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**The Estimation of Parameters in Nonlinear,
Implicit Measurement Error Models with
Experiment-wide Measurements**

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Summary

Measurement error modeling is a statistical approach to the estimation of unknown model parameters which takes into account the measurement errors in all of the data. Approaches which ignore the measurement errors in so-called independent variables may yield inferior estimates of unknown model parameters. At the same time, experiment-wide variables (such as physical constants) are often treated as known without error, when in fact they were produced from prior experiments. Realistic assessments of the associated uncertainties in the experiment-wide variables can be utilized to improve the estimation of unknown model parameters.

A maximum likelihood approach to incorporate measurements of experiment-wide variables and their associated uncertainties is presented here. An iterative algorithm is presented which yields estimates of unknown model parameters and their estimated covariance matrix. Further, the algorithm can be used to assess the sensitivity of the estimates and their estimated covariance matrix to the given experiment-wide variables and their associated uncertainties.

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Introduction

In parameter estimation problems associated with the analysis of experimental data, measurements of experiment-wide variables are often available. These experiment-wide variables, such as atmospheric conditions or other "known" physical constants, which enter the models, are typically treated as if they are known without error. Ignoring the measurement error in the experiment-wide variables has varying impact on the estimates of unknown parameters and the estimates of their uncertainties depending on the relative measurement error variances for those variables. This report presents a method to take account of these measurement errors in the context of fitting nonlinear, implicit models.

The analysis of experimental data using measurement error modeling was discussed by Deuver et. al. (1987). A critical issue is the distinction between the theoretical or "true" value of a variable and the measured value of that variable. This obvious distinction is what separates a sound statistical analysis from an *ad hoc* data analysis; is an appropriate statistical error model superimposed on the underlying physical model? A sound statistical analysis takes into account the errors in all measurements in an appropriately weighted fashion.

In the following sections, the general functional model is described, the maximum likelihood estimation algorithm is presented, and examples are discussed.

The Measurement Error Model

At the foundation of measurement error modeling is a physical/theoretical model which gives the relation between the fixed, true values of the measured variables, variables which are known without error, and the unknown parameters. In this report, the model is

$$\mathbf{g}(\mathbf{z}_i, \mathbf{w}, \boldsymbol{\beta}; \mathbf{x}_i) = \mathbf{0} \quad \text{for } i = 1, \dots, N. \quad (1)$$

The vector-valued function $\mathbf{g}$ has dimension n_g , while vectors $\mathbf{z}_i$, $\mathbf{w}$, $\boldsymbol{\beta}$, and $\mathbf{x}_i$ have dimensions n_z , n_w , n_β , and n_x , respectively, with $n_z \geq n_g$. The available measured data are

$$\mathbf{W} = \mathbf{w} + \boldsymbol{\eta} \quad \text{and} \quad \mathbf{Z}_i = \mathbf{z}_i + \boldsymbol{\varepsilon}_i, \quad i = 1, \dots, N, \quad (2)$$

where the measurement error vectors $\boldsymbol{\eta}$ and $\{\boldsymbol{\varepsilon}_i; i = 1, \dots, N\}$ are assumed pairwise independent and normally distributed with zero means and known covariance matrices Σ_w and Σ_z , respectively. The true values, $\mathbf{w}$ and the $\mathbf{z}_i$, are assumed to be fixed unknown constants, thus making the model a functional measurement error model (Fuller 1987). The $\mathbf{x}_i$ are auxiliary variables assumed to be known without error. The n_β -dimensional parameter $\boldsymbol{\beta}$ is the vector of unknown parameters to be estimated.

The vector $\mathbf{w}$ is similar to the vector $\boldsymbol{\beta}$ in that it is unknown and constant over i . In fact, were it not for the availability of the one experiment-wide measurement $\mathbf{W}$, the analyst could consider estimating the variables in $\mathbf{w}$ by including them in $\boldsymbol{\beta}$. However, any components of $\mathbf{w}$ that are known without error (or that have measurement errors which turn out to be negligible compared to their standard errors of estimation) could be included in $\mathbf{x}_i$.

The model is a special case of the model considered by Britt and Luecke (1973), and therefore their estimation algorithm could be used to estimate the unknown parameters, $\boldsymbol{\beta}$, $\mathbf{w}$, and the $\mathbf{z}_i$. However, the special form of this model allows the use of smaller matrices, thus permitting a numerically simpler algorithm, which is presented in the next section. Fuller (1987) considered another special form of the Britt and Luecke model without the $\mathbf{w}$ variables and with a one-dimensional relation $\mathbf{g}$. The derivations of the two algorithms are similar.

Some extensions and further generalizations of this model are:

- the covariance matrices need only be known up to an unknown common multiplier σ^2 ; that is, $\Sigma_z = \sigma^2 \Psi_z$ and $\Sigma_w = \sigma^2 \Psi_w$ with Ψ_z and Ψ_w known;
- the covariance matrices can vary with i , if the measurement process changes over the data collection period;
- the model can be extended to data from multiple experiments of the same nature; that is, $\mathbf{z}_i$ and possibly all or part of $\mathbf{w}$ can be subscripted with j to indicate the j -th experiment; and
- prior knowledge of $\boldsymbol{\beta}$ can be accounted for, using a penalized likelihood approach.

Maximum Likelihood Estimation Algorithm

The maximum likelihood estimators for the model in Equations (1) and (2) are those values, $\hat{\beta}$, $\hat{\mathbf{w}}$, and $\hat{\mathbf{z}}_i$, which minimize the sums of squares

$$\sum_{i=1}^N (\mathbf{Z}_i - \mathbf{z}_i)' \Sigma_z^{-1} (\mathbf{Z}_i - \mathbf{z}_i) + (\mathbf{W} - \mathbf{w})' \Sigma_w^{-1} (\mathbf{W} - \mathbf{w}) \quad (3)$$

subject to the N nonlinear constraints in Equation (1). Britt and Luecke (1973) developed an iterative algorithm for the maximum likelihood estimators of a general nonlinear, implicit measurement error model. The specific form of the model in Equations (1) and (2) can be used to provide a computationally simpler iterative algorithm. The algorithm is similar to one developed by Anderson (1989) for an approximate Bayesian extension of the Britt and Luecke (1973) technique. The key idea of these algorithms is to solve the nonlinearly constrained optimization by linearizing the constraints and solving a linear Lagrange multiplier minimization problem at each step.

The iterative algorithm can be initialized with a starting value $\tilde{\beta}$ provided by the analyst and the data $\mathbf{W}$ and $\mathbf{Z}_i$. Then, at each iteration of the algorithm, given the current values, $\tilde{\beta}$, $\tilde{\mathbf{w}}$, and $\tilde{\mathbf{z}}_i$, the constraints in Equation (1) can be linearized as

$$\mathbf{g}(\tilde{\mathbf{z}}_i, \tilde{\mathbf{w}}, \tilde{\beta}; \mathbf{x}_i) + \tilde{\mathbf{G}}_{iz}(\mathbf{z}_i - \tilde{\mathbf{z}}_i) + \tilde{\mathbf{G}}_{iw}(\mathbf{w} - \tilde{\mathbf{w}}) + \tilde{\mathbf{G}}_{i\beta}(\beta - \tilde{\beta}) = \mathbf{0} \quad \text{for } i = 1, \dots, N, \quad (4)$$

where $\tilde{\mathbf{G}}_{i\beta}$, $\tilde{\mathbf{G}}_{iw}$, and $\tilde{\mathbf{G}}_{iz}$ are the Jacobians of $\mathbf{g}$ with respect to β , $\mathbf{w}$, and $\mathbf{z}_i$, respectively, evaluated at $(\tilde{\mathbf{z}}_i, \tilde{\mathbf{w}}, \tilde{\beta}; \mathbf{x}_i)$. The next values in the iteration are values of β , $\mathbf{w}$, and $\mathbf{z}_i$ which minimize Equation (3) subject to Equation (4), using Lagrange multipliers. The details of this minimization are omitted. The optimal values of β , $\mathbf{w}$, and $\mathbf{z}_i$ are

$$\begin{bmatrix} \tilde{\beta} \\ \tilde{\mathbf{w}} \end{bmatrix} + \tilde{\Delta}$$

and

$$\mathbf{Z}_i - \Sigma_z \tilde{\mathbf{G}}_{iz}' \tilde{\mathbf{T}}_i^{-1} \left[\mathbf{g}(\tilde{\mathbf{z}}_i, \tilde{\mathbf{w}}, \tilde{\beta}; \mathbf{x}_i) + \tilde{\mathbf{G}}_{iz}(\mathbf{Z}_i - \tilde{\mathbf{z}}_i) + \tilde{\mathbf{G}}_{i\theta} \tilde{\Delta} \right],$$

respectively, where $\tilde{\mathbf{T}}_i = \tilde{\mathbf{G}}_{iz} \Sigma_z \tilde{\mathbf{G}}_{iz}'$, $\tilde{\Delta}$ is the vector which satisfies the equation

$$\tilde{\mathbf{B}} \tilde{\Delta} = \begin{bmatrix} \mathbf{0} \\ \Sigma_w^{-1} (\mathbf{W} - \tilde{\mathbf{w}}) \end{bmatrix} - \sum_{i=1}^N \tilde{\mathbf{G}}_{i\theta}' \tilde{\mathbf{T}}_i^{-1} \left[\mathbf{g}(\tilde{\mathbf{z}}_i, \tilde{\mathbf{w}}, \tilde{\beta}; \mathbf{x}_i) + \tilde{\mathbf{G}}_{iz}(\mathbf{Z}_i - \tilde{\mathbf{z}}_i) \right],$$

$$\tilde{\mathbf{B}} = \begin{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \Sigma_w^{-1} \end{bmatrix} + \sum_{i=1}^N \tilde{\mathbf{G}}_{i\theta}' \tilde{\mathbf{T}}_i^{-1} \tilde{\mathbf{G}}_{i\theta} \end{bmatrix},$$

and $\tilde{\mathbf{G}}_{i\theta}$ is the $n_g \times (n_\beta + n_w)$ partitioned matrix $(\tilde{\mathbf{G}}_{i\beta} \tilde{\mathbf{G}}_{iw})$. The "primes" indicate matrix transposition. The iteration continues in this way until the estimates converge to the values $\hat{\beta}$, $\hat{\mathbf{w}}$,

and $\hat{z}_i$. One can stop when the changes in subsequent values of $\tilde{\beta}$, $\tilde{w}$, and $\tilde{z}_i$ are negligible and the nonlinear constraints in Equation (1) are satisfied numerically.

An estimate of the variance of $\hat{\beta}$ is the upper-left, $n_\beta \times n_\beta$ submatrix of the inverse of the last calculated $\tilde{B}$. This variance estimate is the extension of the Britt and Luecke (1973) variance estimate.

If it assumed that $\Sigma_z = \sigma^2 \Psi_z$ and $\Sigma_w = \sigma^2 \Psi_w$ and the known matrices Ψ_z and Ψ_w are used in Equation (3) and the iteration in place of Σ_z and Σ_w , respectively, then the minimum value for Equation (3) divided by the degrees of freedom $N - n_\beta$ provides an estimate, s^2 , of the unknown common multiplier σ^2 . Furthermore, in this case, the submatrix of the inverse of $\tilde{B}$ must be multiplied by s^2 to obtain an estimate of the variance of $\hat{\beta}$.

Examples

In this section, we consider two examples: one where an independent experiment-wide measurement of a variable aids in the estimation of the unknown variables and another, a degenerate case, where the data provide no information on a variable which is "known precisely." In the latter case, the estimation algorithm presented here includes the uncertainty in the independent experiment-wide measurement in the uncertainties of the other estimated parameters.

As the first example, consider the problem of determining the acceleration due to gravity given by Barlow (1989). In this example, a ball-bearing is released by switching off an electromagnet, and the time t and distance d through which it falls are measured. Here, $z_i' = (t_i, d_i)$, $\beta' = (a, c)$, and the one-dimensional g function model is

$$d_i - 0.5a(t_i + c)^2 = 0,$$

where a is the acceleration due to gravity (m/s/s) and c is a constant time offset used to model the time it takes the field in the magnet to die away.

Assuming $\Sigma_z = \sigma^2 \Psi_z$ with σ^2 unknown and $\Psi_z = \text{diag}(1.0, 0.25)$, the data in Table 1 can be analyzed by the Britt and Lueck (1973) technique to provide estimates (with standard errors) of 9.86 ± 0.37 and 0.049 ± 0.013 for a and c , respectively.

Table 1. Time and Distance Measurements

Time (seconds)	0.16	0.40	0.58	0.72	0.97
Distance (meters)	0.2	1.0	2.0	3.0	5.0

Now suppose we wish to take into account an independent prior determination of a , $W = 9.815$, with uncertainty assumed to be of the same magnitude as the uncertainty in the time measurements, that is, $\Sigma_w = \sigma^2 \Psi_w$ with $\Psi_w = 1.0$. Then, the algorithm presented here yields estimates (with standard errors) of 9.8150 ± 0.0098 and 0.0507 ± 0.0044 for a and c , respectively, and $s^2 = (0.0098)^2$.

The estimate of a does not change noticeably from the given W value because the data do not contribute much towards improving the estimate. The time and distance data alone yield an estimate of a with a standard error of 0.37 m/s/s, while the W measurement was assumed to have a much tighter standard deviation of approximately 0.01 m/s/s, which in this case is almost like knowing a without error. The estimation of c benefits from taking into account W ; its standard error is reduced by a factor of three.

The second example involves the ideal gas law $PV = nRT$, where P is the pressure (in millimeters of mercury, torr), V is the volume (in cubic centimeters), n is the number of moles of gas, R is the gas constant, and T is the temperature (in degrees Kelvin). A particular laboratory performed the following experiments in order to calibrate the reference volume for each of six noble gas transfer lines. For each transfer line, sets of sequentially measured

pressure and temperature pairs on five gas samples of unknown size are taken; first, in the reference volume; second, in the reference volume and an unknown connector volume; and third, in the reference volume, the connector volume, and a calibrated flask of "known" volume determined by gravimetric means. One such calibrated flask and a total of 30 gas samples are used throughout the calibration procedure. The model is expressed as

$$p_{ijk} v_{ik} - m_{ij} t_{ijk} = 0, \quad (5)$$

where p_{ijk} and t_{ijk} are the pressure and temperature of the j -th gas sample in the k -th volume on transfer line i ; and m_{ij}/R is the number of moles of the j -th gas sample on transfer line i . v_{ik} is the k -th volume on transfer line i ; that is,

$$v_{i1} = v_{Ri}, \quad v_{i2} = v_{Ri} + v_{Ci}, \text{ and } v_{i3} = v_{Ri} + v_{Ci} + v_F \quad (6)$$

where v_{Ri} and v_{Ci} are the reference and connector volumes of transfer line i and v_F is the calibrated flask volume.

The parameters to be estimated are the six transfer line reference volumes, the six transfer line connector volumes, and the 30 m_{ij} values corresponding to the 30 gas samples used. These 42 parameters are included in β .

The paired pressure and temperature data in Table 2 in the Appendix were used to estimate β . We assumed that the measurement errors of the paired pressure and temperature data were independent, with relative variances of 1 and 10000, respectively. An independent measurement of 25.647 cubic centimeters for the flask volume v_F was assumed to have a measurement error with relative variance 1. The estimates $\hat{\beta}$ and their estimated standard errors are listed in the Appendix, Tables 3 and 4.

It follows from Equations (5) and (6) that without a flask volume measurement, only relative values for the volumes and the m_{ij} values could be estimated. Hence, the estimation algorithm presented here cannot provide an improved estimate of the flask volume. However, the estimated covariance matrix of $\hat{\beta}$ does reflect the uncertainty in the flask volume measurement. To assess the sensitivity of the estimated standard errors to the assumed flask volume measurement uncertainty, we analyzed the data again, with different uncertainty levels. When we used a relative variance of 0.1 for the flask volume measurement error, the standard errors of $\hat{\beta}$ decreased by approximately 1.1%. When we used a relative variance of 10.0, the standard errors of $\hat{\beta}$ increased by approximately 10.4%. Thus, this example is mildly sensitive to assumed uncertainty in the experiment-wide measurement.

Conclusions

Data analysts often have available to them independent measurements of some of the variables in the models they are fitting to data. These experiment-wide variables may include such things as physical constants or laboratory conditions at the time of the experiment. Their values may have been measured in a previous experiment or measured independently at the time of the experiment. Depending on the relative variances, the practice of ignoring the measurement error in these independent measurements can have significant impact on the parameter estimates and the estimates of their uncertainties. Typically, ignoring the measurement error leads to underestimates of the uncertainties of the estimated parameters. A rigorous statistical treatment produces more realistic estimates and uncertainties.

We presented such a rigorous statistical treatment through a maximum likelihood approach to incorporate the independent measurements of the experiment-wide variables into the problem of estimating parameters of nonlinear, implicit measurement error models. An algorithm was given which can be used to estimate model parameters and their uncertainties.

The modeling approach presented here can be utilized to assess the impact of the experiment-wide variables and their uncertainties. Examples were presented to demonstrate the impact experiment-wide variables can have on the estimation of the other parameters in the model.

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APPENDIX

Gas Data and Analysis Results

Table 2. Gas Pressure/Temperature Data

Transfer Line	Gas Sample	Volume	Pressure	Temperature
1	1	1	13.561	296.2
1	1	2	12.236	296.3
1	1	3	7.128	296.3
1	2	1	13.616	296.2
1	2	2	12.288	296.1
1	2	3	7.157	296.1
1	3	1	13.258	296.3
1	3	2	11.972	296.3
1	3	3	6.971	296.3
1	4	1	13.338	296.3
1	4	2	12.036	296.2
1	4	3	7.011	296.2
1	5	1	14.371	296.2
1	5	2	12.984	296.3
1	5	3	7.558	296.3
2	1	1	11.520	295.5
2	1	2	10.419	295.5
2	1	3	6.052	295.5
2	2	1	13.103	295.5
2	2	2	11.850	295.5
2	2	3	6.886	295.5
2	3	1	12.502	295.5
2	3	2	11.306	295.5
2	3	3	6.570	295.5
2	4	1	12.415	295.6
2	4	2	11.227	295.6
2	4	3	6.523	295.6
2	5	1	12.157	295.6
2	5	2	10.993	295.6
2	5	3	6.387	295.6

Table 2. Continued

Transfer Line	Gas Sample	Volume	Pressure	Temperature
3	1	1	12.314	296.0
3	1	2	11.131	296.0
3	1	3	6.512	296.0
3	2	1	12.207	296.1
3	2	2	11.017	296.1
3	2	3	6.452	296.1
3	3	1	12.567	296.1
3	3	2	11.342	296.2
3	3	3	6.641	296.2
3	4	1	13.051	296.1
3	4	2	11.778	296.1
3	4	3	6.895	296.1
3	5	1	11.528	296.1
3	5	2	10.405	296.1
3	5	3	6.092	296.1
4	1	1	12.559	295.8
4	1	2	11.339	295.8
4	1	3	6.634	295.8
4	2	1	12.254	295.8
4	2	2	11.062	295.8
4	2	3	6.473	295.8
4	3	1	12.836	295.8
4	3	2	11.589	295.9
4	3	3	6.782	295.9
4	4	1	13.232	295.9
4	4	2	11.945	296.0
4	4	3	6.992	296.0
4	5	1	11.944	295.9
4	5	2	10.783	295.9
4	5	3	6.310	295.9

Table 2. Continued

Transfer Line	Gas Sample	Volume	Pressure	Temperature
5	1	1	12.772	296.3
5	1	2	11.552	296.3
5	1	3	6.716	296.3
5	2	1	13.003	296.3
5	2	2	11.760	296.3
5	2	3	6.833	296.4
5	3	1	12.488	296.4
5	3	2	11.296	296.4
5	3	3	6.563	296.4
5	4	1	12.825	296.4
5	4	2	11.605	296.4
5	4	3	6.742	296.4
5	5	1	12.237	296.3
5	5	2	11.076	296.4
5	5	3	6.432	296.4
6	1	1	12.793	296.2
6	1	2	11.647	296.2
6	1	3	6.958	296.2
6	2	1	12.448	296.2
6	2	2	11.335	296.2
6	2	3	6.770	296.2
6	3	1	12.114	296.2
6	3	2	11.028	296.2
6	3	3	6.587	296.2
6	4	1	12.372	296.3
6	4	2	11.263	296.3
6	4	3	6.729	296.3
6	5	1	12.710	296.3
6	5	2	11.570	296.3
6	5	3	6.913	296.3

Table 3. Gas Analysis Results: Volume Estimates and Standard Errors.

Volume Estimate	Transfer Line					
	1	2	3	4	5	6
$\hat{v}_{Ri}$	32.285	32.164	32.693	32.660	32.168	34.644
Standard Error	(0.011)	(0.012)	(0.012)	(0.012)	(0.012)	(0.013)
$\hat{v}_{Ci}$	3.4787	3.4023	3.5223	3.5216	3.3916	3.4094
Standard Error	(0.0051)	(0.0053)	(0.0054)	(0.0053)	(0.0052)	(0.0056)

Table 4. Gas Analysis Results: $\hat{m}_{ij}$ Estimates and Standard Errors.

$\hat{m}_{ij}$ Estimate	Gas Sample				
	1	2	3	4	5
$\hat{m}_{1j}$	1.47748	1.48418	1.44480	1.45335	1.56671
Standard Error	(0.00053)	(0.00054)	(0.00052)	(0.00053)	(0.00056)
$\hat{m}_{2j}$	1.25390	1.42627	1.36082	1.35082	1.32270
Standard Error	(0.00048)	(0.00054)	(0.00052)	(0.00051)	(0.00050)
$\hat{m}_{3j}$	1.36094	1.34771	1.38713	1.44072	1.27273
Standard Error	(0.00052)	(0.00052)	(0.00053)	(0.00055)	(0.00049)
$\hat{m}_{4j}$	1.38678	1.35303	1.41716	1.46035	1.31843
Standard Error	(0.00053)	(0.00051)	(0.00054)	(0.00055)	(0.00050)
$\hat{m}_{5j}$	1.38668	1.41142	1.35527	1.39212	1.32858
Standard Error	(0.00052)	(0.00053)	(0.00051)	(0.00052)	(0.00050)
$\hat{m}_{6j}$	1.49633	1.45606	1.41679	1.44656	1.48606
Standard Error	(0.00058)	(0.00056)	(0.00055)	(0.00056)	(0.00057)

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