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Least-squares estimation using Lagrange multipliers

L. Nielsen

Abstract. This paper presents a general formulation of least-squares estimation using Lagrange multipliers. It is general in the sense that it takes into account the covariance matrix of all measured quantities and allows any known constraint to be imposed on the quantities being estimated. The technique may be used to estimate parameters of a calibration curve for a transducer taking into account the uncertainty and correlation coefficients of the measured stimuli and responses. It may also be used to adjust measured fundamental constants to a coherent set obeying the appropriate physical laws.

1. Introduction

Least-squares estimation is a very powerful data-analysis tool. One of its advantages is that no assumptions on the statistical distributions of data are necessary. Another advantage is that the covariances of the estimated parameters are easily calculated.

Linear least-squares estimation taking into account the uncertainty in the dependent variable is described in textbooks on data analysis [1]. However, in many metrological applications the uncertainty in the independent variable has to be taken into account. In order to do so, nonlinear least-squares estimation has to be applied [2, 3], although in special cases other least-squares techniques may be applied [4].

When applying least-squares estimation in metrology, the quantities to be estimated may be subject to constraints reflecting, for example, physical laws. Different solutions to this problem have been published [5, 6].

In this paper a nonlinear least-squares technique is presented in which Lagrange multipliers are introduced in order to fix all the constraints imposed on the quantities involved in a measurement. The technique provides estimates of the values and covariances of all the quantities involved taking into account the covariances of the measured quantities.

2. Measurement model

Consider a measurement in which m quantities $\zeta = (\zeta_1, \dots, \zeta_m)^T$ are being measured. Due to measurement uncertainty the values $z = (z_1, \dots, z_m)^T$ obtained by measurement of these quantities should be considered as an m -dimensional random variable $Z = (Z_1, \dots, Z_m)^T$

with expectation $E(Z) = \zeta$ and covariance matrix $V(Z) = \Sigma$. Assuming that the standard uncertainty $u(z_i)$ of each measured value z_i as well as any correlation coefficient $r(z_i, z_j)$ between two measured values z_i and z_j have been estimated in accordance with the ISO *Guide to the Expression of Uncertainty in Measurement* [7], the elements of the covariance matrix Σ can be estimated by

$$\Sigma_{ij} = u(z_i) r(z_i, z_j) u(z_j), \quad i, j = 1, \dots, m. \quad (1)$$

Assume that n constraints between the quantities ζ are known or have been assumed. The constraints may involve $k \geq 0$ additional quantities $\beta = (\beta_1, \dots, \beta_k)^T$, which have not been subject to direct measurement. The constraints between the quantities ζ and β may reflect known or assumed physical laws. If, for example, corresponding values of stimuli and responses have been measured on a transducer, for which a certain transfer function may be known or assumed, the quantities β may be parameters in this transfer function. In any case, it is assumed that the n constraints can be written in the form

$$f(\beta, \zeta) = \begin{pmatrix} f_1(\beta, \zeta) \\ f_2(\beta, \zeta) \\ \vdots \\ f_n(\beta, \zeta) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad (2)$$

where $f_i : \Omega \rightarrow R$, $i = 1, \dots, n$, are C^1 functions defined in a region $\Omega \subset R^{k+m}$ around (β, ζ) .

3. Normal equations

Given the measured values z , the least-squares estimates $\hat{\zeta}$ and $\hat{\beta}$ of the quantities ζ and β are found by minimizing the quadratic form

$$\chi^2(\zeta; z) = (z - \zeta)^T \Sigma^{-1} (z - \zeta) \quad (3)$$

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with respect to ζ under the condition $f(\beta, \zeta) = 0$. If such a minimum exists (which is certainly the case if the constraints are properly defined), the quantities $\hat{\zeta}$ and $\hat{\beta}$ satisfy the identity

$$\nabla_{(\beta, \zeta, \lambda)} \Phi(\hat{\beta}, \hat{\zeta}, \lambda; z) = 0, \quad (4)$$

where

$$\begin{aligned} \Phi(\beta, \zeta, \lambda; z) = \\ (z - \zeta)^T \Sigma^{-1} (z - \zeta) + 2\lambda^T f(\beta, \zeta), \end{aligned} \quad (5)$$

and where $\lambda = (\lambda_1, \dots, \lambda_n)^T$ are the so-called Lagrange multipliers [8]. By inserting (5) into (4) and carrying out the differentiation, the normal equations for $\hat{\zeta}$, $\hat{\beta}$ and λ are obtained:

$$\begin{aligned} f(\hat{\beta}, \hat{\zeta}) &= 0 \\ -\Sigma^{-1} (z - \hat{\zeta}) + \nabla_{\zeta} f(\hat{\beta}, \hat{\zeta})^T \lambda &= 0 \\ \nabla_{\beta} f(\hat{\beta}, \hat{\zeta})^T \lambda &= 0, \end{aligned} \quad (6)$$

where the (n, k) -dimensional functional matrix $\nabla_{\beta} f$ and (n, m) -dimensional functional matrix $\nabla_{\zeta} f$ are defined by

$$\begin{aligned} \nabla_{\beta} f &= \begin{pmatrix} \frac{\partial f_1}{\partial \beta_1} & \dots & \frac{\partial f_1}{\partial \beta_k} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial \beta_1} & \dots & \frac{\partial f_n}{\partial \beta_k} \end{pmatrix} \\ \nabla_{\zeta} f &= \begin{pmatrix} \frac{\partial f_1}{\partial \zeta_1} & \dots & \frac{\partial f_1}{\partial \zeta_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial \zeta_1} & \dots & \frac{\partial f_n}{\partial \zeta_m} \end{pmatrix}. \end{aligned} \quad (7)$$

The $m + k + n$ normal equations are, in the general case, nonlinear and have to be solved numerically. The existence of a solution requires, however, that two necessary conditions are fulfilled:

First, the covariance matrix Σ has to be non-singular; otherwise it cannot be inverted and the quadratic form (3) is not defined. Note that Σ will be singular if one of the correlation coefficients $r(z_i, z_j)$ is equal to ± 1 for $i \neq j$.

Second, the number n of constraints has to be larger than or equal to the number k of elements in the unknown β , but smaller than the total number $m + k$ of quantities to be adjusted: $k \leq n < m + k$.

4. Solving the normal equations

Assume that a solution $(\hat{\beta}, \hat{\zeta}, \lambda) \in \Omega$ to the normal equations (6) exists and that the $(n + m + k, n + m + k)$ -dimensional matrix*

$$\begin{aligned} D(\beta_l, \zeta_l) \\ = \begin{pmatrix} \nabla_{\beta} f(\beta_l, \zeta_l) & \nabla_{\zeta} f(\beta_l, \zeta_l) & \mathbf{0}^{(n, n)} \\ \mathbf{0}^{(m, k)} & \Sigma^{-1} & \nabla_{\zeta} f(\beta_l, \zeta_l)^T \\ \mathbf{0}^{(k, k)} & \mathbf{0}^{(k, m)} & \nabla_{\beta} f(\beta_l, \zeta_l)^T \end{pmatrix} \end{aligned} \quad (8)$$

is non-singular for all $(\beta_l, \zeta_l) \in \Omega$. Then the recursion formula

$$\begin{aligned} \begin{pmatrix} \beta_{l+1} \\ \zeta_{l+1} \\ \lambda_{l+1} \end{pmatrix} &= \begin{pmatrix} \beta_l \\ \zeta_l \\ \mathbf{0} \end{pmatrix} + D(\beta_l, \zeta_l)^{-1} \begin{pmatrix} -f(\beta_l, \zeta_l) \\ \Sigma^{-1} (z - \zeta_l) \\ \mathbf{0}^{(k, 1)} \end{pmatrix}; \\ l &= 1, \dots, \infty \end{aligned} \quad (9)$$

defines an iteration procedure, which converges towards $(\hat{\beta}, \hat{\zeta}, \lambda)$, provided that suitable starting values (β_1, ζ_1) are applied (for the quantities $\hat{\zeta}$ the starting values $\zeta_1 = z$ are the obvious choice!). That is:

$$\begin{pmatrix} \hat{\beta} \\ \hat{\zeta} \\ \lambda \end{pmatrix} = \lim_{l \rightarrow \infty} \begin{pmatrix} \beta_l \\ \zeta_l \\ \lambda_l \end{pmatrix}. \quad (10)$$

The iteration procedure (9) is similar to the Newton-Raphson method, except that the second-order partial derivatives of the functions f have been neglected, as is usually done in nonlinear least-squares estimation [3].

5. Properties of the least-squares estimator

The estimates $(\hat{\beta}, \hat{\zeta})$ of the expectations (β, ζ) depend on the actual outcome z of the measurement. The estimates can therefore be regarded as a multivariate random variable (estimator), which depends on the random variables \mathbf{Z} . To first order, the functional dependency is given by an equation similar to the recursion formula (9) but with (β_l, ζ_l) replaced by the expectations (β, ζ) , $(\beta_{l+1}, \zeta_{l+1})$ replaced by the estimators $(\hat{\beta}, \hat{\zeta})$, and with the measured values z replaced by the random variables \mathbf{Z} :

$$\begin{pmatrix} \hat{\beta} \\ \hat{\zeta} \\ \lambda \end{pmatrix} = \begin{pmatrix} \beta \\ \zeta \\ \mathbf{0} \end{pmatrix} + D(\beta, \zeta)^{-1} \begin{pmatrix} \mathbf{0}^{(n, 1)} \\ \Sigma^{-1} (\mathbf{Z} - \zeta) \\ \mathbf{0}^{(k, 1)} \end{pmatrix}. \quad (11)$$

* The notation $\mathbf{0}^{(m, k)}$ is used to indicate a zero matrix of dimension (m, k) .

According to this first-order approximation, the expectation and the variance of the multivariate estimator are given by

$$E \begin{pmatrix} \hat{\beta} \\ \hat{\zeta} \\ \hat{\lambda} \end{pmatrix} = \begin{pmatrix} \beta \\ \zeta \\ 0 \end{pmatrix}, \quad (12)$$

$$V \begin{pmatrix} \hat{\beta} \\ \hat{\zeta} \\ \hat{\lambda} \end{pmatrix} = D(\beta, \zeta)^{-1} \begin{pmatrix} 0^{(n,n)} & 0^{(n,m)} & 0^{(n,k)} \\ 0^{(m,n)} & \Sigma^{-1} & 0^{(m,k)} \\ 0^{(k,n)} & 0^{(k,m)} & 0^{(k,k)} \end{pmatrix} \times (D(\beta, \zeta)^{-1})^T. \quad (13)$$

Due to the zero matrices in the matrix product, (13) can be simplified by introducing the $(n + m + k, m)$ -dimensional matrix $C(\beta, \zeta)$ which contains the columns $n + 1$ through $n + m$ of the matrix $D(\beta, \zeta)^{-1}$:

$$V \begin{pmatrix} \hat{\beta} \\ \hat{\zeta} \\ \hat{\lambda} \end{pmatrix} = C(\beta, \zeta) \Sigma^{-1} C(\beta, \zeta)^T. \quad (14)$$

Equation (12) shows that $(\hat{\beta}, \hat{\zeta})$ are central estimators in a first-order approximation. This means that the recursion formula (9) on average will provide the expectations (β, ζ) . The covariance matrix of the estimate provided by the recursion formula are calculated by (14) by replacing the unknown matrix $C(\beta, \zeta)$ with the matrix $C(\hat{\beta}, \hat{\zeta})$, the elements of which have already been calculated as part of the iteration procedure. From this covariance matrix the standard uncertainties and the correlation coefficients of the estimated quantities can be calculated. The standard uncertainties and correlation coefficients provided this way comply with the philosophy of the ISO Guide [7].

6. Checking consistency of measurement model

Once the estimates $(\hat{\beta}, \hat{\zeta})$ have been calculated, the consistency of the imposed constraints (described by the functions f) and the measured values z should be checked. This can be done by calculating the quantity

$$\chi^2(\hat{\zeta}; z) = (z - \hat{\zeta})^T \Sigma^{-1} (z - \hat{\zeta}). \quad (15)$$

If the random variables Z describing the measurement follow a multivariate normal distribution, then $\chi^2(\hat{\zeta}, Z)$ follows (to a first-order approximation) a $\chi^2(\nu)$ distribution with ν degrees of freedom. The degrees of freedom ν are equal to the number of measured quantities (m) minus the number of estimated quantities ($m + k$) plus the number of constraints (n), or $\nu = n - k$. In this case

$$E(\chi^2(\hat{\zeta}; Z)) = \nu; \quad V(\chi^2(\hat{\zeta}; Z)) = 2\nu. \quad (16)$$

If the calculated quantity $\chi^2(\hat{\zeta}; z)$ is significantly larger than its expectation ν , the measurement model

has to be rejected. Objective rejection criteria can be set up by calculating the probability $P\{\chi^2(\nu) > \chi^2(\hat{\zeta}; z)\}$; if this probability is less than, say, 5%, the measurement model should be rejected. This check may be carried out even if some of the measured values are known not to be normally distributed. Note that if $n = k$, then $\chi^2(\hat{\zeta}; z) = 0$ and no check of consistency can be performed.

7. Numerical example

This example shows how a transfer function for a nonlinear weighing instrument can be determined in the range 0 g to 20 g using one known mass standard of nominal mass 10 g and two unknown mass standards of nominal masses 5 g.

The mass m_1 and density ρ_1 of the 10 g mass standard are known a priori with specified standard uncertainties and correlation coefficient $r(m_1, \rho_1)$. The masses m_2 and m_3 of the two 5 g mass standards are unknown, but their densities are assumed to have a common value ρ_{23} , which is known with a specified standard uncertainty. Seven different combinations of the three mass standards are repeatedly applied to the weighing instrument. For each combination the mean reading I_i , $i = 1, \dots, 7$, and the standard deviation of the mean $s(I_i)$ are calculated; $s(I_i)$ is used as the standard uncertainty of the mean reading. The air density a is assumed to be constant during the measurement and is measured with a specified standard uncertainty.

The transfer function, transforming the indication I of the weighing instrument into the load $L = M(1 - a/\rho)$ generated by a mass standard with mass M and density ρ in air with density a , is assumed to be a homogeneous third-order polynomial in the indication I with coefficients A , B and C . In this case $\zeta = (m_1, \rho_1, \rho_{23}, a, I_1, \dots, I_7)^T$, $\beta = (m_2, m_3, A, B, C)^T$, and there are seven constraints:

$$AI_i + BI_i^2 + CI_i^3 - \sum_{j=1}^2 X_{ij} m_j (1 - a/\rho_j) = 0, \quad i = 1, \dots, 7, \quad (17)$$

where $\rho_2 = \rho_3 = \rho_{23}$ and where X_{ij} are the elements of the load matrix X :

$$X = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix}^T. \quad (18)$$

The measured values z_i , $i = 1, \dots, 11$, and associated standard uncertainties $u(z_i)$ are summarized in Table 1. All measured values are assumed to be uncorrelated, except the mass m_1 and density ρ_1 for which $r(m_1, \rho_1) = -0.312$ is assumed. From these standard uncertainties and correlation coefficients the covariance matrix Σ is calculated using (1).

Table 1. Measured and estimated values and associated standard uncertainties.

	m_1/g	$\rho_1/(\text{g}/\text{cm}^3)$	$\rho_{23}/(\text{g}/\text{cm}^3)$	$a/(\text{g}/\text{cm}^3)$	I_1/div	I_2/div
z	9.999 989	7.983	6.68	0.001 178	4.999 652	4.999 658
$u(z)$	0.000 011	0.017	0.29	0.000 060	0.000 013	0.000 015
$\hat{\zeta}$	9.999 989	7.983	6.68	0.001 178	4.999 659	4.999 666
$u(\hat{\zeta})$	0.000 011	0.017	0.29	0.000 060	0.000 010	0.000 011
	I_3/div	I_4/div	I_5/div	I_6/div	I_7/div	
z	9.999 907	10.000 021	15.000 230	15.000 234	19.999 885	
$u(z)$	0.000 012	0.000 015	0.000 011	0.000 012	0.000 011	
$\hat{\zeta}$	9.999 899	10.000 007	15.000 234	15.000 240	19.999 882	
$u(\hat{\zeta})$	0.000 011	0.000 013	0.000 009	0.000 010	0.000 011	
	m_2/g	m_3/g	$A/(\text{g}/\text{div})$	$B/(\text{g}/\text{div}^2)$	$C/(\text{g}/\text{div}^3)$	
$\hat{\beta}$	5.000 087	5.000 081	1.000 0039	-2.305e-05	7.72e-07	
$u(\hat{\beta})$	0.000 057	0.000 058	0.000 0056	6.8e-07	2.3e-08	

The estimates $\hat{\zeta}_i$, $i = 1, \dots, 11$, of the measured quantities and the estimates $\hat{\beta}_i$, $i = 1, \dots, 5$ of the unknown quantities, obtained by applying the recursion formula (9), are also shown in Table 1. Note that for the quantities m_1 , ρ_1 , ρ_{23} and a the estimated values are identical to the measured values, whereas all the indications I_i have been adjusted slightly. The fact that, for example, the mass value of m_1 has not been adjusted is obvious from the physical point of view, since m_1 is the only mass standard for which a mass value has been assigned a priori. In other words, there is no information available which suggests that the specified mass of m_1 should be changed. If values of m_2 and m_3 had been known a priori and had been included in the data analysis, the mass of m_1 would also have been adjusted to some extent, depending on the specified uncertainties.

The standard uncertainties $u(\hat{\zeta}_i)$, $i = 1, \dots, 11$, and $u(\hat{\beta}_i)$, $i = 1, \dots, 5$, derived from the covariance matrix (14), are also given in Table 1. Note that $u(\hat{\zeta}_i) = u(z_i)$ for the quantities where $\hat{\zeta}_i = z_i$, whereas $u(\hat{\zeta}_i) < u(z_i)$ when $\hat{\zeta}_i \neq z_i$. Selected correlation coefficients are given in Table 2. Note that m_2 and m_3 as well as A , B and C are highly correlated.

Table 2. Correlation coefficients of selected estimated values.

	m_1	m_2	m_3	ρ_1	ρ_{23}	A	B	C
m_1	1	0.083	0.083	-0.312	0.000	0.171	0.000	0.000
m_2	0.083	1	0.976	-0.001	-0.663	0.030	-0.098	0.096
m_3	0.083	0.976	1	-0.001	-0.663	0.039	-0.103	0.099
ρ_1	-0.312	-0.001	-0.001	1	0.000	-0.001	0.000	0.000
ρ_{23}	0.000	-0.663	-0.663	0.000	1	0.000	0.000	0.000
A	0.171	0.030	0.039	-0.001	0.000	1	-0.950	0.919
B	0.000	-0.098	-0.103	0.000	0.000	-0.950	1	-0.991
C	0.000	0.096	0.099	0.000	0.000	0.919	-0.991	1

From (15) the value $\chi^2 = 2.5$ is calculated; the associated degrees of freedom are $\nu = 7 - 5 = 2$. Since $P\{\chi^2(2) > 2.5\} = 29\%$, the assumed measurement model cannot be rejected.

8. Conclusion

A general formulation of least-squares estimation using Lagrange multipliers has been presented. The formulation allows any constraints (linear or nonlinear) to be imposed on the quantities being estimated and takes into account the covariances of all measured quantities. An iterative procedure for calculation of the least-square estimates and the associated covariance matrix has been described. The applicability of the technique has been demonstrated by an example in which a nonlinear weighing instrument was calibrated using one known and two unknown mass standards.

References

1. Jenkins G. M. et al., *Spectral Analysis and its Applications*, San Francisco, Holden-Day, 1977.
2. Fuller W. A., *Measurement Error Models*, New York, John Wiley, 1987.
3. Press W. P. et al., *Numerical Recipes in C*, 2nd ed., Cambridge, Cambridge University Press, 1992.
4. Premoli A. et al., A New Approach to Total Least-Squares Techniques for Metrological Applications, In *Advanced Mathematical Tools in Metrology II* (Edited by P. Ciarlini, M. G. Fox, F. Pavese and D. Richter) Singapore, World Scientific Publishing Co., 1996.
5. *Basic Concepts of Measurements, Treatment of Uncertainties in the Evaluation of Measurements* [Preliminary translation of the German Draft Standard DIN 1319 Part 4, June 1984].
6. Forbes A. B., Generalized Regression Problems in Metrology, *Numerical Algorithms*, 1993, **5**, 523-533.
7. *Guide to the Expression of Uncertainty in Measurement*, 1st ed., Geneva, International Organization for Standardization, 1993.
8. Jensen H. E., *Matematisk Analyse*, Bind 4, 2. udgave, København, Matematisk Institut, 1976.

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