma}_e^2\) is:

\[
[I(\psi)]^{-1} = \begin{pmatrix}
\mu^2 + \frac{\sigma^4}{\sigma^2 + \sigma^2_{\delta}} & -\mu & \frac{2 \mu \sigma^2 \sigma^2_{\delta}}{(\sigma^2 + \sigma^2_{\delta})} \\
\frac{T}{n \sigma^4} & \frac{\beta \sigma^2 \sigma^2_{\delta} (\sigma^2 + \sigma^2_{\delta})}{T} & 2 \beta \sigma^2 \sigma^2_{\delta} \sigma^2_{\delta} (\sigma^2 + \sigma^2_{\delta}) \\
\frac{2 \beta \mu \sigma^2 \sigma^2_{\delta}}{\sigma^2 + \sigma^2_{\delta}} & \frac{2 \beta \sigma^2 \sigma^2_{\delta}}{\sigma^2 + \sigma^2_{\delta}} & \frac{2MT}{(\sigma^2 + \sigma^2_{\delta})^2} \\
\end{pmatrix}
\]

(16)

From (17), the asymptotic variances of \(\hat{\beta}, \hat{\alpha}\) and \(\hat{\sigma}_e^2\) are obtained as:

\[
\text{var}(\hat{\beta}) = \frac{1}{n \sigma^4} \left\{ \sigma^2 (\beta^2 \sigma^2_{\delta} + \sigma^2_{e}) + \sigma^2_{\delta} \sigma^2_{e} \right\},
\]

(18)

\[
\text{var}(\hat{\alpha}) = \left\{ \mu^2 + \frac{\sigma^4}{(\sigma^2 + \sigma^2_{\delta})} \right\} \text{var}(\hat{\beta}),
\]

(19)

\[
\text{var}(\hat{\sigma}_e^2) = \frac{2MT}{(\sigma^2 + \sigma^2_{\delta})^2} \text{var}(\hat{\beta}).
\]

(20)

A comparison of the above expressions (18 and 19) with the asymptotic variances of \(\hat{\beta}\) and \(\hat{\alpha}\), where only \(\sigma^2_{\delta}\) is known, shows that the further knowledge of \(\sigma^2\) leads to smaller variances for the maximum likelihood estimates.

Methodology

Simulation Study

A simulation study was carried out using R statistical software to investigate the effect of sample size on the accuracy of the derived maximum likelihood estimates of \(\alpha, \beta\) and \(\sigma^2_{e}\) (14) and their corresponding asymptotic variances (18 – 20). Taking into account examples of data used for method comparison studies and the fact that, depending on the type of analyte considered, the sample size of a method comparison study will vary from a minimum of 17 to more than 500 (Bland & Altman, 1986; Stockl, Dewitte & Thienpont, 1998; Linnet, 1999), this simulation study considered sample sizes ranging from a minimum of 20 to a maximum of 1,000. This was also done in order to assess the effect of a sample size on the accuracy of the derived estimates. Ten thousand simulations have been considered in this study and particular attention was given to the estimates of \(\alpha\) and \(\beta\) because the values of these can allow for the estimation of possible constant and proportional interference biases in a biological test material. In all cases considered an interference bias of 10% was allowed so that \(\alpha = 0.10\) and \(\beta = 1.10\).

Because there is a tendency for practitioners to use methods with which they are more familiar, such as the ordinary least square (OLS) estimation for the simple linear
regression model (Westgard & Hunt, 1973), the simulation study also compared the OLS estimates with the derived MLEs (14). The accuracy of these estimates is based on the mean squared error (MSE) criterion; some of the obtained results are presented in Tables 1 – 3 below.

Results
The results are in agreement with what was expected, namely:

1. Increasing the sample size leads to a decrease in the bias of the maximum likelihood estimates and - as expected in such cases - the mean squared error reduces to the variance of the estimate.

2. The mean squared errors of the maximum likelihood estimates are less than the mean squared errors of the least squares estimates irrespectively of the sample size. It is clear that the OLS are inappropriate to use in a method comparison study where errors are assumed in both assays.

3. The accuracy of the maximum likelihood estimates particularly for \( \hat{\beta} \) and \( \hat{\alpha} \) can be achieved with samples as small as 20.

4. The expressions for the asymptotic variances have been verified for samples greater than 100 with biases less than 0.0001.

Conclusion
Under the assumption that the parameters specifying the underlying incidental distribution \( \left( \mu, \sigma^2 \right) \), the maximum likelihood estimates of the unknown parameters \( \alpha, \beta \) and \( \sigma^2 \) are obtained: these are consistent, asymptotically normal and efficient. The asymptotic variances of the estimates were obtained by the inversion of the information matrix. It has been shown that the asymptotically equivalent estimator of the slope is a function of \( \sigma^2 \) and \( \sigma^2_\delta \) thus utilizing the known information about the variances. The derived solution is in agreement with the case where only \( \sigma^2_\delta \) is known. In the latter case the asymptotically equivalent estimator of the slope is a function of the known variance \( \sigma^2_\delta \) (Ketellapper, 1983). A simulation study verified the accuracy of the maximum likelihood estimates with samples as small as 20. This study also verified the accuracy of the asymptotic variances with biases less than 0.0001.

Acknowledgements
The author would like to thank her colleague David Jarrett for his valuable comments on this article and Professor Bob Gilchrist for suggesting the use of the software R for the simulation work included in this study.

References
Table 1: MLEs and OLS Estimates and Their Corresponding Mean Squared Errors; Simulated Variances \(\{\cdot\}\) and Derived Asymptotic Variances of the MLEs \([\cdot]\) \((\mu = 3, \sigma = 0.45, \sigma_\delta = 0.4, \sigma_\epsilon = 0.6)\)

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## MLE FOR LINEAR STRUCTURAL RELATIONSHIP: THREE KNOWN PARAMETERS

Table 2: MLEs and OLS Estimates and their Corresponding Mean Squared Errors; Simulated Variances \( \{.\} \) and Derived Asymptotic Variances of the MLEs \([.]\) \((\mu = 3, \sigma = 0.35, \sigma_\varepsilon = 0.4, \sigma_\varepsilon = 0.6)\)

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<th>MLE</th>
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