Stochastic Regression with Errors in Both Variables

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Abstract

Linear structural models are linear relationships between two stochastic (random) variates in which both of the variates are subject to measurement errors. Structural models are common in experimental work but are typically fit using least squares. In this paper maximum likelihood estimators for linear structural models are presented and contrasted with the corresponding least squares estimators. Practical suggestions are made for application of the proposed techniques.

Key words: Errors in Variables, Least Squares, Maximum Likelihood

Introduction

Analysis of experimental results frequently requires the fitting of straight lines to data in which both the response and the predictor variables are measured with error. While least squares is most commonly used to estimate the slope and intercept parameters, such estimates are known to be biased when the predictor variable is measured with error. In this article we discuss maximum likelihood estimation of slope and intercept parameters of linear models which are subject to measurement errors.

In order to focus on the complications which arise when linear regression models are subject to measurement errors consider the scattergram shown in Figure 1. Displayed in this graph are 96 100-minute radiation counts from the Carbon-14 decay of a 650 year-old sample of charcoal. The measurements on the vertical and horizontal axes represent counts from two channels of the same decay counter; however, Channel B obtains decay counts over a narrower energy band of radiation than does Channel A. The scatterplot suggests that the two sets of measurements are linearly related and one is tempted to use least squares to obtain a straight line fit to the data.

[Insert Figure 1]

Least squares estimators are usually justified either by reference to the Gauss-Markov theorem or by their derivation using maximum likelihood under normality assumptions on the error term of the model (e.g., Draper and Smith (1981, Chapter 2), Gunst and Mason (1980, Chapter 6)). In either case the predictor-variable values must be assumed to be known constants which are measured without error or one must be willing to make inferences conditional on the observed predictor-variable values (which reduces this latter situation to the former one of known, error-free constants).

Suppose now that two variates (Y,X) are linearly related as

$$Y_i = \alpha + \beta X_i , \qquad i = 1, 2, \ldots, n \tag{1}$$

but that each of these variates is only measureable with error; i.e., (y,x) is observable, where

$$y_i = Y_i + v_i \quad \text{and} \quad x_i = X_i + u_i , \qquad i = 1, 2, \ldots, n. \tag{2}$$

Substituting (2) into (1) yields the observable regression

$$y_i = \alpha + \beta x_i + e_i, \qquad e_i = v_i - \beta u_i \ . \tag{3}$$

Although equation (3) appears to be that of the usual regression model, neither the Gauss-Markov theorem not traditional maximum likelihood derivations constitute theoretically correct justifications for using least squares. These arguments are not valid because the predictor variable x_i in (3) is stochastic and is correlated with the error term e_i (both x_i and e_i contain u_i). These statements suggest that the least squares estimator no longer enjoys the properties of unbiasedness and minimum variance (among unbiased estimators) which accompany its use when the predictor variable values are error-free constants. We demonstrate below that these properties are lost when both variates are measured with error.

Before discussing the estimation of the model parameters in (1), a further specification of the nature of the true, unobservable predictor variable X must be made. In this article we assume that X is stochastic. This assumption is reasonable for the data in Figure 1 since the 100-minute Carbon-14 decay counts (X_i) for a single sample, apart from any measurement error due to the counting equipment, fluctuate around some constant mean decay rate μ_X.

These data can be contrasted with the average counts per minute of 32 different samples displayed in Figure 2. A straight line fit to these points might be made in order to calibrate one of the channels relative to the other, with the samples intentionally chosen to cover the useful range of the counter. In this case one might consider the unobservable X_i to be the (constant) mean decay rates μ_i for each sample. This latter type of model was discussed by Mandel (1984).

When the unobservable X_i are assumed to be random variables as in Figure 1 the model defined by (1) and (2) is referred to as a "linear structural model." When the X_i are considered to be unknown constants as in Figure 2, the corresponding models are called "linear functional models." In the discussions below we concentrate attention on linear structural models, with reference to similarities between functional and structural models when appropriate. More detailed discussions on functional and structural models can be found in Kendall and Stuart (1977, Chapter 29), Madansky (1959), and Moran (1971).

[Insert Figure 2]

Linear Structural Models

We now add to the model defined by equations (1) and (2) the assumption that X is distributed independently of (u,v) and that

$$X \sim N(\mu_X, \sigma_X^2) \text{ and } \begin{pmatrix} v \\ u \end{pmatrix} \sim N\left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \sigma_v^2 & \rho\sigma_u\sigma_v \\ \rho\sigma_u\sigma_v & \sigma_u^2 \end{pmatrix} \right\}. \quad (4)$$

If the measurement errors are themselves independently distributed then $\rho = 0$ in (4). With these assumptions the joint distribution of the observable variates x and y is

$$\begin{pmatrix} y \\ x \end{pmatrix} \sim N\left\{ \begin{pmatrix} \alpha - \beta\mu_X \\ \mu_X \end{pmatrix}, \begin{pmatrix} \beta^2\sigma_X^2 + \sigma_v^2 & \beta\sigma_X^2 + \theta\sigma_u^2 \\ \beta\sigma_X^2 + \theta\sigma_u^2 & \sigma_X^2 + \sigma_u^2 \end{pmatrix} \right\}, \quad (5)$$

where $\theta = \rho\lambda^{\frac{1}{2}}$ and $\lambda = \sigma_v^2/\sigma_u^2$ is the ratio of the error variances. The maximum likelihood estimating equations for the parameters in this joint distribution can be obtained by equating sample moments to the respective parameters:

$$\bar{y} = \tilde{\alpha} + \tilde{\beta}\tilde{\mu}_X \qquad s_{yy} = \tilde{\beta}^2\tilde{\sigma}_X^2 + \tilde{\sigma}_v^2 \qquad s_{xy} = \tilde{\beta}\tilde{\sigma}_X^2 + \theta\tilde{\sigma}_u^2$$
$$\bar{x} = \tilde{\mu}_X \qquad s_{xx} = \tilde{\sigma}_X^2 + \tilde{\sigma}_u^2 \tag{6}$$

where $\bar{y} = n^{-1}\Sigma y_i$, $\bar{x} = n^{-1}\Sigma x_i$, $s_{yy} = n^{-1}\Sigma(y_i - \bar{y})^2$, $s_{xx} = n^{-1}\Sigma(x_i - \bar{x})^2$, and $s_{xy} = n^{-1}\Sigma(x_i - \bar{x})(y_i - \bar{y})$.

Immediately a problem arises in attempting to solve for the maximum likelihood estimators: there are only five estimating equations for the seven model parameters. Even if the correlation between the measurement errors is assumed to be zero there are six parameters to be estimated from the five equations. This difficulty arises because of the additivity of independent normal distributions. For example, the observable predictor variable x is the sum of two independent normal variates. Its mean and variance are, respectively, μ_X and $\sigma_X^2 + \sigma_u^2$. Thus the sample mean $\bar{x}$ can be used to estimate μ_X and the sample variance s_{xx} can be used to estimate the sum of $\sigma_X^2 + \sigma_u^2$ but the individual variance components σ_X^2 and σ_u^2 cannot be estimated using only the marginal distribution of x.[1]

Since α, β, μ_X, and σ_X^2 are the parameters of primary interest in fitting the structural model, one is required to know some information about the error variances and the correlation between the errors in order to obtain appropriate estimators of the remaining model parameters. We focus attention in this discussion on the assumption that the ratio of the error variances $\lambda = \sigma_v^2/\sigma_u^2$ and the correlation ρ are known.

Knowledge of the ratio of the error variances does not necessarily require explicit knowledge of either of the individual error variances. For the Carbon-14 dating examples of the previous section it is reasonable to assume that the error variances are equal ($\lambda = 1$) since the counts are from two channels of the same counter. It is also reasonable to assume that the measurement errors made by the two counters are not correlated. Mandel (1984) presents an example on interlaboratory testing in which a functional model is assumed and the ratio of error variances and the correlation are known. These are but two examples demonstrating the applicability of assuming known values for the ratio of the error variances and the error correlation.

With the assumption that λ and ρ are known the solution to the likelihood equations (6) for $\tilde{\alpha}$ and $\tilde{\beta}$ are

$$\tilde{\alpha} = \bar{y} - \tilde{\beta}\bar{x}$$

and (7)

$$\tilde{\beta} = S \pm \{S^2 + T\}^{\frac{1}{2}} ,$$

where

$$S = (s_{yy} - \lambda s_{xx})/2U \qquad T = (\lambda s_{xy} - \theta s_{yy})/U$$

$$U = s_{xy} - \theta s_{xx} \qquad \theta = \rho\lambda^{\frac{1}{2}}$$

and the sign (+ or -) in the expression for $\tilde{\beta}$ is the same as that of U. The estimators of the remaining model parameters are

$$\tilde{\sigma}_u^2 = (s_{yy} - 2\tilde{\beta}s_{xy} + \tilde{\beta}^2 s_{xx})/(\tilde{\beta}^2 + \lambda - 2\tilde{\beta}\theta) \tag{8}$$

$$\tilde{\sigma}_X^2 = s_{xx} - \tilde{\sigma}_u^2 \qquad \tilde{\sigma}_v^2 = \lambda\tilde{\sigma}_u^2 \qquad \text{and } \tilde{\mu}_X = \bar{x}\ .$$

Estimates of the variance components obtained from equations (8) are non-negative, a property not necessarily guaranteed if one makes an alternative assumption that one or both of the error variances are known instead of their ratio. Frequently a degrees of freedom adjustment is made in the estimation of the variance components by dividing the sample variances and covariances by n-2 rather than n.

The estimators of α and β given in equations (7) are the same for functional and structural models (e.g., Patefield (1978))[2]. Appendix A contains formulae for approximate asymptotic variances for the maximum likelihood estimators $\tilde{\alpha}$ and $\tilde{\beta}$. These asymptotic variance formulae differ slightly for functional and structural models; the differences are pointed out in the appendix.

Least Squares Estimators

The usual least squares estimators of the intercept and slope parameters are $\hat{\alpha} = \bar{y} - \hat{\beta}\bar{x}$ and $\hat{\beta} = s_{xy}/s_{xx}$. While the maximum likelihood estimators $\tilde{\alpha}$ and $\tilde{\beta}$ are consistent (i.e., $\tilde{\alpha} \to \alpha$ and $\tilde{\beta} \to \beta$ as $n \to \infty$), the least squares estimators are not consistent for the parameters in model (1) when the predictor variable is subject to measurement error. The least squares slope estimator tends to underestimate the true slope, thereby biasing the intercept estimator as well. Appendix B contains asymptotic limits for the least squares estimators $\hat{\alpha}$ and $\hat{\beta}$ as well as approximate asymptotic variance formulae.

Reilman, et al. (1985) compare the large-sample performance of the least squares estimator and the maximum likelihood estimator by deriving an expression for $R = \mathrm{var}(\tilde{\beta})/\mathrm{mse}(\hat{\beta})$.[3] They show that $R > 1$ when

$$\psi < (1 + \gamma)(2 + \gamma)/(n - 2 - \gamma) , \tag{9}$$

where $\psi = (\phi - \rho)^2/(1 - \rho^2)$, $\phi = \beta\lambda^{-\frac{1}{2}}$ is the "sensitivity" measure defined by Mandel and Stiehler (1954), and $\gamma = \sigma_u^2/\sigma_X^2$ is the "noise-to-signal ratio" of the observable predictor variable x. Thus the asymptotic variance of the maximum likelihood estimator exceeds the mean squared error of the least squares estimator when inequality (9) is satisfied. Denote the right side of (9) by c(n). Then least squares is preferable to the maximum likelihood estimator when

$$\rho - \{(1 - \rho^2)c(n)\}^{\frac{1}{2}} < \phi < \rho + \{(1 - \rho^2)c(n)\}^{\frac{1}{2}} . \tag{9'}$$

Note that when $\rho = 0$, inequalities (9) and (9') quantify Mandel's (1984) condition $|\phi| \ll 1$ for the appropriateness of least squares estimation when errors occur in both y and x: $\phi^2 < c(n)$. Note too from inequality (9) when $\rho = 0$ that $\phi^2 < 2/(n - 2)$ is a sufficient condition for least squares to have a smaller mean squared error than the maximum likelihood estimator for all values of the noise-to-signal ratio γ. This is the same condition cited by Anderson (1976) for the distribution of the least squares estimator to be more concentrated about β than that of the maximum likelihood estimator.

Radiocarbon Dating Example

The sample statistics for the n = 96 100-minute Carbon-14 counts plotted in Figure 1 are:

$\bar{y} = 3111.95 \qquad s_{yy} = 2525.65 \qquad s_{xy} = 2103.02$

$\bar{x} = 2326.47 \qquad s_{xx} = 2467.94 .$

The least squares estimates are $\hat{\alpha} = 1129.47$ and $\hat{\beta} = 0.8521$ while the maximum likelihood estimates with $\lambda = 1$ and $\rho = 0$ are $\tilde{\alpha} = 753.34$ and $\tilde{\beta} = 1.0138$. The straight line fits corresponding to these two sets of estimates are shown in Figure 3. Both fits appear to represent the observed scatter of points well, although there are obvious differences at the extremes of the scatterplot.

[Insert Figure 3]

Geometrically, the least squares fit minimizes the sum of the squared residuals, $\Sigma(y_i - \hat{y}_i)^2$, measured in the vertical direction. The ratio of the sum of the squared residuals for the maximum likelihood fit to that for the least squares fit is 1.09. Since $\lambda = 1$, the maximum likelihood estimator minimizes the sum of the squared residuals measured perpendicular to the fitted line (e.g., Hawkins (1973), Malinvaud (1970)). The ratio of the sum of the squared perpendicular residuals for the maximum likelihood estimator to that of the least squares estimator is 0.93. Since both of these ratios area close to 1 for this data set, the two fits again appear to be about equivalent.

A convenient way to assess differences between maximum likelihood estimates and least squares estimates, especially when there is some uncertainty about the correct value of the variance ratio λ, is to calculate estimates of the intercept and slope parameters for a range of values of λ and/or ρ. When $\rho = 0$, the two extremes are least squares ($\lambda = \infty$) and "reverse least squares" ($\lambda = 0$). The latter estimator is obtained by regressing x on y and solving the resulting least squares fit for y, yielding $\alpha' = \bar{y} - \beta'\bar{x}$ and $\beta' = s_{yy}/s_{xy}$.

Table 1 displays estimates of the intercept and slope parameters for a range of values of λ, assuming $\rho = 0$. The estimated standard errors are obtained by taking the square roots of the variance formulae in Appendices A and B after inserting the parameter estimates from each fit into the respective equations. While the estimates and their standard errors clearly change as λ is varied, the estimates do not appear to be drastically different for this data set. In such circumstances one might elect to use least squares unless the differences in the predicted responses for extreme values of predictor variable are judged to be substantial from a practical viewpoint.

[Insert Table 1]

Another assessment of the choice between least squares and maximum likelihood estimates can be made by estimating the quantities in inequality (9). From the summary information in Table 1 corresponding to $\lambda = 1$, $\tilde{\phi}^2 = \tilde{\beta}^2 = 1.028$ and $c(n) = .0278$. This comparison suggests that the least squares estimator is inappropriate for these data. While appearing to be in conflict with the previous conclusions, this recommendation is based on a comparison of the theoretical properties of the two slope estimators while the discussion of the previous two paragraphs focused on practical differences in the predicted responses and parameter estimates.

A final comparison between the two fits is made in Figure 4. In this figure 356 100-minute counts from several samples are combined. Those samples combined in Figure 4 correspond to the samples in the upper right corner of Figure 2, samples which have similar radiocarbon decay activity. The two fits are superimposed on the scatterplot and while both appear to lie below the middle of the swarm of points, the maximum likelihood fit appears to be somewhat closer to the center than the least squares fit. Indeed, the ratio of the sum of squared residuals for the two fits indicates that the maximum likelihood fit is better in both the vertical (ratio = 0.84) and the perpendicular (ratio = 0.72) directions.

[Insert Figure 4]

The foregoing discussions demonstrate the importance of carefully evaluating several measures of the adequacy of least squares and maximum likelihood fits when errors occur in both variables. Generally, least squares will provide a visually acceptable fit to the data from which the model estimates are obtained, in this case to the data for Sample #1277. Note, however, that the maximum likelihood estimator not only provides a visually acceptable fit to the estimation data but it also provides a better fit than least squares to the enlarged prediction data set. This empirical evidence of a superior fit coupled with the evaluation of inequality (9) leads one to prefer the maximum likelihood fit for this data set.

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Footnotes

[1]Riersol (1950) showed that no consistent estimators of the model parameters exist under the normality assumptions (4) unless one or more of the model parameters is known. Exceptions to this general result occur if (a) the true predictor variable X has a nonnormal distribution, (b) replicated observations are available, or (c) one or more additional "instrumental variables" is available. It is beyond the scope of this paper to discuss these alternatives but the interested reader is referred to Kendall and Stuart (1977, Chapter 29) for a survey of some of the more important alternatives.

[2]Estimators for some of the other model parameters differ from those shown in equations (8). For example, one does not estimate μ_X and σ_X^2 in the functional model but one must estimate the n unknown constants X_i. The estimator (7) is also the solution to equations (10a) and (10b) of Mandel (1984).

[3]The asymptotic mean squared error $mse(\hat{\beta})$ is compared to the asymptotic variance $var(\tilde{\beta})$ because the estimator $\tilde{\beta}$ is consistent; therefore, asymptotically $mse(\tilde{\beta}) = var(\tilde{\beta})$.

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Appendix A: Maximum Likelihood Large Sample Properties

The maximum likelihood estimators in equations (7) and (8) are consistent for their respective parameters; e.g., $\tilde{\alpha} \to \alpha$ and $\tilde{\beta} \to \beta$ as $n \to \infty$. Approximate asymptotic variances for the estimators of α and β are given in Reilman, et al. (1985):

$$\mathrm{var}(\tilde{\alpha}) = n^{-1}\sigma_u^2(\beta^2 + \lambda - 2\beta\theta) + \mu_X^2 \mathrm{var}(\tilde{\beta}) \tag{A.1}$$

and

$$\mathrm{var}(\tilde{\beta}) = n^{-1}\gamma\{(\beta - \theta)^2 + (1 + \gamma)(\lambda - \theta^2)\} , \tag{A.2}$$

where $\gamma = \sigma_u^2/\sigma_X^2$ is the "noise-to-signal ratio" for the observable predictor variable x. Lakshminarayanan and Gunst (1984) and Reilman, et. al. (1985) report on simulation studies which investigate the adequacy of the asymptotic variance formula (A.2) for the slope parameter. These simulations indicate that relatively large sample sizes (say, $n = 200$) are usually needed before the asymptotic variance formula is an adequate indicator of the variation of the maximum likelihood estimator over a wide range of model parameters. However, if the models of interest have relatively small noise-to-signal ratios (say, $\gamma \le .1$) and the scaled slope (sensitivity) parameter $\phi = \beta\lambda^{-\frac{1}{2}}$ is not too small (say, $|\phi| > 1$), samples of size $n = 50$ generally result in ratios of sample mean squared errors to the variance formula (A.2) which are less than 2.

Asymptotic variance formulae for $\tilde{\alpha}$ and $\tilde{\beta}$ for functional models (e.g., Patefield (1978)) are very similar to those shown in equations (A.1) and (A.2). The main differences are that μ_X and σ_X^2 are replaced by, respectively,

$$\nu_X = \lim_{n\to\infty} n^{-1}\Sigma X_i \quad \text{and} \quad \tau_X^2 = \lim_{n\to\infty} n^{-1}\Sigma(X_i - \bar{X})^2 .$$

Appendix B: Least Squares Large Sample Properties

The least squares estimators $\hat{\alpha}$ and $\hat{\beta}$ converge to the following limits when $\rho = 0$ and the predictor variable is subject to measurement error:

$$\hat{\alpha} \to \alpha + \beta\gamma(1 + \gamma)^{-1}\mu_X \quad \text{and} \quad \hat{\beta} \to \beta(1 + \gamma)^{-1}.$$

The usual estimators of $\mathrm{var}(\hat{\alpha})$ and $\mathrm{var}(\hat{\beta})$ are not valid when the predictor variable is subject to measurement error. The variance of $\hat{\alpha}$ is given by equation (A.1) with $\mathrm{var}(\tilde{\beta})$ replaced by $\mathrm{var}(\hat{\beta})$. An asymptotic expression for the latter variance can be obtained from the mean squared error formula of Reilman, et. al. (1985) as

$$\begin{aligned} \mathrm{var}(\hat{\beta}) &= n^{-1}\gamma(1 + \gamma)^{-2}\{(\beta - \theta)^2 + (1 + \gamma)(\lambda - \theta^2)\} \\ &= (1 + \gamma)^{-2}\ \mathrm{var}(\tilde{\beta})\ . \end{aligned} \tag{B.1}$$

The corresponding expression for the functional model is derivable from the results of Halperin and Gurian (1971) and Richardson and Wu (1970). With ν_X and τ_X^2 replacing μ_X and σ_X^2, the only change in (B.1) for functional model estimators is the insertion of $-2(\beta - \theta)^2\gamma^2(1 + \gamma)^{-4}$ within the braces $\{\cdot\}$. The asymptotic mean squared error of the least squares slope estimator is $\mathrm{var}(\hat{\beta}) + (\beta - \theta)^2\gamma^2(1 + \gamma)^{-2}$.

Table Title

Table 1. Maximum Likelihood Fits to Carbon-14 Data, Sample #1277.

Figure Titles

TABLE 1. Maximum Likelihood Fits to Carbon-14 Data, Sample #1277.

Estimator	Intercept	Std. Error	Slope	Std. Error
Least Squares	1129.47	130.85	.8521	.0562
$\lambda = \infty$				
Max. Likelihood				
$\lambda = 10$	1073.08	133.17	.8764	.0572
$\lambda = 8$	1059.77	134.04	.8821	.0576
$\lambda = 6$	1038.29	135.44	.8913	.0582
$\lambda = 4$	997.85	138.08	.9087	.0593
$\lambda = 2$	895.14	144.78	.9529	.0622
$\lambda = 1$	753.34	154.04	1.0138	.0662
$\lambda = 0.8$	703.93	157.27	1.0351	.0676
$\lambda = 0.6$	641.51	161.35	1.0619	.0693
$\lambda = 0.4$	561.23	166.59	1.0964	.0716
$\lambda = 0.2$	456.35	173.44	1.1415	.0745
Reverse L.S.				
$\lambda = 0$	317.95	182.48	1.2010	.0784

<u>Estimates for $\lambda = 1$</u>

$\tilde{\alpha} = 753.34$ $\quad\tilde{\beta} = 1.0138$ $\quad\tilde{\sigma}_u^2 = \tilde{\sigma}_v^2 = 393.57$ $\quad\tilde{\sigma}_X^2 = 2074.36$