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LEAST-SQUARES WITH UNCERTAINTIES IN BOTH COORDINATES

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Abstract. This paper addresses the problem of least-squares curve adjustment in the case of uncertain measurement data. Compact matrix analysis is used to derive an iterative solution for the parameters of the adjusted curve. An expression for the uncertainty matrix of these parameters is also given.
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1 INTRODUCTION

Consider two quantities $X(t)$ and $Y(t)$, where t is a parameter that represents the measurement conditions. Let these conditions be varied discretely and define the vectors (column matrices) **X** and **Y** with elements $X_i = X(t_i)$ and $Y_i = Y(t_i)$, $i = 1,...,I$. The measurement results are the estimated values $\mathbf{x}_e$ and $\mathbf{y}_e$. (In this paper we denote quantities by upper case letters and values of the quantities with the corresponding lower case letters).

Let now $\mathbf{f}(x)$ be a column matrix of J given functions of one variable, with $J<I$. It is desired to infer the values of the J coefficients **Z** that define the adjustment curve

$$Y(t) = \mathbf{f}[X(t)]^T\mathbf{Z} = f_1[X(t)]\,Z_1 + ... + f_J[X(t)]\,Z_J. \tag{1}$$

The classical solution proceeds by minimizing the sum of squares

$$\chi_c^2 = (\mathbf{y} - \mathbf{y}_e)^T(\mathbf{y} - \mathbf{y}_e) \tag{2}$$

subject to

$$\mathbf{y} = \mathbf{F}(\mathbf{x}_e)\mathbf{z} \tag{3}$$

where $\mathbf{F}(\mathbf{x}_e)$ is an $I \times J$ matrix whose elements are $f_j(x_{ei})$.

The minimum value of χ_c^2 is obtained for the adjusted values

$$\mathbf{y}_c = \mathbf{F}(\mathbf{x}_e)\mathbf{z}_c \tag{4}$$

where

$$\mathbf{z}_c = [\,\mathbf{F}(\mathbf{x}_e)^T\,\mathbf{F}(\mathbf{x}_e)\,]^{-1}\,\mathbf{F}(\mathbf{x}_e)^T\,\mathbf{y}_e. \tag{5}$$

Suppose now that the measurement uncertainty is not negligible. Let $\mathbf{U}(\mathbf{x}_e)$ and $\mathbf{U}(\mathbf{y}_e)$ be the $I \times I$ uncertainty (or covariance) matrices, the diagonal elements of which are the squares of the standard uncertainties associated with the estimated values and the off-diagonal elements are the mutual uncertainties. Under this condition, the quantity to be minimized is

$$\chi^2 = (\mathbf{y} - \mathbf{y}_e)^T\,\mathbf{U}(\mathbf{y}_e)^{-1}\,(\mathbf{y} - \mathbf{y}_e) + (\mathbf{x} - \mathbf{x}_e)^T\,\mathbf{U}(\mathbf{x}_e)^{-1}\,(\mathbf{x} - \mathbf{x}_e) \tag{6}$$

subject to

$$\mathbf{y} = \mathbf{F}(\mathbf{x})\mathbf{z}. \tag{7}$$

In case there is no uncertainty associated with the measurement of **X**, the solution is

$\mathbf{x}^* = \mathbf{x}_e$ and

$$\mathbf{y}^* = \mathbf{F}(\mathbf{x}_e)\mathbf{z}^* \tag{9}$$

where

$$\mathbf{z}^* = [\,\mathbf{F}(\mathbf{x}_e)^T\,\mathbf{U}(\mathbf{y}_e)^{-1}\,\mathbf{F}(\mathbf{x}_e)\,]^{-1}\,\mathbf{F}(\mathbf{x}_e)^T\,\mathbf{U}(\mathbf{y}_e)^{-1}\,\mathbf{y}_e \tag{10}$$

with an uncertainty matrix

$$\mathbf{U}(\mathbf{z}^*) = [\,\mathbf{F}(\mathbf{x}_e)^T\,\mathbf{U}(\mathbf{y}_e)^{-1}\,\mathbf{F}(\mathbf{x}_e)\,]^{-1}. \quad (11)$$

The more general case when both coordinates are subject to measurement uncertainty does not have a closed form solution. This problem may be solved using the procedure above with $\mathbf{U}(\mathbf{y}_e)$ replaced by the so-called "effective variance" matrix [1]

$$\mathbf{U}(\mathbf{y}_e)' = \mathbf{U}(\mathbf{y}_e) + \mathbf{F}_x(\mathbf{x}_e,\mathbf{z})\,\mathbf{U}(\mathbf{x}_e)\,\mathbf{F}_x(\mathbf{x}_e,\mathbf{z}) \quad (12)$$

where $\mathbf{F}_x(\mathbf{x}_e,\mathbf{z})$ is an $I \times I$ diagonal matrix, whose elements are $\mathbf{f}_x(x_{ei})^T\mathbf{z}$ and $\mathbf{f}_x(x_{ei})$ are column matrices whose elements are the derivatives of the functions $\mathbf{f}$ evaluated at x_{ei}. The solution is iterative: as an initial approximation to the coefficients $\mathbf{z}$ in (12) those obtained from (10) are used. This vector, as well as the effective variance matrix $\mathbf{U}(\mathbf{y}_e)'$, are used in (9) to obtain a new vector $\mathbf{y}$ which is then used in (10) to update the vector $\mathbf{z}$. A new effective variance matrix is next calculated and the process is repeated until convergence, which is very rapid. No general proof of the validity of this method has been found by this author, other than that given in [1] for the case where both uncertainty matrices are diagonal.

2 THE PROPOSED ALGORITHM

A method for the general problem of least-squares adjustment under uncertainty is given in [2] and [3]. A procedure specifically designed to the problem of curve adjustment is presented next. Substitution of (7) into (6) gives χ^2 as a function of $\mathbf{z}$ and $\mathbf{x}$ only. Differentiating with respect to both these quantities and setting the results equal to zero gives

$$\mathbf{F}(\mathbf{x})^T\,\mathbf{U}(\mathbf{y}_e)^{-1}\,[\,\mathbf{F}(\mathbf{x})\mathbf{z} - \mathbf{y}_e\,] = 0 \quad (13)$$

and

$$\mathbf{U}(\mathbf{x}_e)^{-1}\,(\mathbf{x} - \mathbf{x}_e) + \mathbf{F}_x(\mathbf{x},\mathbf{z})\,\mathbf{U}(\mathbf{y}_e)^{-1}\,[\,\mathbf{F}(\mathbf{x})\mathbf{z} - \mathbf{y}_e\,] = 0. \quad (14)$$

Solving for $\mathbf{z}$ in (13) and substituting into (14) gives an equation for $\mathbf{x}$. Its solution follows by writing

$$\mathbf{F}(\mathbf{x})\mathbf{z} \approx \mathbf{y}_n + \mathbf{F}_x(\mathbf{x}_n,\mathbf{z}_n)\,(\mathbf{x}_{n+1} - \mathbf{x}_n) \quad (15)$$

where

$$\mathbf{y}_n = \mathbf{F}(\mathbf{x}_n)\mathbf{z}_n \quad (16)$$

$$\mathbf{z}_n = [\,\mathbf{F}(\mathbf{x}_n)^T\,\mathbf{U}(\mathbf{y}_e)^{-1}\,\mathbf{F}(\mathbf{x}_n)\,]^{-1}\,\mathbf{F}(\mathbf{x}_n)^T\,\mathbf{U}(\mathbf{y}_e)^{-1}\,\mathbf{y}_e \quad (17)$$

and n denotes the iteration step. Then, using the Newton-Raphson method, the vector $\mathbf{x}_n$ is updated according to

$$\mathbf{x}_{n+1} = \mathbf{x}_n - [\,\mathbf{U}(\mathbf{x}_e)^{-1} + \mathbf{F}_x(\mathbf{x}_n,\mathbf{z}_n)\,\mathbf{U}(\mathbf{y}_e)^{-1}\,\mathbf{F}_x(\mathbf{x}_n,\mathbf{z}_n)\,]^{-1}\,[\,\mathbf{U}(\mathbf{x}_e)^{-1}(\,\mathbf{x}_n - \mathbf{x}_e\,) + \mathbf{F}_x(\mathbf{x}_n,\mathbf{z}_n)\,\mathbf{U}(\mathbf{y}_e)^{-1}\,(\,\mathbf{y}_n - \mathbf{y}_e\,)\,]. \quad (18)$$

The algorithm starts with $\mathbf{x}_1 = \mathbf{x}_e$. After convergence, the uncertainty matrix of the coefficients is obtained from the equations in [2] and [3]. The result is

$$\mathbf{U}(\mathbf{z}^*) = \{\,\mathbf{F}(\mathbf{x}^*)^T\,[\mathbf{U}(\mathbf{y}_e) + \mathbf{F}_x(\mathbf{x}^*,\mathbf{z}^*)\,\mathbf{U}(\mathbf{x}_e)\,\mathbf{F}_x(\mathbf{x}^*,\mathbf{z}^*)\,]^{-1}\,\mathbf{F}(\mathbf{x}^*)\}^{-1} \quad (19)$$

where $\mathbf{x}^*$ and $\mathbf{z}^*$ denote the convergence values. (Note the similarity of the matrix within the square brackets in (19) with the effective variance matrix).

One advantage of this algorithm over the method in [2] and [3] is that it does not require starting values for $\mathbf{z}$. Its convergence is rather slow, but this is of no importance since its computer implementation is normally fast and easy using readily available software.

3 EXAMPLE

This example uses the data (taken from [1]) shown in Table 1. It concerns the determination of the inductance l and the internal resistance r of a black box connected in series with a capacitor for which g = 0.02 µF. A sinusoidal voltage was applied to the combination at several frequency settings ν, which in this context is identified with the parameter t. The phase shift q of the capacitor voltage with respect to the applied voltage was read off an oscilloscope. With Y = cot q, X = ν / ν_o and ν_o = 1 rad/s being a reference frequency, the adjustment curve is

$$Y = X Z_1 - X^{-1} Z_2$$

where $Z_1 = \nu_o\, l / r$ and $Z_2 = (\nu_o\, r\, g)^{-1}$.

Table 1. Data

I	x_{ei}	$u(x_{ei})$	y_{ei}	$u(y_{ei})$
1	22 000	440	–4.0170	0.50
2	22 930	470	–2.7420	0.25
3	23 880	500	–1.1478	0.08
4	25 130	530	1.4910	0.09
5	26 390	540	6.8730	1.90

Results are shown in Table 2, where $r(z_1,z_2) = u(z_1,z_2)/[\,u(z_1)\, u(z_2)\,]$ is the correlation coefficient. According to the proposed algorithm, the values and relative standard uncertainties of the measurands are

$$r = \frac{1}{z_2 \nu_o g} = 80\ \Omega$$

$$l = \frac{z_1 r}{\nu_o} = 85.9\ \text{mH}$$

$$\frac{u(r)}{r} = \frac{u(z_2)}{z_2} = 0.203$$

$$\frac{u(l)}{l} = \left[\frac{u(z_1)^2}{z_1^2} + \frac{u(z_2)^2}{z_2^2} - 2\frac{u(z_1,z_2)}{z_1 z_2}\right]^{1/2} = 0.023$$

$$\frac{u(r,l)}{r\,l} = \frac{u(z_2)^2}{z_2^2} - \frac{u(z_1,z_2)}{z_1 z_2} = -0.0017$$

4 CONCLUSIONS

An iterative algorithm to calculate the coefficients of a least-squares adjusted curve has been derived. The algorithm is presented in compact matrix notation and applies to the case where measurement uncertainties and correlations affect both sets of data points.

Table 2. Results

	$z_1 / 10^{-3}$	$z_2 / 10^5$	$u(z_1) / 10^{-3}$	$u(z_2) / 10^5$	$r(z_1,z_2)$
Conventional procedure	1.20	6.91			
Effective variance	1.01	5.92	0.10	0.60	0.990
Proposed algorithm	1.07	6.3	0.23	1.3	0.995

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