NPL Report CMSC 24/03

Report to the National Measurement System Directorate, Department of Trade and Industry

From the Software Support for Metrology Programme

The classification and solution of regression problems for calibration

By
M G Cox, A B Forbes, P M Harris and I M Smith

Revised August 2004

The classification and solution of regression problems for calibration

M G Cox, A B Forbes, P M Harris and I M Smith
Centre for Mathematics and Scientific Computing

Revised August 2004

ABSTRACT

Many experiments in metrology involve the use of instruments or measuring systems that measure values of a *response* variable corresponding to given values of a *stimulus* variable. The *calibration* of such instruments requires using a set of measurements of stimulus and response variables, along with their associated uncertainties, to determine estimates of the parameters that best describe the relationship between them, along with their associated uncertainty matrix.

Algorithms for determining the *calibration parameters* for problems where measurements of the stimulus variable can be assumed to be accurate relative to those of the response variable are well known. However, there is much less awareness in the metrology community of solution algorithms for more generalised problems.

Many standards that deal with calibration, while identifying the types of *regression* problems to be solved, offer only limited advice regarding the selection and use of solution algorithms. There is also a need for guidance regarding uncertainty evaluation.

The aim of this report is to provide more assistance to the metrologist, allowing the calibration problem to be easily classified according to the uncertainty structure associated with the measurement data, providing solution algorithms for the main types of calibration problems, and describing the evaluation of uncertainties associated with the calibration parameters.

The report will also act as input to JCGM-WG1 and ISO TC69/SC6/WG7.

ISSN 1471–0005

Authorised by Dr Dave Rayner,
Head of the Centre for Mathematics and Scientific Computing

National Physical Laboratory,
Queens Road, Teddington, Middlesex, United Kingdom TW11 0LW

Contents

1 Introduction

Experimental data analysis is a key activity in metrology. It involves developing a mathematical model of a physical system in terms of mathematical equations involving parameters that describe all relevant aspects of the system. The model specifies how the system is expected to respond to input data and the nature of the uncertainties associated with this data. Given measured data, estimates of the model parameters are determined by solving the mathematical equations constructed as part of the model, and this requires developing an algorithm (or estimator) to determine values for the parameters that best explain the data.

In many areas of metrology the relationship between a "stimulus" variable and a "response" variable is used as the basis for the calibration of an instrument or measuring system. Actual measurements consisting of the observed response for settings of the stimulus variable are fitted by an appropriate calibration curve to quantify the required relationship. In cases where the measurements of the stimulus variable can be considered to be accurate compared with those of the response variable, ordinary least squares or other procedures can be used to provide the "regression" curve. The uncertainties associated with the curve and its subsequent usage can also readily be determined. However, in many applications, such as dimensional metrology, gas-standards work and analytical chemistry, the uncertainties associated with the measurements of the stimulus variable can be appreciable, and ignoring them can yield invalid results and unreliable uncertainties associated with the calibration curve.

The motivation for this report is as follows:

- Calibration problems occur widely in metrology and algorithms for problems where measurements of the stimulus variable can be assumed to be accurate relative to those of the response variable are well known. However, there is much less awareness in the metrology community of solution algorithms for more generalised problems and this lack of awareness needs to be addressed.

- A recent Software Support for Metrology (SS*f*M) survey [17] has investigated the extent to which metrology algorithms are used within standards. This survey has identified the need for more comprehensive advice regarding the selection and use of such algorithms. For example, there is a generic standard [8] on regression, but it has a limited scope, dealing only with straight line calibration curves. Also identified is the need for more guidance regarding uncertainty evaluation and a recommendation that reliable software be provided. The survey identifies the requirement for generic standards that specify the statistical methods that should be used in all the calibration cases that occur in metrology, with appropriate guidance on uncertainty evaluation.

- NPL has representation on JCGM-WG1[1] and ISO TC69/SC6/WG7[2], both of which have identified a need for increased guidance relating to calibration problems. In the case of JCGM-WG1, it is expected that guidance will be provided in the form of a supplemental guide to the GUM [3] on least squares adjustment.

The main aims of this report are therefore:

- To describe the main types of uncertainty models encountered by metrologists, and provide a basic classification of the resulting calibration problems into which metrologists can characterise their own problems.
- To provide algorithms for the estimation of calibration parameters and their associated uncertainties.
- To describe the "application" of the calibration curve to the evaluation of other quantities and their associated uncertainties.
- To act as input to the work of JCGM-WG1 and ISO TC69/SC6/WG7.

The layout of the remainder of this report is as follows. Section 2 introduces many of the relevant terms and the mathematical notation. Section 3 describes the formulation of the calibration problem and introduces a classification of calibration problems based on the structure of the uncertainty matrix associated with the stimulus and response variables. Sections 4 and 5 describe algorithms for estimating the calibration curve parameters and their associated uncertainties when the response variable is respectively a linear function and a non-linear function of the stimulus variable. In both these sections, it is shown that the calibration problems require the solution of a number of "standard" problems to which standard algorithmic tools can be applied. In section 6, the application of the calibration curve to function evaluation, inverse function evaluation and the evaluation of other derived quantities is detailed. Section 7 discusses some of the issues concerning polynomial calibration curves, a class of calibration curve widely used in metrology. Concluding remarks are given in Section 8.

August 2004 revision
This revised version of the report contains corrections to formulæ concerning Chebyshev polynomials in section 7.1.

[1] Joint Committee for Guides in Metrology, Working group 1 (Measurement Uncertainty)
[2] Technical committee 69/Subcommittee 6/Working group 7 (Application of statistical methods/Measurement methods and results/Uncertainty of measurement)

2 Terms and definitions

Throughout the report, the following notation is used:

m	number of measurements.
n	number of model parameters.
$\mathbf{a}$	vector of model parameters $\mathbf{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}$.
$\{x_i\}_1^m$	set of m elements indexed by $i = 1, \ldots, m$.
$\mathbf{a}^{\mathrm{T}}$, A^{T}	transpose of a vector or matrix.
$\mathbf{0}$	zero matrix.
I	identity matrix.
$\mathrm{diag}\{\alpha, \beta, \ldots, \omega\}$	diagonal matrix $\begin{bmatrix} \alpha & & & \\ & \beta & & \\ & & \ddots & \\ & & & \omega \end{bmatrix}$.
$\|\mathbf{a}\|$	the 2-norm of the vector $\mathbf{a}$: $\|\mathbf{a}\| = (a_1^2 + \cdots + a_n^2)^{\frac{1}{2}}$.
$\sum_{i=1}^{m} x_i$	sum of elements of the vector $\mathbf{x}$: $\sum_{i=1}^{m} x_i = x_1 + \cdots + x_m$.
$\frac{\partial h}{\partial t}(t_0)$	partial derivative of the function $h = h(t)$ with respect to t, evaluated at $t = t_0$.
$\frac{\partial h}{\partial a_j}(\mathbf{a}_0)$	partial derivative of the function $h = h(\mathbf{a})$ with respect to a_j, evaluated at $\mathbf{a} = \mathbf{a}_0$.
$\frac{\partial h}{\partial t}(t_0, \mathbf{a}_0)$	partial derivative of the function $h = h(t, \mathbf{a})$ with respect to t, evaluated at $t = t_0, \mathbf{a} = \mathbf{a}_0$.
$\frac{\partial h}{\partial a_j}(t_0, \mathbf{a}_0)$	partial derivative of the function $h = h(t, \mathbf{a})$ with respect to a_j, evaluated at $t = t_0, \mathbf{a} = \mathbf{a}_0$.
$\nabla_{\mathbf{a}} h(\mathbf{a}_0)$	vector of partial derivatives of the function $h = h(\mathbf{a})$ with respect to the parameters $\mathbf{a}$, evaluated at $\mathbf{a} = \mathbf{a}_0$: $\nabla_{\mathbf{a}} h(\mathbf{a}_0) = \begin{bmatrix} \frac{\partial h}{\partial a_1}(\mathbf{a}_0) \\ \vdots \\ \frac{\partial h}{\partial a_n}(\mathbf{a}_0) \end{bmatrix}$.

$\nabla_{\mathbf{a}} h(t_0, \mathbf{a}_0)$	vector of partial derivatives of the function $h = h(t, \mathbf{a})$ with respect to the parameters $\mathbf{a}$, evaluated at $t = t_0, \mathbf{a} = \mathbf{a}_0$: $\nabla_{\mathbf{a}} h(t_0, \mathbf{a}_0) = \begin{bmatrix} \frac{\partial h}{\partial a_1}(t_0, \mathbf{a}_0) \\ \vdots \\ \frac{\partial h}{\partial a_n}(t_0, \mathbf{a}_0) \end{bmatrix}$.
J	Jacobian matrix associated with a set of functions $\{h_i(\mathbf{a})\}_1^m$ of parameters $\mathbf{a}$ with general element $J_{ij} = \frac{\partial h_i}{\partial a_j}$.
u_x	standard uncertainty associated with the estimate x of random variable X.
$\mathrm{var}(x)$	variance associated with the estimate x of random variable X: $\mathrm{var}(x) = u_x^2$.
$\mathrm{cov}(x, y)$	covariance associated with the estimates x and y of random variables X and Y. Note: $\mathrm{cov}(x, x) = \mathrm{var}(x)$.
U (or $U_{\mathbf{a}}$)	uncertainty matrix (also known as covariance matrix) associated with $\mathbf{a}$ having general element $U_{ij} = U_{\mathbf{a},ij} = \mathrm{cov}(a_i, a_j)$ if $i \neq j$, $U_{ij} = U_{\mathbf{a},ij} = \mathrm{var}(a_i)$ if $i = j$.

3 Problem formulation

3.1 Functional models

Many metrology experiments involve determining the behaviour of a response variable v as a function of a stimulus variable t. Model building involves establishing the functional relationship between these quantities, usually involving a set of model parameters

$$\mathbf{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix},$$

i.e.,

$$v = h(t, \mathbf{a}). \tag{1}$$

The terms $\mathbf{a}$ parametrize the range of possible response behaviour, and the actual behaviour is specified by determining values for these parameters from measurement data. Equation (1) defines a *calibration curve* and $\mathbf{a}$ is sometimes referred to as the vector of *calibration coefficients*.

The functional model is *linear* (in the parameters $\mathbf{a}$) if h can be expressed in the form

$$h(t, \mathbf{a}) = \sum_{j=1}^{n} a_j h_j(t) = a_1 h_1(t) + a_2 h_2(t) + \cdots + a_n h_n(t),$$

where $\{h_j(t)\}_1^n$ is a set of basis functions, and is *non-linear* otherwise.

Often the same curve can be expressed in a number of ways by choosing different basis functions. The problem of choosing an appropriate set of basis functions to represent the calibration curve is one of *parametrisation*; a fuller discussion is available [7]. Section 7 contains a brief discussion of parametrisation issues that arise when working with polynomials which constitute a class of calibration curves widely used in metrology.

Example: Calibration of a thermometer. The response v of a thermometer to temperature t is modelled as

$$v = a_1 + a_2(t - t_0),$$

where t_0 is a fixed temperature. This is a linear calibration curve with basis functions

$$h_1(t) = 1, \quad h_2(t) = t - t_0$$

and

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}.$$

♯

Example: Calibration of a hydrophone. As part of the calibration of an underwater electroacoustic transducer, measurements are made of the response of the transducer to a sinusoidal drive signal of frequency f. Assuming that the system behaves as a linear damped harmonic oscillator, the response v is modelled as a function of time as follows:

$$v = A_1 \sin(2\pi f t + \phi_1) + \sum_{k=2}^{1+n_r} A_k e^{d_k t} \sin(2\pi f_k t + \phi_k),$$

where the first term represents the steady-state behaviour of the device, and the remaining terms are used to represent its resonant behaviour. The coefficients $\mathbf{a}$ comprise the amplitudes $\{A_k\}_1^{1+n_r}$, resonant frequencies $\{f_k\}_2^{2+n_r}$, damping factors $\{d_k\}_2^{2+n_r}$ and phase angles $\{\phi_k\}_1^{2+n_r}$. The calibration curve is a non-linear function of the coefficients $\mathbf{a}$.

♯

3.2 Least squares analysis/adjustment

In this section, we describe the general approach to the least squares analysis or adjustment (LSA) of calibration data. Suppose, in a calibration of a measurement system, that the response of the system is modelled as $v = h(t, \mathbf{a})$ and that measurements

$$\mathbf{x} = \begin{bmatrix} \mathbf{v} \\ \mathbf{t} \end{bmatrix},$$

comprising of measurements

$$\mathbf{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_m \end{bmatrix} \text{ and } \mathbf{t} = \begin{bmatrix} t_1 \\ \vdots \\ t_m \end{bmatrix}$$

of the response and stimulus variables, are gathered.

Associated with $\mathbf{x}$ is its uncertainty matrix $U_{\mathbf{x}}$, a $2m \times 2m$ symmetric matrix. Suppose U_x can be factored as

$$U_{\mathbf{x}} = GG^{\mathrm{T}},$$

where G is an $2m \times k$ matrix. G could be derived from an eigenvalue decomposition of $U_{\mathbf{x}}$, for example, but often the nature of the experiment provides $U_{\mathbf{x}}$ in

this form. In a least squares analysis, estimates of the calibration parameters $\mathbf{a}$ are determined by solving the optimisation problem

$$\min_{\mathbf{a},\mathbf{q},\mathbf{y}} \mathbf{y}^{\mathrm{T}}\mathbf{y} \tag{2}$$

subject to the constraints

$$\begin{bmatrix} \mathbf{v} \\ \mathbf{t} \end{bmatrix} = \begin{bmatrix} \mathbf{h}(\mathbf{q},\mathbf{a}) \\ \mathbf{q} \end{bmatrix} + G\mathbf{y}, \tag{3}$$

where the ith element of the m-vector $\mathbf{h}(\mathbf{q},\mathbf{a})$ is $h(q_i,\mathbf{a})$. This optimisation problem implicitly defines $\mathbf{a} = \mathbf{a}(\mathbf{x})$ as a function of the input data $\mathbf{x}$ and the general principles of the GUM [8] can be applied to determine the uncertainty matrix $U_{\mathbf{a}}$ associated with $\mathbf{a}$, given the uncertainty matrix $U_{\mathbf{x}}$.

LSA methods are used widely throughout metrology (and science in general) and can be justified for a wide range of applications. For measurement data modelled in terms of Gaussian distributions, the LSA estimate of the parameters $\mathbf{a}$ provides the most likely explanation of the data, i.e., the maximum likelihood estimate. The Gauss Markov theorem [13] states that, with some mild qualifications, the LSA approach makes the best use of the available data $\mathbf{x}$ and $U_{\mathbf{x}}$.

While (2) defines the LSA estimate in completely general terms, in many regression problems the uncertainty matrix $U_{\mathbf{x}}$ has a structure that allows the optimisation problem to be reformulated in a more simple way. In this report, we list some of the most common uncertainty structures and describe corresponding estimation algorithms. The algorithms employ numerically stable procedures such as orthogonal factorisation methods in order to avoid the unnecessary loss of accuracy in the computed estimates.

The LSA method assumes that the data uncertainty matrix $U_{\mathbf{x}}$ is known. However, the solution $\tilde{\mathbf{a}}$ for data $\mathbf{x}$ and $U_{\mathbf{x}}$ is the same as that for $\mathbf{x}$ and $\sigma^2 U_{\mathbf{x}}$, $\sigma^2 > 0$, i.e., changing $U_{\mathbf{x}}$ by a scale factor does not change the solution $\tilde{\mathbf{a}}$. In this way, LSA methods can be applied to data $\mathbf{x}$ and $U_{\mathbf{x}} = \sigma^2 GG^{\mathrm{T}}$, where the factor G is known but the scale σ^2 is unknown. In this situation, the uncertainty matrix $U_{\tilde{\mathbf{a}}}$ associated with the estimated parameters can be written as

$$U_{\tilde{\mathbf{a}}} = \sigma^2 UU^{\mathrm{T}},$$

where U is known. Often, once the LSA estimate $\tilde{\mathbf{a}}$ has been determined, an estimate $\hat{\sigma}$ of σ can be derived and then used to specify $U_{\tilde{\mathbf{a}}}$ and $U_{\mathbf{x}}$ completely.

3.3 Uncertainty models

The uncertainties associated with the measurement data

$$\mathbf{x} = \begin{bmatrix} \mathbf{v} \\ \mathbf{t} \end{bmatrix}$$

are described by the uncertainty matrix

$$U_{\mathbf{x}} = \begin{bmatrix} U_{\mathbf{v}} & U_{\mathbf{vt}} \\ U_{\mathbf{vt}}^{\mathrm{T}} & U_{\mathbf{t}} \end{bmatrix}.$$

The ith diagonal element of sub-matrix $U_{\mathbf{t}}$ [$U_{\mathbf{v}}$] is $\mathrm{var}(t_i)$ [$\mathrm{var}(v_i)$], the variance of t_i [v_i], while the i, j $(i \neq j)$ element of $U_{\mathbf{t}}$ [$U_{\mathbf{v}}$] is $\mathrm{cov}(t_i, t_j)$ [$\mathrm{cov}(v_i, v_j)$], the covariance of t_i and t_j [v_i and v_j].

The sub-matrix $U_{\mathbf{vt}}$ contains the covariance of the stimulus and response variables, i.e., the i, j element of $U_{\mathbf{vt}}$ is $\mathrm{cov}(v_i, t_j)$.

Common examples of calibration problems where the measurements of the stimulus variable are assumed to be accurate relative to the measurements of the response variable are those where the measurements of the response variable are:

1. uncorrelated but have *unknown* equal variances s^2, i.e., $U_{\mathbf{v}} = s^2 I$ with s unknown,
2. uncorrelated but have *known* equal variances σ^2, i.e., $U_{\mathbf{v}} = \sigma^2 I$ with σ known,
3. uncorrelated with the ith measurement having known variance σ_i^2, i.e., $U_{\mathbf{v}} = \mathrm{diag}\{\sigma_1^2, \ldots, \sigma_m^2\}$,
4. correlated with general uncertainty matrix $U_{\mathbf{v}}$,

while typical examples of more generalised uncertainty structures include cases where:

5. the measurements are uncorrelated but the measurements of the stimulus and response variables have *unknown* equal variances r^2 and s^2, respectively, but the ratio of r to s *is* known, i.e., $U_{\mathbf{t}} = r^2 I$, $U_{\mathbf{v}} = s^2 I$, $U_{\mathbf{vt}} = \mathbf{0}$, $\frac{r}{s} = \alpha$ known,
6. the measurements are uncorrelated and the measurements of the stimulus and response variables have *known* equal variances ρ^2 and σ^2, respectively, i.e., $U_{\mathbf{t}} = \rho^2 I$, $U_{\mathbf{v}} = \sigma^2 I$, $U_{\mathbf{vt}} = \mathbf{0}$,
7. the measurements are uncorrelated and the ith measurements of the stimulus and response variables have *known* variances ρ_i^2 and σ_i^2 respectively, i.e., $U_{\mathbf{t}} = \mathrm{diag}\{\rho_1^2, \ldots, \rho_m^2\}$, $U_{\mathbf{v}} = \mathrm{diag}\{\sigma_1^2, \ldots, \sigma_m^2\}$, $U_{\mathbf{vt}} = \mathbf{0}$,
8. as 7, but the ith measurements t_i and v_i are correlated with *known* covariance $\mathrm{cov}(v_i, t_i) = \alpha_i$, i.e., $U_{\mathbf{t}} = \mathrm{diag}\{\rho_1^2, \ldots, \rho_m^2\}$, $U_{\mathbf{v}} = \mathrm{diag}\{\sigma_1^2, \ldots, \sigma_m^2\}$, $U_{\mathbf{vt}} = \mathrm{diag}\{\alpha_1, \ldots, \alpha_m\}$,

9. all the response variable measurements are (generally) correlated with *known* uncertainty matrix $U_{\mathbf{v}}$, all the stimulus variable measurements are (generally) correlated with *known* uncertainty matrix $U_{\mathbf{t}}$ and there is no correlation between stimulus and response variable measurements, i.e., $U_{\mathbf{vt}} = \mathbf{0}$,

10. all the measurements are (generally) correlated with *known* uncertainty matrix $U_{\mathbf{x}}$.

Note that any uncertainty model can be considered to belong to at least one of types 3, 4, 8 or 10. In particular, *any* uncertainty model can be classified as the most general (case 10), but the provision of information to it, and its numerical handling, will not necessarily be efficient.

The above list is not exhaustive and it is not the intention of this report to provide individual solution algorithms for each. In the following sections we will focus on the four distinct types of statistical model that we consider to be the most important, viz., 3, 4, 8 and 10. Algorithms for each of the resulting calibration problems, namely [9]:

I. diagonally weighted least squares problems (uncertainty models 1, 2 and 3), i.e., $U_{\mathbf{v}}$ diagonal, $U_{\mathbf{t}} = U_{\mathbf{vt}} = \mathbf{0}$,

II. Gauss-Markov regression problems (uncertainty model 4), i.e., $U_{\mathbf{t}} = U_{\mathbf{vt}} = \mathbf{0}$,

III. generalised distance regression problems (uncertainty models 5, 6, 7 and 8) [2], i.e., $U_{\mathbf{v}}$, $U_{\mathbf{t}}$ and $U_{\mathbf{vt}}$ diagonal,

IV. generalised Gauss-Markov regression problems (uncertainty models 9 and 10), i.e., $U_{\mathbf{x}}$ a full matrix,

are described along with details of the evaluation of the uncertainties associated with the solutions to these problems.

Note that while the same algorithm is therefore used to find parameter estimates for uncertainty model 1 (5) as for uncertainty models 2 and 3 (6, 7 and 8), evaluation of the uncertainty matrix associated with the solution parameters requires an estimate of the unknown variance(s) to be incorporated; see, for example, [7].

Table 1 relates the four main types of calibration problem listed above to the appropriate parts of Sections 4 and 5.

For calibration problems of types I and II, direct methods are used to obtain the solution parameters, and different algorithms are recommended for the cases where the calibration function h is linear and non-linear. For calibration problems of

Calibration problem	Calibration function	Section
I	Linear	4.1
I	Non-linear	5.1
II	Linear	4.2
II	Non-linear	5.2
III	Linear	5.3
III	Non-linear	5.3
IV	Linear	5.4
IV	Non-linear	5.4

Table 1: Location in this report of descriptions of solution algorithms corresponding to the four main types of calibration problem, for linear and non-linear calibration functions.

---

types III and IV, where non-direct methods involving the application of the Gauss-Newton algorithm [11] are recommended, there is no clear advantage in distinguishing between linear and non-linear calibration functions.

Example: Preparation of primary standard natural gas mixtures Within the Centre for Optical and Analytical Measurement at NPL, one part of the work of the Environmental Standards Group is to prepare primary standard natural gas mixtures. Cylinders containing natural gas are prepared gravimetrically to contain known compositions of each of the 11 constituent components (methane, ethane, propane, l-butane, n-butane, l-pentane, n-pentane, neo-pentane, hexane, nitrogen and carbon dioxide). Mixtures are prepared to cover various concentration ranges, e.g., methane: $64\% - 98\%$. These primary standard mixtures are used as the basis for determining the composition of a new mixture and hence its calorific value.

Given a number of primary standard natural gas mixtures containing known concentrations of one of the constituent components (e.g., CO_2), the detector response for each mixture and the detector response for the new mixture, it is required to determine the concentration of CO_2 in the new mixture.

An approach to solving this problem is firstly to use the calibration data (relating to the primary gas mixtures) to calibrate the detector and, secondly, to use the calibration curve so constructed with the new measurement to predict the concentration in the new mixture.

Uncertainties to be accounted for are:

- the process of preparing the primary standards means that they are known inexactly, and indeed the uncertainties in the standards may be correlated

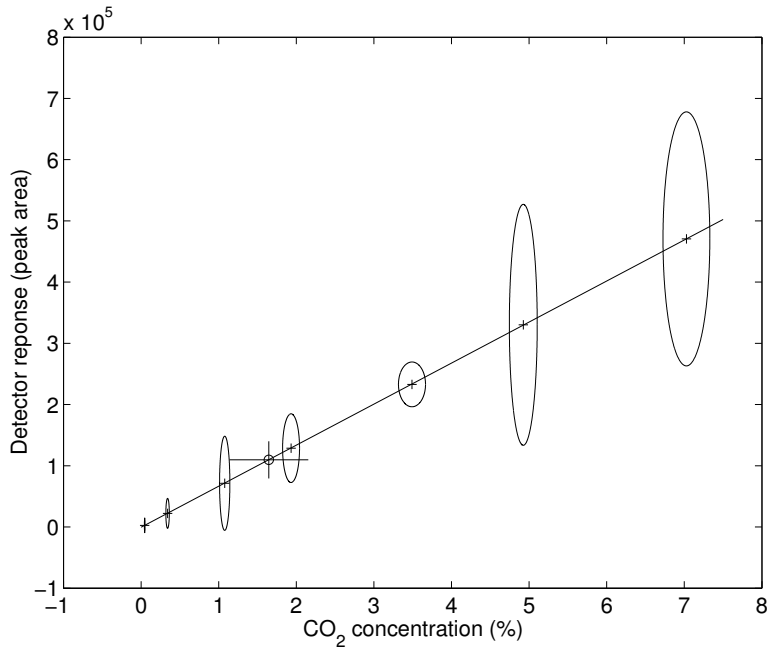

Figure 1: Sample data (+), fitted calibration curve and predicted measurement (○).

(this is a consequence of the gravimetric process used to prepare the standard mixtures which involves comparing on a balance each standard mixture at each stage of preparation against calibrated masses selected from a common set of masses),

- the data returned by the detector (which is based on the analytical technique of chromatography) is subject to measurement uncertainty.

The data analysis has to account for the inexactness of the measurement data and quantify the resulting uncertainty associated with the final measurement result.

Figure 1 shows a sample set of measurement data, with the ellipses around the calibration points illustrating the uncertainties in the concentrations and detector responses. (The uncertainty ellipses have been magnified greatly for illustrative purposes.) The figure also shows a linear calibration curve which is used to estimate the concentration of the component for which the detector response (and its uncertainty) is known.

Note that of the ten models described earlier in this section, this example is classified as uncertainty model 9 (and the resulting calibration problem therefore is classified as type IV).

♯

4 Linear models

In this section, we assume that the calibration function is linear in the parameters $\mathbf{a}$, i.e.,

$$h(t_i, \mathbf{a}) = \sum_{j=1}^{n} a_j h_j(t_i),$$

and define C to be the $m \times n$ matrix whose ith row is $\mathbf{c}_i^{\mathrm{T}}$, where

$$\mathbf{c}_i = \begin{bmatrix} h_1(t_i) \\ \vdots \\ h_n(t_i) \end{bmatrix}.$$

4.1 Linear diagonally weighted least squares problems

Consider the case where the measurements $\{t_i\}_1^m$ of the stimulus variable are assumed to be accurate relative to the measurements $\{v_i\}_1^m$ of the response variable, the response variable measurements being uncorrelated and therefore having (diagonal) uncertainty matrix

$$U_{\mathbf{v}} = \mathrm{diag}\{\sigma_1^2, \ldots, \sigma_m^2\}, \quad \sigma_i > 0.$$

The LSA problem is

$$\min_{\mathbf{a}} \ (\mathbf{h}(\mathbf{t}, \mathbf{a}) - \mathbf{v})^{\mathrm{T}} U_{\mathbf{v}}^{-1} (\mathbf{h}(\mathbf{t}, \mathbf{a}) - \mathbf{v}).$$

The matrix $U_{\mathbf{v}}$ can be written as

$$U_{\mathbf{v}} = LL^{\mathrm{T}},$$

where $L = \mathrm{diag}\{\sigma_1, \ldots, \sigma_m\}$.

Setting $\tilde{C} = L^{-1}C$ and $\tilde{\mathbf{v}} = L^{-1}\mathbf{v}$, the LSA problem takes the form of a (weighted) linear least squares problem, and estimates of $\mathbf{a}$ are found by solving

$$\min_{\mathbf{a}} \ \left(\tilde{C}\mathbf{a} - \tilde{\mathbf{v}}\right)^{\mathrm{T}} \left(\tilde{C}\mathbf{a} - \tilde{\mathbf{v}}\right),$$

i.e.,

$$\min_{\mathbf{a}} \ \|\tilde{C}\mathbf{a} - \tilde{\mathbf{v}}\|^2.$$

4.1.1 Solution algorithm

For reasons of numerical stability and efficiency, the use of orthogonal factorisation is generally recommended to solve this problem. The matrix $\tilde{C}$ has QR factorisation [12]

$$\tilde{C} = \tilde{Q} \begin{bmatrix} \tilde{R} \\ \mathbf{0} \end{bmatrix}, \tag{4}$$

where $\tilde{Q}$ is $m \times m$ orthogonal, i.e., $\tilde{Q}^{\mathrm{T}}\tilde{Q} = I$, the $m \times m$ identity matrix, and $\tilde{R}$ is $n \times n$ upper-triangular.

Using the fact that $\|\tilde{Q}^{\mathrm{T}}\mathbf{x}\| = \|\mathbf{x}\|$, we have

$$\|\tilde{C}\mathbf{a} - \tilde{\mathbf{v}}\| = \|\tilde{Q}^{\mathrm{T}}\tilde{C}\mathbf{a} - \tilde{Q}^{\mathrm{T}}\tilde{\mathbf{v}}\| = \left\| \begin{bmatrix} \tilde{R} \\ \mathbf{0} \end{bmatrix} \mathbf{a} - \begin{bmatrix} \tilde{\mathbf{q}}_1 \\ \tilde{\mathbf{q}}_2 \end{bmatrix} \right\|,$$

where $\tilde{\mathbf{q}}_1$ is the first n and $\tilde{\mathbf{q}}_2$ the last $m - n$ elements of $\tilde{Q}^{\mathrm{T}}\tilde{\mathbf{v}}$. From this it is seen that $\|\tilde{C}\mathbf{a} - \tilde{\mathbf{v}}\|$ is minimised if $\mathbf{a}$ solves the upper-triangular system

$$\tilde{R}\mathbf{a} = \tilde{\mathbf{q}}_1.$$

$\tilde{C}$ and $\tilde{\mathbf{v}}$ can be calculated efficiently from C and v by row scaling:

$$\tilde{\mathbf{c}}_i = \frac{\mathbf{c}_i}{\sigma_i}, \quad \tilde{v}_i = \frac{v_i}{\sigma_i}.$$

4.1.2 Uncertainties associated with solution parameters

$U_{\tilde{\mathbf{a}}}$, the uncertainty matrix associated with the solution parameters $\tilde{\mathbf{a}}$, is given by [13]

$$U_{\tilde{\mathbf{a}}} = UU^{\mathrm{T}},$$

where U is the solution of the upper-triangular system

$$\tilde{R}U = I.$$

A fuller derivation of this expression can be found in Appendix D.

4.2 Linear Gauss-Markov regression problems

Consider the case where the measurements $\{t_i\}_1^m$ of the stimulus variable are assumed to be accurate relative to the measurements $\{v_i\}_1^m$ of the response variable, the response variable measurements being correlated and therefore having (general) uncertainty matrix $U_{\mathbf{v}}$ with $\mathrm{rank}(U_{\mathbf{v}}) = m$.

The LSA problem is

$$\min_{\mathbf{a}} \ (\mathbf{h}(\mathbf{t},\mathbf{a}) - \mathbf{v})^{\mathrm{T}} U_{\mathbf{v}}^{-1} (\mathbf{h}(\mathbf{t},\mathbf{a}) - \mathbf{v}),$$

and takes the form of a linear Gauss-Markov regression problem, with estimates of $\mathbf{a}$ found by solving

$$\min_{\mathbf{a}} \ (C\mathbf{a} - \mathbf{v})^{\mathrm{T}} U_{\mathbf{v}}^{-1} (C\mathbf{a} - \mathbf{v}).$$

4.2.1 Solution algorithms

The Gauss-Markov estimate can be found by forming the Cholesky decomposition [12] of $U_{\mathbf{v}}$,

$$U_{\mathbf{v}} = LL^{\mathrm{T}},$$

where L is $m \times m$ lower-triangular, and then solving

$$\min_{\mathbf{a}} \ \left\| \tilde{C}\mathbf{a} - \tilde{\mathbf{v}} \right\|^2, \tag{5}$$

where $\tilde{C}$ and $\tilde{\mathbf{v}}$ solve the upper-triangular systems

$$L\tilde{C} = C, \quad L\tilde{\mathbf{v}} = \mathbf{v}.$$

This problem can be solved using the approach described in section 4.1.1.

However, if $U_{\mathbf{v}}$ is poorly conditioned (a consequence of strong correlation effects) the formation of $\tilde{C}$ and $\tilde{\mathbf{v}}$ may introduce significant numerical instability.

A stable approach to solving this type of problem is provided by *generalised QR factorisation*. This section will list the main points in the application of this method. More details can be found in Appendix A.

Evaluate the generalised QR factorisation of the pair (C, L), i.e., find $m \times m$ orthogonal matrix Q, $n \times n$ upper-triangular matrix R, $m \times m$ upper-triangular matrix T and $m \times m$ orthogonal matrix Z such that

$$C = Q \begin{bmatrix} R \\ \mathbf{0} \end{bmatrix}, \quad Q^{\mathrm{T}} L = TZ.$$

Partition Q and T:

$$Q = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix}, \quad T = \begin{bmatrix} T_{11} & T_{12} \\ \mathbf{0} & T_{22} \end{bmatrix},$$

where Q_1, Q_2, T_{11}, T_{12} and T_{22} are respectively $m \times n$, $m \times (m-n)$, $n \times n$ upper-triangular, $n \times (m-n)$ and $(m-n) \times (m-n)$ upper-triangular.

Let $(m-n) \times (m-n)$ matrix $\tilde{T}_{22}$ be the solution of the upper-triangular system

$$T_{22}\tilde{T}_{22} = I.$$

The solution parameters $\tilde{\mathbf{a}}$ are then given by the solution of the upper-triangular system

$$R\tilde{\mathbf{a}} = \left(Q_1^{\mathrm{T}} - T_{12}\tilde{T}_{22}Q_2^{\mathrm{T}}\right)\mathbf{v}.$$

The generalised QR factorisation can also be applied in the case where $U_{\mathbf{v}}$ is not full rank, but we do not consider this case further here.

4.2.2 Uncertainties associated with solution parameters

$U_{\tilde{\mathbf{a}}}$, the uncertainty matrix associated with the solution parameters $\tilde{\mathbf{a}}$, is given by

$$U_{\tilde{\mathbf{a}}} = UU^{\mathrm{T}},$$

where U is the solution of the upper-triangular system

$$RU = T_{11}.$$

A fuller derivation of this expression can be found in Appendix D.

5 Non-linear models

5.1 Non-linear diagonally weighted least squares problems

Consider the case where the measurements $\{t_i\}_1^m$ of the stimulus variable are assumed to be accurate relative to the measurements $\{v_i\}_1^m$ of the response variable, the response variable measurements being uncorrelated and therefore having associated uncertainty matrix

$$U_{\mathbf{v}} = \mathrm{diag}\{\sigma_1^2, \ldots, \sigma_m^2\}, \quad \sigma_i > 0.$$

The LSA problem is

$$\min_{\mathbf{a}} \ (\mathbf{h}(\mathbf{t}, \mathbf{a}) - \mathbf{v})^{\mathrm{T}} U_{\mathbf{v}}^{-1} (\mathbf{h}(\mathbf{t}, \mathbf{a}) - \mathbf{v}) .$$

If the calibration function is non-linear in the parameters $\mathbf{a}$, then the above LSA problem takes the form of a weighted non-linear least squares problem, and estimates of the parameters $\mathbf{a}$ can be found by solving

$$\min_{\mathbf{a}} \ \sum_{i=1}^{m} \tilde{f}_i^2(\mathbf{a}), \tag{6}$$

where

$$\tilde{f}_i(\mathbf{a}) = \frac{h(t_i, \mathbf{a}) - v_i}{\sigma_i}.$$

5.1.1 Solution algorithm

Let

$$\tilde{\mathbf{f}}(\mathbf{a}) = \begin{bmatrix} \tilde{f}_1(\mathbf{a}) \\ \vdots \\ \tilde{f}_m(\mathbf{a}) \end{bmatrix}.$$

Then the minimisation problem (6) can be written as

$$\min_{\mathbf{a}} \ \tilde{\mathbf{f}}^{\mathrm{T}}(\mathbf{a}) \tilde{\mathbf{f}}(\mathbf{a}).$$

Estimates of the solution parameters can be found by applying the Gauss-Newton algorithm (see Appendix B) to $\tilde{\mathbf{f}}(\mathbf{a})$.

At each iteration of the Gauss-Newton algorithm we are required to solve, in the least squares sense,

$$\tilde{J}\mathbf{p} = -\tilde{\mathbf{f}},$$

where $\tilde{J}$ is the $m \times n$ Jacobian matrix associated with $\tilde{\mathbf{f}}$, evaluated at the current estimate $\widehat{\mathbf{a}}$ of the solution parameters.

An updated estimate of the calibration curve parameters is now given by $\widehat{\mathbf{a}} + \mathbf{p}$.

5.1.2 Uncertainties associated with solution parameters

$U_{\tilde{\mathbf{a}}}$, the uncertainty matrix associated with the solution parameters $\tilde{\mathbf{a}}$, is given by

$$U_{\tilde{\mathbf{a}}} = \left(\tilde{J}^{\mathrm{T}}\tilde{J}\right)^{-1},$$

where $\tilde{J}$ is the $m \times n$ Jacobian matrix associated with $\tilde{\mathbf{f}}(\tilde{\mathbf{a}})$.

Let $\tilde{J}$ have QR factorisation

$$\tilde{J} = \tilde{Q}\begin{bmatrix} \tilde{R} \\ \mathbf{0} \end{bmatrix},$$

where $\tilde{Q}$ is $m \times m$ orthogonal and $\tilde{R}$ is $n \times n$ upper-triangular.

Since

$$\tilde{J}^{\mathrm{T}}\tilde{J} = \tilde{R}^{\mathrm{T}}\tilde{R},$$

$U_{\tilde{\mathbf{a}}}$ is given by

$$U_{\tilde{\mathbf{a}}} = UU^{\mathrm{T}},$$

where U is the solution of the upper-triangular system

$$\tilde{R}U = I.$$

5.2 Non-linear Gauss-Markov regression problems

Consider the case where the measurements $\{t_i\}_1^m$ of the stimulus variable are assumed to be accurate relative to the measurements $\{v_i\}_1^m$ of the response variable, the response variable measurements being correlated and therefore having associated uncertainty matrix $U_{\mathbf{v}}$ with $\mathrm{rank}(U_{\mathbf{v}}) = m$.

The LSA problem is

$$\min_{\mathbf{a}} \ (\mathbf{h}(\mathbf{t},\mathbf{a}) - \mathbf{v})^{\mathrm{T}} U_{\mathbf{v}}^{-1} (\mathbf{h}(\mathbf{t},\mathbf{a}) - \mathbf{v}).$$

If the calibration function is non-linear in the parameters $\mathbf{a}$, then the above LSA problem takes the form of a non-linear Gauss-Markov problem, and estimates of the parameters $\mathbf{a}$ can be found by solving

$$\min_{\mathbf{a}} \ \mathbf{f}(\mathbf{a})^{\mathrm{T}} U_{\mathbf{v}}^{-1} \mathbf{f}(\mathbf{a}), \tag{7}$$

where

$$\mathbf{f}(\mathbf{a}) = \begin{bmatrix} f_1(\mathbf{a}) \\ \vdots \\ f_m(\mathbf{a}) \end{bmatrix} = \begin{bmatrix} h(t_1, \mathbf{a}) - v_1 \\ \vdots \\ h(t_m, \mathbf{a}) - v_m \end{bmatrix}.$$

5.2.1 Solution algorithms

Calculate the Cholesky factorisation $U_{\mathbf{v}} = LL^{\mathrm{T}}$, where L is $m \times m$ lower-triangular, and let

$$L\tilde{\mathbf{f}}(\mathbf{a}) = \mathbf{f}(\mathbf{a}).$$

Then the minimisation problem (7) can be written as

$$\min_{\mathbf{a}} \ \tilde{\mathbf{f}}^{\mathrm{T}}(\mathbf{a})\tilde{\mathbf{f}}(\mathbf{a}).$$

Estimates of the solution parameters can be found by applying the Gauss-Newton algorithm (see Appendix B) to $\tilde{\mathbf{f}}(\mathbf{a})$.

At each iteration of the Gauss-Newton algorithm we are required to solve, in the least squares sense,

$$\tilde{J}\mathbf{p} = -\tilde{\mathbf{f}}, \quad L\tilde{J} = J,$$

where J is the $m \times n$ Jacobian matrix associated with $\mathbf{f}$, evaluated at the current estimate $\widehat{\mathbf{a}}$ of the solution parameters.

As in the linear case, if L is well conditioned this represents a satisfactory approach to solving (7). Otherwise, the formation of $\tilde{J}$ and $\tilde{\mathbf{f}}$ can introduce numerical instability.

A stable approach to finding the update step is provided by generalised QR factorisation. This section will list here only the main points in the application of this method. More details can be found in Appendix A.

Evaluate the generalised QR factorisation of the pair (J, L), i.e., find $m \times m$ orthogonal matrix Q, $n \times n$ upper-triangular matrix R, $m \times m$ upper-triangular matrix T and $m \times m$ orthogonal matrix Z such that

$$J = Q \begin{bmatrix} R \\ \mathbf{0} \end{bmatrix}, \quad Q^{\mathrm{T}} L = TZ.$$

Partition Q and T:

$$Q = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix}, \quad T = \begin{bmatrix} T_{11} & T_{12} \\ \mathbf{0} & T_{22} \end{bmatrix},$$

where Q_1, Q_2, T_{11}, T_{12} and T_{22} are respectively $m \times n$, $m \times (m-n)$, $n \times n$ upper-triangular, $n \times (m-n)$ and $(m-n) \times (m-n)$ upper-triangular.

Let $(m-n) \times (m-n)$ matrix $\tilde{T}_{22}$ be the solution of the upper-triangular system

$$T_{22}\tilde{T}_{22} = I.$$

The Gauss-Newton step $\mathbf{p}$ is then given by the solution of the upper-triangular system

$$R\mathbf{p} = \left(T_{12}\tilde{T}_{22}Q_2^{\mathrm{T}} - Q_1^{\mathrm{T}}\right)\mathbf{f}.$$

An updated estimate of the calibration curve parameters is now given by $\widehat{\mathbf{a}} + \mathbf{p}$.

We note that, unlike the linear case in Section 4.2, the case where $U_{\mathbf{v}}$ is not full rank cannot in general be solved using the Gauss-Newton algorithm and generalised QR factorisation since the optimisation problem involves non-linear constraints.

5.2.2 Uncertainties associated with solution parameters

$U_{\tilde{\mathbf{a}}}$, the uncertainty matrix associated with the solution parameters $\tilde{\mathbf{a}}$ is given by

$$U_{\tilde{\mathbf{a}}} = \left(\tilde{J}^{\mathrm{T}}\tilde{J}\right)^{-1},$$

where $L\tilde{J} = J$, J being the Jacobian matrix evaluated at the solution parameters $\tilde{\mathbf{a}}$.

A similar analysis to that carried out in Section 4.2.2 (see also Appendix D for a fuller derivation) gives

$$U_{\tilde{\mathbf{a}}} = UU^{\mathrm{T}},$$

where U is the solution of the upper-triangular problem

$$RU = T_{11}.$$

5.3 Generalised distance regression problems

Consider the case where the the stimulus variable measurements are uncorrelated and have uncertainty matrix $U_{\mathbf{t}} = \mathrm{diag}\{\rho_1^2, \ldots, \rho_m^2\}$, the response variable measurements are uncorrelated and have uncertainty matrix $U_{\mathbf{v}} = \mathrm{diag}\{\sigma_1^2, \ldots, \sigma_m^2\}$ and the ith measurements t_i and v_i are correlated with $\mathrm{cov}(v_i, t_i) = \alpha_i$, i.e., $U_{\mathbf{vt}} = \mathrm{diag}\{\alpha_1, \ldots, \alpha_m\}$, $\sigma_i^2\rho_i^2 - \alpha_i^2 \neq 0$.

The LSA problem is

$$\min_{\mathbf{a},\mathbf{q}} \begin{bmatrix} \mathbf{h}(\mathbf{q},\mathbf{a}) - \mathbf{v} \\ \mathbf{q} - \mathbf{t} \end{bmatrix}^{\mathrm{T}} U_{\mathbf{x}}^{-1} \begin{bmatrix} \mathbf{h}(\mathbf{q},\mathbf{a}) - \mathbf{v} \\ \mathbf{q} - \mathbf{t} \end{bmatrix},$$

where

$$U_{\mathbf{x}} = \begin{bmatrix} U_{\mathbf{v}} & U_{\mathbf{vt}} \\ U_{\mathbf{vt}}^{\mathrm{T}} & U_{\mathbf{t}} \end{bmatrix}.$$

Estimates of $\mathbf{a}$ and $\mathbf{q}$ can be found by solving

$$\min_{\mathbf{a},\mathbf{q}} \sum_{i=1}^{m} \begin{bmatrix} h(q_i,\mathbf{a}) - v_i \\ q_i - t_i \end{bmatrix}^{\mathrm{T}} U_i^{-1} \begin{bmatrix} h(q_i,\mathbf{a}) - v_i \\ q_i - t_i \end{bmatrix}, \tag{8}$$

where

$$U_i = \begin{bmatrix} \sigma_i^2 & \alpha_i \\ \alpha_i & \rho_i^2 \end{bmatrix}.$$

5.3.1 Solution algorithm

Generalised distance regression problems can be solved efficiently by taking advantage of the fact that the parameter q_i appears *only* in the ith summand in (8), allowing the application of a structured approach to solve the Jacobian system [5, 6].

For each $i = 1, \ldots, m$, calculate the Cholesky factorisation $U_i = L_i^{\mathrm{T}} L_i$, where L is 2×2 lower-triangular.

Let

$$L_i \tilde{\mathbf{f}}_i(q_i,\mathbf{a}) = \begin{bmatrix} h(q_i,\mathbf{a}) - v_i \\ q_i - t_i \end{bmatrix},$$

and

$$\tilde{\mathbf{f}}(\mathbf{q},\mathbf{a}) = \begin{bmatrix} \tilde{\mathbf{f}}_1(q_1,\mathbf{a}) \\ \vdots \\ \tilde{\mathbf{f}}_m(q_m,\mathbf{a}) \end{bmatrix}.$$

Then the minimisation problem (8) can be written as

$$\min_{\mathbf{a},\mathbf{q}} \tilde{\mathbf{f}}^{\mathrm{T}}(\mathbf{q},\mathbf{a}) \tilde{\mathbf{f}}(\mathbf{q},\mathbf{a}).$$

Estimates of the solution parameters can be found by applying the Gauss-Newton algorithm (see Appendix B) to $\tilde{\mathbf{f}}(\mathbf{q},\mathbf{a})$.

At each iteration of the Gauss-Newton algorithm we are required to solve, in the least squares sense,

$$\tilde{J}\mathbf{p} = -\tilde{\mathbf{f}}, \tag{9}$$

where $\tilde{J}$ is the $2m \times (m+n)$ Jacobian matrix associated with $\tilde{\mathbf{f}}$, evaluated at the current estimates

$$\widehat{\zeta} = \begin{bmatrix} \widehat{\mathbf{q}} \\ \widehat{\mathbf{a}} \end{bmatrix}$$

of the solution parameters.

$\tilde{J}$ can be written as

$$\tilde{J} = \begin{bmatrix} \tilde{K}_1 & & & \tilde{J}_1 \\ & \ddots & & \vdots \\ & & \tilde{K}_m & \tilde{J}_m \end{bmatrix},$$

i.e., $\tilde{J}$ is composed of the 2×1 blocks $\{\tilde{K}_i\}_1^m$ and $2 \times n$ blocks $\{\tilde{J}_i\}_1^m$ where

$$L_i\tilde{K}_i = \begin{bmatrix} \frac{\partial h}{\partial q}(q_i, \mathbf{a}) \\ 1 \end{bmatrix}$$

and

$$L_i\tilde{J}_i = \begin{bmatrix} \frac{\partial h}{\partial a_1}(q_i, \mathbf{a}) & \cdots & \frac{\partial h}{\partial a_n}(q_i, \mathbf{a}) \\ 0 & \cdots & 0 \end{bmatrix}.$$

The update step $\mathbf{p}$ can be found using QR factorisation[3] as follows:

1. Find $2m \times 2m$ orthogonal matrix $\tilde{Q}$ and $(m+n) \times (m+n)$ upper-triangular matrix $\tilde{R}$ such that
$$\tilde{J} = \tilde{Q} \begin{bmatrix} \tilde{R} \\ \mathbf{0} \end{bmatrix}. \tag{10}$$

2. $\mathbf{p}$ is the solution of the upper-triangular system
$$\tilde{R}\mathbf{p} = \widehat{\mathbf{f}}_1,$$
where $\widehat{\mathbf{f}}_1$ is the first $m+n$ elements of $\tilde{Q}^{\mathrm{T}}\tilde{\mathbf{f}}$.

An updated estimate of the solution parameters is now given by $\widehat{\zeta} + \mathbf{p}$.

Other approaches to solving generalised distance regression problems are considered in [7, 2].

[3] An efficient approach to finding the update step is described in Appendix D.

5.3.2 Uncertainties associated with solution parameters

Let $\tilde{R}_0$ be the lower-right $n \times n$ block of the upper-triangular factor $\tilde{R}$ of the matrix $\tilde{J}$ as defined in (10).

$U_{\tilde{\mathbf{a}}}$, the uncertainty matrix associated with the solution parameters $\tilde{\mathbf{a}}$, is given by

$$U_{\tilde{\mathbf{a}}} = UU^{\mathrm{T}},$$

where U is the solution of the upper-triangular system

$$\tilde{R}_0 U = I.$$

A fuller derivation of this expression can be found in Appendix D.

5.4 Generalised Gauss-Markov regression problems

Consider the case where the the measurements are generally correlated and have uncertainty matrix $U_{\mathbf{x}}$ with $\mathrm{rank}(U_{\mathbf{x}}) = 2m$.

The LSA problem is

$$\min_{\mathbf{a},\mathbf{q}} \left[\begin{array}{c} \mathbf{h}(\mathbf{q},\mathbf{a}) - \mathbf{v} \\ \mathbf{q} - \mathbf{t} \end{array} \right]^{\mathrm{T}} U_{\mathbf{x}}^{-1} \left[\begin{array}{c} \mathbf{h}(\mathbf{q},\mathbf{a}) - \mathbf{v} \\ \mathbf{q} - \mathbf{t} \end{array} \right]. \tag{11}$$

5.4.1 Solution algorithm

Calculate the Cholesky factorisation $U_{\mathbf{x}} = LL^{\mathrm{T}}$ where L is $2m \times 2m$ lower triangular. Let

$$\mathbf{f}(\mathbf{q},\mathbf{a}) = \left[\begin{array}{c} \mathbf{h}(\mathbf{q},\mathbf{a}) - \mathbf{v} \\ \mathbf{q} - \mathbf{t} \end{array} \right]$$

and

$$L\tilde{\mathbf{f}}(\mathbf{q},\mathbf{a}) = \mathbf{f}(\mathbf{q},\mathbf{a}).$$

Then the minimisation problem (11) can be written as

$$\min_{\mathbf{a},\mathbf{q}} \tilde{\mathbf{f}}^{\mathrm{T}}(\mathbf{q},\mathbf{a})\tilde{\mathbf{f}}(\mathbf{q},\mathbf{a}).$$

Estimates of the solution parameters can be found by applying the Gauss-Newton algorithm (see Appendix B) to $\tilde{\mathbf{f}}(\mathbf{q},\mathbf{a})$.

At each iteration of the Gauss-Newton algorithm we are required to solve, in the least squares sense,

$$\tilde{J}\mathbf{p} = -\tilde{\mathbf{f}}, \quad L\tilde{J} = J, \tag{12}$$

where J is the $2m \times (m+n)$ Jacobian matrix associated with the functions $\mathbf{f}(\mathbf{q}, \mathbf{a})$, evaluated at the current estimates

$$\widehat{\zeta} = \begin{bmatrix} \widehat{\mathbf{q}} \\ \widehat{\mathbf{a}} \end{bmatrix}$$

of the solution parameters.

J can be written as

$$J = \begin{bmatrix} K_1 & & J_1 \\ & \ddots & \vdots \\ & K_m & J_m \end{bmatrix},$$

i.e., J is composed of the 2×1 blocks $\{K_i\}_1^m$ and $2 \times n$ blocks $\{J_i\}_1^m$ where

$$K_i = \begin{bmatrix} \frac{\partial h}{\partial q}(q_i, \mathbf{a}) \\ 1 \end{bmatrix}$$

and

$$J_i = \begin{bmatrix} \frac{\partial h}{\partial a_1}(q_i, \mathbf{a}) & \cdots & \frac{\partial h}{\partial a_n}(q_i, \mathbf{a}) \\ 0 & \cdots & 0 \end{bmatrix}.$$

If L is poorly conditioned, the formation of $\tilde{J}$ and $\tilde{\mathbf{f}}$ can be numerically unstable. A stable approach to finding the update step is provided by generalised QR factorisation. This section will list here only the main points in the application of this method. More details can be found in Appendix A.

Evaluate the generalised QR factorisation[4] of the pair (J, L), i.e., find $2m \times 2m$ orthogonal matrix Q, $(m+n) \times (m+n)$ upper-triangular matrix R, $2m \times 2m$ upper-triangular matrix T and $2m \times 2m$ orthogonal matrix Z such that

$$J = Q \begin{bmatrix} R \\ \mathbf{0} \end{bmatrix}, \quad Q^{\mathrm{T}} L = TZ.$$

Partition Q and T:

$$Q = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix}, \quad T = \begin{bmatrix} T_{11} & T_{12} \\ \mathbf{0} & T_{22} \end{bmatrix},$$

where Q_1, Q_2, T_{11}, T_{12} and T_{22} are respectively $2m \times (m+n)$, $2m \times (m-n)$, $(m+n) \times (m+n)$ upper-triangular, $(m+n) \times (m-n)$ and $(m-n) \times (m-n)$ upper-triangular.

[4] An efficient approach to evaluating the QR factorisation is described in Appendix D.

Let $(m-n) \times (m-n)$ matrix $\tilde{T}_{22}$ be the solution of the upper-triangular system

$$T_{22}\tilde{T}_{22} = I.$$

Then the Gauss-Newton step $\mathbf{p}$ is then given by the solution of the upper-triangular system

$$R\mathbf{p} = \left(T_{12}\tilde{T}_{22}Q_2^{\mathrm{T}} - Q_1^{\mathrm{T}}\right)\mathbf{f}.$$

An updated estimate of the calibration curve parameters is now given by $\widehat{\mathbf{a}} + \mathbf{p}$.

We note that the case where $U_{\mathbf{x}}$ is not full rank cannot in general be solved using the Gauss-Newton algorithm and generalised QR factorisation since the optimisation problem involves non-linear constraints.

5.4.2 Uncertainties associated with solution parameters

Partition R and T_{11}:

$$R = \begin{bmatrix} R_{11} & R_{12} \\ \mathbf{0} & R_0 \end{bmatrix}, \quad T_{11} = \begin{bmatrix} W_{11} & W_{12} \\ \mathbf{0} & W_{22} \end{bmatrix},$$

where R_{11} and W_{11} are $m \times m$ upper-triangular, R_{12} and W_{12} are $m \times n$ and R_0 and W_{22} are $n \times n$ upper-triangular.

$U_{\tilde{\mathbf{a}}}$, the uncertainty matrix associated with the solution parameters $\tilde{\mathbf{a}}$, is given by

$$U_{\tilde{\mathbf{a}}} = UU^{\mathrm{T}},$$

where U is the solution of the upper-triangular system

$$R_0 U = W_{22}.$$

A fuller derivation of this expression can be found in Appendix D.

6 Applications of the calibration curve

6.1 Function evaluation

One use of a calibration curve obtained by LSA is to estimate the values of the response variable and the associated uncertainty matrix corresponding to given values of the stimulus variable and their associated uncertainty matrix.

In the following, it is assumed that calibration curve parameters $\tilde{\mathbf{a}}$ and their associated uncertainty matrix $U_{\tilde{\mathbf{a}}}$ have been obtained using LSA. Note that often other information associated with the calibration needs to be stored, e.g., in fitting a polynomial curve using Chebyshev polynomials (see Section 7), the values $x_{\min}$ and $x_{\max}$ used to normalise the data abscissae.

The results quoted below are obtained using an approach to uncertainty evaluation consistent with those recommended by the GUM [3].

6.1.1 Linear models

Given a number of values (that may or may not correspond to measurements) $\{t_{0,k}\}_1^p$ of the stimulus variable and associated uncertainty matrix $U_{\mathbf{t}_0}$, the calibration curve can be used to obtain estimates of the corresponding response variables $\{v_{0,k}\}_1^p$:

$$\mathbf{v}_0 = \begin{bmatrix} v_{0,1} \\ \vdots \\ v_{0,p} \end{bmatrix} = C_{\mathbf{t}_0}\tilde{\mathbf{a}},$$

where $C_{\mathbf{t}_0}$ is the $p \times n$ matrix whose kth row is $(h_1(t_{0,k}), \ldots, h_n(t_{0,k}))$.

Assuming that the calibration curve parameters $\tilde{\mathbf{a}}$ and the values $\{t_{0,k}\}_1^p$ are not correlated, $U_{\mathbf{v}_0}$, the uncertainty matrix associated with $\mathbf{v}_0$, is given by

$$U_{\mathbf{v}_0} = J_{\mathbf{t}_0} U_{\mathbf{t}_0} J_{\mathbf{t}_0} + C_{\mathbf{t}_0} U_{\tilde{\mathbf{a}}} C_{\mathbf{t}_0}^{\mathrm{T}},$$

where $J_{\mathbf{t}_0} = \operatorname{diag}\left\{\frac{\partial h}{\partial t}(t_{0,1}), \ldots, \frac{\partial h}{\partial t}(t_{0,p})\right\}$.

In particular, for a single stimulus variable value t_0 with associated uncertainty u_{t_0}, an estimate v_0 of the response variable is

$$v_0 = \mathbf{c}_{t_0}^{\mathrm{T}}\tilde{\mathbf{a}},$$

where

$$\mathbf{c}_{t_0} = \begin{bmatrix} h_1(t_0) \\ \vdots \\ h_n(t_0) \end{bmatrix}.$$

u_{v_0}, the standard uncertainty associated with v_0, is given by

$$u_{v_0} = \left(\left[\frac{\partial h}{\partial t}(t_0) \right]^2 u_{t_0}^2 + \mathbf{c}_{t_0}^{\mathrm{T}} U_{\tilde{\mathbf{a}}} \mathbf{c}_{t_0} \right)^{\frac{1}{2}}.$$

6.1.2 Non-linear models

Given a number of values $\{t_{0,k}\}_1^p$ of the stimulus variable and associated uncertainty matrix $U_{\mathbf{t}_0}$, the calibration curve can be used to obtain estimates of the corresponding response variables $\{v_{0,k}\}_1^p$:

$$\mathbf{v}_0 = \begin{bmatrix} v_{0,1} \\ \vdots \\ v_{0,p} \end{bmatrix} = \begin{bmatrix} h(t_{0,1}, \tilde{\mathbf{a}}) \\ \vdots \\ h(t_{0,p}, \tilde{\mathbf{a}}) \end{bmatrix}.$$

Assuming that the calibration curve parameters $\tilde{\mathbf{a}}$ and the values $\{t_{0,k}\}_1^p$ are not correlated, $U_{\mathbf{v}_0}$, the uncertainty matrix associated with $\mathbf{v}_0$, is given by

$$U_{\mathbf{v}_0} = J_{\mathbf{t}_0} U_{\mathbf{t}_0} J_{\mathbf{t}_0} + J_{\tilde{\mathbf{a}}} U_{\tilde{\mathbf{a}}} J_{\tilde{\mathbf{a}}}^{\mathrm{T}},$$

where $J_{\mathbf{t}_0} = \operatorname{diag}\left\{ \frac{\partial h}{\partial t}(t_{0,1}, \tilde{\mathbf{a}}), \ldots, \frac{\partial h}{\partial t}(t_{0,p}, \tilde{\mathbf{a}}) \right\}$ and $J_{\tilde{\mathbf{a}}}$ is the $p \times n$ matrix whose ith row is $(\nabla_{\mathbf{a}} h(t_{0,i}, \tilde{\mathbf{a}}))^{\mathrm{T}}$.

In particular, for a single stimulus variable value t_0 with associated uncertainty u_{t_0}, an estimate v_0 of the response variable is

$$v_0 = h(t_0, \tilde{\mathbf{a}}).$$

u_{v_0}, the standard uncertainty associated with v_0, is given by

$$u_{v_0} = \left(\left[\frac{\partial h}{\partial t}(t_0, \tilde{\mathbf{a}}) \right]^2 u_{t_0}^2 + \left(\nabla_{\mathbf{a}} h(t_0, \tilde{\mathbf{a}}) \right)^{\mathrm{T}} U_{\tilde{\mathbf{a}}} \left(\nabla_{\mathbf{a}} h(t_0, \tilde{\mathbf{a}}) \right) \right)^{\frac{1}{2}}.$$

6.2 Inverse function evaluation

A problem more frequently encountered is that of inverse function evaluation, i.e., given a value of the response variable and its uncertainty, estimate the value of the stimulus variable and the associated uncertainty.

Given a number of measurements $\{v_{0,k}\}_1^p$ of the response variable and associated uncertainty matrix $U_{\mathbf{v}_0}$, the calibration curve can be used to obtain estimates of the corresponding stimulus variables $\{t_{0,k}\}_1^p$. Typically each estimate $t_{0,k}$ is found using a bisection method (see Appendix C).

Assuming that the calibration curve parameters $\tilde{\mathbf{a}}$ and the values $\{v_{0,k}\}_1^p$ are not correlated, $U_{\mathbf{t}_0}$, the uncertainty matrix associated with

$$\mathbf{t}_0 = \begin{bmatrix} t_{0,1} \\ \vdots \\ t_{0,p} \end{bmatrix}$$

is given by

$$U_{\mathbf{t}_0} = J_{\mathbf{t}_0}^{-1} \left[U_{\mathbf{v}_0} + J_{\tilde{\mathbf{a}}} U_{\tilde{\mathbf{a}}} J_{\tilde{\mathbf{a}}}^{\mathrm{T}} \right] J_{\mathbf{t}_0}^{-1},$$

where $J_{\mathbf{t}_0} = \operatorname{diag}\left\{ \frac{\partial h}{\partial t}(t_{0,1}, \tilde{\mathbf{a}}), \ldots, \frac{\partial h}{\partial t}(t_{0,p}, \tilde{\mathbf{a}}) \right\}$ and $J_{\tilde{\mathbf{a}}}$ is the $p \times n$ matrix whose ith row is $(\nabla_{\mathbf{a}} h(t_{0,i}, \tilde{\mathbf{a}}))^{\mathrm{T}}$.

In particular, for a single response variable value v_0 with associated uncertainty u_{v_0}, an estimate t_0 of the stimulus variable satisfies

$$v_0 = h(t_0, \tilde{\mathbf{a}}).$$

u_{t_0}, the standard uncertainty associated with t_0, is given by

$$u_{t_0} = \left(\left[\frac{\partial h}{\partial t}(t_0, \tilde{\mathbf{a}}) \right]^{-2} u_{v_0}^2 + (\nabla_{\mathbf{a}} h(t_0, \tilde{\mathbf{a}}))^{\mathrm{T}} U_{\tilde{\mathbf{a}}} (\nabla_{\mathbf{a}} h(t_0, \tilde{\mathbf{a}})) \right)^{\frac{1}{2}}.$$

6.3 Derived quantities

In many metrology applications, quantities (other than the function and inverse function values) derived from the calibration coefficients are required.

In the following, we use the fact that for all of the models considered, $U_{\tilde{\mathbf{a}}}$, the uncertainty matrix associated with the solution parameters $\tilde{\mathbf{a}}$, can be written as

$$U_{\tilde{\mathbf{a}}} = UU^{\mathrm{T}}.$$

6.3.1 Linear functions of the parameters

If $f = \mathbf{f}^{\mathrm{T}} \tilde{\mathbf{a}}$ is a linear combination of the parameters, then u_f, the standard uncertainty associated with f, is given by

$$u_f = \|\tilde{\mathbf{f}}\|,$$

where

$$\tilde{\mathbf{f}} = U^{\mathrm{T}} \mathbf{f}.$$

Similarly, if $\mathbf{f} = F\tilde{\mathbf{a}}$ is a vector of linear combinations of the solution parameters, then $U_{\mathbf{f}}$, the uncertainty matrix associated with $\mathbf{f}$ is given by

$$U_{\mathbf{f}} = \tilde{F}\tilde{F}^{\mathrm{T}},$$

where

$$\tilde{F} = FU.$$

6.3.2 Non-linear functions of the parameters

If $f = f(\tilde{\mathbf{a}})$ is a non-linear function of the solution parameters, then u_f, the standard uncertainty associated with f is given by

$$u_f = \|\tilde{\mathbf{f}}\|,$$

where

$$\tilde{\mathbf{f}} = U^{\mathrm{T}}\nabla_{\mathbf{a}} f(\tilde{\mathbf{a}}).$$

Similarly, if

$$\mathbf{f} = \begin{bmatrix} f_1(\tilde{\mathbf{a}}) \\ \vdots \\ f_r(\tilde{\mathbf{a}}) \end{bmatrix}$$

is a vector function of the solution parameters, then $U_{\mathbf{f}}$, the uncertainty matrix associated with $\mathbf{f}$, is given by

$$U_{\mathbf{f}} = \tilde{G}\tilde{G}^{\mathrm{T}},$$

where

$$\tilde{G} = GU,$$

where G is the $r \times n$ matrix whose ith row is $(\nabla_{\mathbf{a}} f_i(\tilde{\mathbf{a}}))^{\mathrm{T}}$.

7 Polynomial calibration curves

Polynomial calibration curves are frequently encountered within metrology. A polynomial of degree n can be written as

$$h(t, \mathbf{a}) = a_0 + a_1 t + a_2 t^2 + \ldots + a_n t^n = \sum_{j=0}^{n} a_j t^j = \sum_{j=0}^{n} a_j h_j(t),$$

where $\{h_j(t) = t^j\}_0^n$ are the *monomial* basis functions.

Section 5.1.3 of [7] describes some of the important aspects associated with polynomial fitting.

There are two problems that arise from representing a curve using monomial basis functions:

1. For values of t significantly greater than one, t^j becomes very large as j increases.

   This problem can be overcome by using the normalised variable

   $$\hat{t} = \frac{(t - t_{\min}) - (t_{\max} - t)}{t_{\max} - t_{\min}}, \tag{13}$$

   where

   $$t_{\min} \leq t \leq t_{\max},$$

   so that $\hat{t}$ (and therefore all its powers) lies in the range $[-1, 1]$.

2. For large j, the function h_j is very similar to h_{j+2} and this can lead to ill-conditioning in the calibration problem.

   This problem can be overcome by the use of basis functions that have better properties. One such set is the *Chebyshev* polynomials [10], denoted by $T_j(x)$, and defined by the recurrence relation

   $$T_0(x) = 1, \quad T_1(x) = x, \quad T_j(x) = 2xT_{j-1}(x) - T_{j-2}(x), \quad j \geq 2.$$

Therefore when a calibration problem involves finding the best-fit polynomial to data, we write

$$h(t, \mathbf{a}) = \tfrac{1}{2} a_0 T_0(\hat{t}) + a_1 T_1(\hat{t}) + a_2 T_2(\hat{t}) + \ldots + a_n T_n(\hat{t}), \tag{14}$$

with $\hat{t}$ defined as in equation (13) and

$$t_{\min} \leq t_i \leq t_{\max}, \quad i = 1, \ldots, m.$$

(The use of the factor $\frac{1}{2}$ in equation (14) allows for a simpler recursion formula when evaluating the partial derivative of $h(t, \mathbf{a})$ with respect to t.)

For non-linear problems, it is required to evaluate $\frac{\partial h}{\partial a_j}(t, \mathbf{a})$, the partial derivatives of $h(t, \mathbf{a})$ with respect to a_j, but it is easily seen that

$$\frac{\partial h}{\partial a_j}(t, \mathbf{a}) = T_j(\hat{t}).$$

For generalised distance regression and generalised Gauss-Markov regression problems, $\frac{\partial h}{\partial t}(t, \mathbf{a})$, the partial derivative of the function $h(t, \mathbf{a})$ with respect to t is also required, and can be expressed as

$$\frac{\partial h}{\partial t}(t, \mathbf{a}) = \tfrac{1}{2} b_0 T_0(\hat{t}) + b_1 T_1(\hat{t}) + b_2 T_2(\hat{t}) + \ldots + b_{n-1} T_{n-1}(\hat{t}),$$

where the set of coefficients

$$\mathbf{b} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ b_{n-1} \end{bmatrix}$$

are defined by the recurrence relation

$$b_{n+1} = 0, \quad b_n = 0, \quad b_{j-1} = b_{j+1} + \frac{4 j a_j}{t_{\max} - t_{\min}}, \quad j = n, n-1, \ldots, 1.$$

7.1 Straight line calibration curves

In straight line polynomial regression, the calibration curve $h(t, \mathbf{a})$ is defined by two parameters a_0 and a_1. Often g_1, the gradient of the straight line, and g_2, the point of interception of the line with the t-axis (and their associated uncertainties) are of interest. Although it is possible to solve the regresion problem using monomial basis functions, i.e., using the representation

$$h(t, \mathbf{a}) = g_1 t + g_2, \tag{15}$$

the fact that software generally employs Chebyshev polynomials to represent the curve means that the parameters

$$\mathbf{a} = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix}$$

and their associated uncertainty matrix $V_{\mathbf{a}}$ need to be converted to the representation

$$\mathbf{g} = \begin{bmatrix} g_1 \\ g_2 \end{bmatrix}$$

and associated uncertainty matrix $V_{\mathbf{g}}$.

The conversion is quite straightforward. Equating equation (15) with

$$\begin{aligned} h(t,\mathbf{a}) &= \tfrac{1}{2}a_0T_0(\hat{t}) + a_1T_1(\hat{t}) \\ &= \tfrac{1}{2}a_0 + a_1\left(\frac{2t-(t_{\max}+t_{\min})}{t_{\max}-t_{\min}}\right) \end{aligned}$$

gives

$$g_1 = \frac{2a_1}{t_{\max}-t_{\min}}, \quad g_2 = \frac{a_0}{2} - a_1\left(\frac{t_{\max}+t_{\min}}{t_{\max}-t_{\min}}\right),$$

i.e.,

$$\mathbf{g} = \begin{bmatrix} g_1 \\ g_2 \end{bmatrix} = \begin{bmatrix} 0 & \dfrac{2}{t_{\max}-t_{\min}} \\ \\ \tfrac{1}{2} & -\dfrac{t_{\max}+t_{\min}}{t_{\max}-t_{\min}} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = G\mathbf{a},$$

where

$$G = \begin{bmatrix} 0 & \dfrac{2}{t_{\max}-t_{\min}} \\ \\ \tfrac{1}{2} & -\dfrac{t_{\max}+t_{\min}}{t_{\max}-t_{\min}} \end{bmatrix}.$$

$U_{\mathbf{g}}$, the uncertainty matrix associated with $\mathbf{g}$, is given by

$$U_{\mathbf{g}} = GU_{\mathbf{a}}G^{\mathrm{T}}.$$

8 Summary

Many metrology experiments require the estimation of a set of calibration parameters that specify the relationship between a stimulus variable and a response variable. In order to obtain reliable parameter estimates, it is important to take account of the uncertainties associated with measured data. In many cases, it can be assumed that the uncertainties associated with measurements of the stimulus variable are small in relation to those associated with measurements of the control variable, and algorithms to obtain parameter estimates in these cases are generally quite well known. For more generalised cases, there is much less awareness of solution algorithms.

This report contains a simple classification of the most common types of uncertainty models from which metrologists can easily identify to which class their problem belongs. For each of four selected classes, algorithms have been provided for evaluation of calibration parameters and their associated uncertainties. The subsequent use of the calibration curve to evaluate related quantities and their associated uncertainties is also described.

Due to their widespread use within metrology, consideration has been given to the particular case of polynomial calibration curves.

As part of the current and future SS*f*M programmes, the algorithms described in this report will be further developed, implemented and made available in METROS, a web-based repository of software for solving metrology problems [1].

9 Acknowledgements

The work described here was supported by the National Measurement System Directorate of the UK Department of Trade and Industry as part of its NMS Software Support for Metrology programme.

We thank Sven Hammarling of NAG Ltd for helpful discussions about this work.

References

[1] R. M. Barker. Software Support for Metrology Best Practice Guide No. 5: Software Re-use: Guide to METROS. Technical report, National Physical Laboratory, Teddington, UK, 2000. 32

[2] M. Bartholomew-Biggs, B. P. Butler, and A. B. Forbes. Optimisation algorithms for generalised regression on metrology. In P. Ciarlini, A. B. Forbes, F. Pavese, and D. Richter, editors, *Advanced Mathematical and Computational Tools in Metrology IV*, pages 21–31, Singapore, 2000. World Scientific. 9, 21

[3] BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, and OIML. Guide to the Expression of Uncertainty in Measurement, 1995. ISBN 92-67-10188-9, Second Edition. 2, 25

[4] A. Björck. *Numerical Methods for Least Squares Problems*. SIAM, Philadelphia, 1996. 36

[5] M. G. Cox. The least-squares solution of linear equations with block-angular observation matrix. In M. G. Cox and S. Hammarling, editors, *Advances in Reliable Numerical Computation*, pages 227–240. Oxford University Press, 1989. 20

[6] M. G. Cox, A. B. Forbes, P. M. Fossati, P. M. Harris, and I. M. Smith. Techniques for the efficient solution of large scale calibration problems. Technical Report CMSC 25/03, National Physical Laboratory, May 2003. 20

[7] M. G. Cox, A. B. Forbes, and P. M. Harris. Software Support for Metrology Best Practice Guide No. 4: Modelling Discrete Data. Technical report, National Physical Laboratory, Teddington, 2000. 5, 9, 21, 29

[8] International Organization for Standardization. Iso 11095: Linear calibration using reference materials, 1996. 1, 7

[9] A. B. Forbes, P. M. Harris, and I. M. Smith. Generalised Gauss-Markov Regression. In J. Levesley, I. Anderson, and J. C. Mason, editors, *Algorithms for Approximation IV*, pages 270–277. University of Huddersfield, 2002. 9

[10] L. Fox and I. B. Parker. *Chebyshev polynomials in numerical analysis*. Oxford University Press, 1968. 29

[11] P. E. Gill, W. Murray, and M. H. Wright. *Practical Optimization*. Academic Press, London, 1981. 10, 38

[12] G. H. Golub and C. F. Van Loan. *Matrix Computations*. John Hopkins University Press, Baltimore, third edition, 1996. 13, 14

[13] K. V. Mardia, J. T. Kent, and J. M. Bibby. *Multivariate Analysis*. Academic Press, London, 1979. 7, 13

[14] C. C. Paige. Fast numerically stable computations for generalized least squares problems. *SIAM J. Numer. Anal.*, 16:165–171, 1979. 36

[15] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vettering. *Numerical Recipes: The Art of Scientific Computing*. Cambridge University Press, Cambridge, 1989. *This book refers to the Fortran version; there are also versions in Pascal and C*. 39

[16] SIAM, Philadelphia. *The LAPACK User's Guide*, third edition, 1999. 36

[17] R. Sym. An assessment of the extent to which metrology algorithms are used in standards. Technical report, signalsfromnoise.com, Abbatsfield, 2002. *http://www.npl.co.uk/ssfm/download/documents/roger_sym_report.pdf*. 1

A Generalised QR factorisation

Generalised QR factorisation [14, 4, 16] represents a stable means of solving linear least squares systems.

Consider the problem

$$\min_{\mathbf{a}} \ \|D^{-1}(E\mathbf{a} - \mathbf{y})\|^2,$$

where $\mathbf{y}$ is $m \times 1$, E is $m \times n$ and D is $m \times m$ and it assumed that $m > n$.

This is equivalent to the problem

$$\min_{\mathbf{a},\mathbf{b}} \ \|\mathbf{b}\|^2$$

subject to the linear constraints

$$\mathbf{y} = E\mathbf{a} + D\mathbf{b}. \tag{16}$$

$m \times m$ orthogonal matrix Q, $n \times n$ upper-triangular matrix R, $m \times m$ orthogonal matrix Z and $m \times m$ upper-triangular T can be found such that

$$E = Q \begin{bmatrix} R \\ \mathbf{0} \end{bmatrix}, \quad D = QTZ.$$

Multiplying the constraint equation (16) by Q^{T} and partitioning into the rows $1 : n$ and $n + 1 : m$ yields

$$\begin{bmatrix} \widehat{\mathbf{y}}_1 \\ \widehat{\mathbf{y}}_2 \end{bmatrix} = \begin{bmatrix} R \\ \mathbf{0} \end{bmatrix} \mathbf{a} + \begin{bmatrix} T_{11} & T_{12} \\ \mathbf{0} & T_{22} \end{bmatrix} \begin{bmatrix} \widehat{\mathbf{b}}_1 \\ \widehat{\mathbf{b}}_2 \end{bmatrix}, \tag{17}$$

where

$$\widehat{\mathbf{y}} = Q^{\mathrm{T}}\mathbf{y} = \begin{bmatrix} \widehat{\mathbf{y}}_1 \\ \widehat{\mathbf{y}}_2 \end{bmatrix},$$

T_{11}, T_{12} and T_{22} are respectively $n \times n$ upper-triangular, $n \times (m - n)$ and $(m - n) \times (m - n)$ upper-triangular and

$$\widehat{\mathbf{b}} = Z\mathbf{b} = \begin{bmatrix} \widehat{\mathbf{b}}_1 \\ \widehat{\mathbf{b}}_2 \end{bmatrix}.$$

If T_{22} is full rank, $\widehat{\mathbf{b}}_2$ is determined as the solution of the upper-triangular system

$$T_{22}\widehat{\mathbf{b}}_2 = \widehat{\mathbf{y}}_2. \tag{18}$$

If R is full rank then, given any $\widehat{\mathbf{b}}$, the first n equations of (17) can be satisfied by chosing $\mathbf{a}$ to solve the upper-triangular system

$$R\mathbf{a} = \widehat{\mathbf{y}}_1 - T_{11}\widehat{\mathbf{b}}_1 - T_{12}\widehat{\mathbf{b}}_2.$$

$\widehat{\mathbf{b}}_2$ is fixed by (18) but we are free to choose any $\widehat{\mathbf{b}}_1$. Since the aim is to minimise $\|\mathbf{b}\| = \|\widehat{\mathbf{b}}\| = \|Z^{\mathrm{T}}\mathbf{b}\|$, we set $\widehat{\mathbf{b}}_1 = \mathbf{0}$.

Let $(m-n) \times (m-n)$ matrix $\tilde{T}_{22}$ be the solution of the upper-triangular system

$$T_{22}\tilde{T}_{22} = I,$$

so that the solution parameters $\tilde{\mathbf{a}}$ are given by

$$\widehat{\mathbf{b}}_2 = \tilde{T}_{22}\widehat{\mathbf{y}}_2, \quad R\tilde{\mathbf{a}} = \widehat{\mathbf{y}}_1 - T_{12}\widehat{\mathbf{b}}_2.$$

Let

$$Q = \left[\begin{array}{cc} Q_1 & Q_2 \end{array} \right],$$

where Q_1 and Q_2 are respectively the first n and final $m-n$ columns of Q.

Then the solution parameters $\tilde{\mathbf{a}}$ are given by the solution of the upper-triangular system

$$R\tilde{\mathbf{a}} = \left(Q_1^{\mathrm{T}} - T_{12}\tilde{T}_{22}Q_2^{\mathrm{T}}\right)\mathbf{y}.$$

B Gauss-Newton algorithm

Non-linear least squares problems are generally solved using some variant of the Gauss-Newton algorithm [11] which we now briefly describe.

Given m non-linear functions $f_i(\mathbf{a})$ of parameters $\mathbf{a}$, we wish to minimise

$$F(\mathbf{a}) = \sum_{i=1}^{m} f_i^2(\mathbf{a}) = \mathbf{f}^{\mathrm{T}}\mathbf{f},$$

where

$$\mathbf{f} = \begin{bmatrix} f_1(\mathbf{a}) \\ \vdots \\ f_m(\mathbf{a}) \end{bmatrix},$$

with respect to parameters $\mathbf{a} = (a_1, \ldots, a_n)^{\mathrm{T}}$ where $m \geq n$.

If J is the associated *Jacobian matrix* defined at an estimate $\mathbf{a}$ of the solution parameters by

$$J_{ij} = \frac{\partial f_i}{\partial a_j},$$

then an updated estimate is given by $\mathbf{a} + \mathbf{p}$, where $\mathbf{p}$ (known as the *Gauss-Newton step*) solves the matrix equation

$$J\mathbf{p} = -\mathbf{f}$$

in the least squares sense. This is a linear least squares problem and can be solved using an orthogonal factorisation approach, for example, see section 4.1.1.

In practice, the update step is often of the form $\mathbf{a} = \mathbf{a} + t\mathbf{p}$ where the step length parameter t is chosen to ensure there is a sufficient decrease in the value of the objective function $F(\mathbf{a})$ at each iteration.

Software implementing the Gauss-Newton algorithm typically requires:

- modules to evaluate both the functions $f_i(\mathbf{a})$ and their first derivatives with respect to the model parameters $\mathbf{a}$ for provided values of $\mathbf{a}$, and
- an initial estimate of $\mathbf{a}$.

Within the iterative process used to find updated estimates, the parameter values are deemed to be acceptable when convergence conditions on the update step and/or the gradient are satisfied.

C Bisection algorithm

Given a measurement v_0 of the response variable and the set $\mathbf{a}$ of calibration parameters, the solution t_0 of the problem $h(t_0, \mathbf{a}) = v_0$ can be obtained via the following steps [15]:

1. Find t_A and t_B such that $(h(t_A, \mathbf{a}) - v_0)(h(t_B, \mathbf{a}) - v_0) \leq 0$. (If this product is exactly zero, then clearly one or both of t_A and t_B must satisfy $h(t_0, \mathbf{a}) = v_0$.)
2. Let $t_C = \frac{1}{2}(t_A + t_B)$. If $h(t_C, \mathbf{a}) = v_0$, then t_C is the required solution, otherwise:
   - if $(h(t_A, \mathbf{a}) - v_0)(h(t_C, \mathbf{a}) - v_0) < 0$, the solution t_0 lies in the interval (t_A, t_C). Set the value of t_B to t_C.
   - if $(h(t_B, \mathbf{a}) - v_0)(h(t_C, \mathbf{a}) - v_0) < 0$, the solution t_0 lies in the interval (t_C, t_B). Set the value of t_A to t_C.
3. If the length of the interval (t_A, t_B) (i.e., $t_B - t_A$) is less than a chosen tolerance, then t_A can be regarded as an acceptable solution, otherwise repeat step 2.

D Derivation of expressions for uncertainty evaluation

D.1 Linear diagonally weighted least squares problems

Note that this appendix uses the notation of section 4.1.

The solution parameters $\tilde{\mathbf{a}}$ are given explicitly by

$$\tilde{\mathbf{a}} = \left(\tilde{C}^{\mathrm{T}}\tilde{C}\right)^{-1}\tilde{C}^{\mathrm{T}}\tilde{\mathbf{v}}.$$

$U_{\tilde{\mathbf{a}}}$, the uncertainty matrix associated with the solution parameters $\tilde{\mathbf{a}}$, is given by

$$U_{\tilde{\mathbf{a}}} = \left(\left(\tilde{C}^{\mathrm{T}}\tilde{C}\right)^{-1}\tilde{C}^{\mathrm{T}}\right)\left(\left(\tilde{C}^{\mathrm{T}}\tilde{C}\right)^{-1}\tilde{C}^{\mathrm{T}}\right)^{\mathrm{T}} = \left(\tilde{C}^{\mathrm{T}}\tilde{C}\right)^{-1}.$$

Since

$$\tilde{C}^{\mathrm{T}}\tilde{C} = \left[\begin{array}{cc} \tilde{R}^{\mathrm{T}} & \mathbf{0} \end{array}\right]\tilde{Q}^{\mathrm{T}}\tilde{Q}\left[\begin{array}{c} \tilde{R} \\ \mathbf{0} \end{array}\right] = \tilde{R}^{\mathrm{T}}\tilde{R},$$

$U_{\tilde{\mathbf{a}}}$ is given by

$$U_{\tilde{\mathbf{a}}} = UU^{\mathrm{T}},$$

where U is the solution of the upper-triangular system

$$\tilde{R}U = I.$$

D.2 Linear Gauss-Markov regression problems

Note that this appendix uses the notation of section 4.2.

$U_{\tilde{\mathbf{a}}}$, the uncertainty matrix associated with the solution parameters $\tilde{\mathbf{a}}$, is given by

$$U_{\tilde{\mathbf{a}}} = \left(\tilde{C}^{\mathrm{T}}\tilde{C}\right)^{-1} = \left(\left(L^{-1}C\right)^{\mathrm{T}}\left(L^{-1}C\right)\right)^{-1}.$$

Now

$$L^{-1}C = Z^{-1}T^{-1}Q^{-1}Q\left[\begin{array}{c} R \\ \mathbf{0} \end{array}\right] = Z^{-1}T^{-1}\left[\begin{array}{c} R \\ \mathbf{0} \end{array}\right],$$

since $Q^{-1}Q = I$.

Therefore

$$\begin{aligned}\tilde{C}^{\mathrm{T}}\tilde{C} &= \left(Z^{-1}T^{-1}\begin{bmatrix} R \\ \mathbf{0} \end{bmatrix}\right)^{\mathrm{T}}\left(Z^{-1}T^{-1}\begin{bmatrix} R \\ \mathbf{0} \end{bmatrix}\right) \\ &= \begin{bmatrix} R^{\mathrm{T}} & \mathbf{0} \end{bmatrix} T^{-\mathrm{T}}Z^{-\mathrm{T}}Z^{-1}T^{-1}\begin{bmatrix} R \\ \mathbf{0} \end{bmatrix} \\ &= \begin{bmatrix} R^{\mathrm{T}} & \mathbf{0} \end{bmatrix} T^{-\mathrm{T}}T^{-1}\begin{bmatrix} R \\ \mathbf{0} \end{bmatrix},\end{aligned}$$

since $Z^{-\mathrm{T}}Z^{-1} = I$.

Consider the product $T^{-1}\begin{bmatrix} R \\ \mathbf{0} \end{bmatrix}$. Since T is upper-triangular, T^{-1} is upper-triangular, i.e.,

$$T^{-1} = \begin{bmatrix} T_{11} & T_{12} \\ \mathbf{0} & T_{22} \end{bmatrix}^{-1} = \begin{bmatrix} \tilde{T}_{11} & \tilde{T}_{12} \\ \mathbf{0} & \tilde{T}_{22} \end{bmatrix},$$

where $\tilde{T}_{12}$ has dimensions $n \times (m-n)$ and $\tilde{T}_{11}$ and $\tilde{T}_{22}$ are respectively $n \times n$ and $(m-n) \times (m-n)$ upper-triangular.

Furthermore

$$\tilde{T}_{11} = T_{11}^{-1} \text{ and } \tilde{T}_{22} = T_{22}^{-1}.$$

Therefore

$$T^{-1}\begin{bmatrix} R \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} T_{11}^{-1} & \tilde{T}_{12} \\ \mathbf{0} & T_{22}^{-1} \end{bmatrix}\begin{bmatrix} R \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} T_{11}^{-1}R \\ \mathbf{0} \end{bmatrix}$$

and

$$\begin{aligned}\tilde{C}^{\mathrm{T}}\tilde{C} &= \begin{bmatrix} R^{\mathrm{T}} & \mathbf{0} \end{bmatrix} T^{-\mathrm{T}}T^{-1}\begin{bmatrix} R \\ \mathbf{0} \end{bmatrix} \\ &= \begin{bmatrix} R^{\mathrm{T}}T_{11}^{-\mathrm{T}} & \mathbf{0} \end{bmatrix}\begin{bmatrix} T_{11}^{-1}R \\ \mathbf{0} \end{bmatrix} \\ &= R^{\mathrm{T}}T_{11}^{-\mathrm{T}}T_{11}^{-1}R.\end{aligned}$$

$U_{\tilde{\mathbf{a}}}$ is given by

$$\begin{aligned}U_{\tilde{\mathbf{a}}} &= \left(R^{\mathrm{T}}T^{-\mathrm{T}}T^{-1}R\right)^{-1} \\ &= R^{-1}T_{11}T_{11}^{\mathrm{T}}R^{-\mathrm{T}} \\ &= UU^{\mathrm{T}},\end{aligned}$$

where U is the solution of the upper-triangular system

$$RU = T_{11}.$$

D.3 Generalised distance regression problems

Note that this appendix uses the notation of section 5.3.

In section 5.3.1 we showed that the update step $\mathbf{p}$ in the Gauss-Newton algorithm solves, in the least squares sense,

$$\tilde{J}\mathbf{p} = -\tilde{\mathbf{f}},$$

where

$$\tilde{J} = \begin{bmatrix} \tilde{K}_1 & & \tilde{J}_1 \\ & \ddots & \vdots \\ & \tilde{K}_m & \tilde{J}_m \end{bmatrix}$$

is composed of the 2×1 blocks $\{\tilde{K}_i\}_1^m$ and $2 \times n$ blocks $\{\tilde{J}_i\}_1^m$.

The update step $\mathbf{p}$ can be calculated efficiently as follows:

1. For each $i = 1, \ldots, m$, find the 2×2 orthogonal matrix $\tilde{Q}_i$ and the $2\times(n+1)$ matrix
$$\tilde{R}_i = \begin{bmatrix} \tilde{r}_i & \tilde{J}_{i1} \\ \mathbf{0} & \tilde{J}_{i2} \end{bmatrix}$$
where $\tilde{r}_i$ is a scalar and $\tilde{J}_{i1}$ and $\tilde{J}_{i2}$ are both $1 \times n$ arrays, such that
$$\tilde{Q}_i\tilde{R}_i = \tilde{Q}_i \begin{bmatrix} \tilde{r}_i & \tilde{J}_{i1} \\ \mathbf{0} & \tilde{J}_{i2} \end{bmatrix} = \begin{bmatrix} \tilde{K}_i & \tilde{J}_i \end{bmatrix}.$$
Evaluate
$$\begin{bmatrix} \tilde{f}_{i1} \\ \tilde{f}_{i2} \end{bmatrix} = \tilde{Q}_i^{\mathrm{T}}\tilde{\mathbf{f}}_i.$$

2. Find the $m \times m$ orthogonal matrix $\tilde{Q}_0$ and the $n \times n$ upper-triangular matrix $\tilde{R}_0$ such that
$$\tilde{Q}_0 \begin{bmatrix} \tilde{R}_0 \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \tilde{J}_{12} \\ \vdots \\ \tilde{J}_{m2} \end{bmatrix}.$$
Evaluate
$$\hat{\mathbf{f}} = \tilde{Q}_0^{\mathrm{T}} \begin{bmatrix} \tilde{f}_{12} \\ \vdots \\ \tilde{f}_{m2} \end{bmatrix},$$
and partition into elements $1 : n$ and $n + 1 : m$ to obtain
$$\hat{\mathbf{f}} = \begin{bmatrix} \hat{\mathbf{f}}_1 \\ \hat{\mathbf{f}}_2 \end{bmatrix}$$

3. The update step $\mathbf{p}$ is found by solving the upper-triangular system

$$\tilde{R}\mathbf{p} = -\tilde{\mathbf{q}},$$

where

$$\tilde{R} = \begin{bmatrix} \tilde{r}_1 & & & \tilde{J}_{11} \\ & \ddots & & \vdots \\ & & \tilde{r}_m & \tilde{J}_{m1} \\ & & & \tilde{R}_0 \end{bmatrix}$$

and

$$\tilde{\mathbf{q}} = \begin{bmatrix} \tilde{f}_{11} \\ \vdots \\ \tilde{f}_{m1} \\ \hat{\mathbf{f}}_1 \end{bmatrix}.$$

$U_{\tilde{\zeta}}$, the uncertainty matrix associated with the solution parameters

$$\tilde{\zeta} = \begin{bmatrix} \tilde{\mathbf{q}} \\ \tilde{\mathbf{a}} \end{bmatrix},$$

is given by

$$U_{\tilde{\zeta}} = \left(\tilde{J}^{\mathrm{T}}\tilde{J}\right)^{-1},$$

where $\tilde{J}$ is the $2m \times (m+n)$ Jacobian matrix associated with $\tilde{\mathbf{f}}(\tilde{\mathbf{q}}, \tilde{\mathbf{a}})$.

A similar analysis to that carried out in Section 5.1.2 gives

$$U_{\tilde{\zeta}} = U_1 U_1^{\mathrm{T}},$$

where U_1 is the solution of the upper-triangular system

$$\tilde{R}U_1 = I.$$

$U_{\tilde{\mathbf{a}}}$, the uncertainty matrix of the solution parameters $\tilde{\mathbf{a}}$, is the lower-right $n \times n$ block of $U_{\tilde{\zeta}}$ and is given by

$$U_{\tilde{\mathbf{a}}} = UU^{\mathrm{T}},$$

where U is the solution of the upper-triangular system

$$\tilde{R}_0 U = I.$$

D.4 Generalised Gauss-Markov regression problems

Note that this appendix uses the notation of section 5.4.

The QR factorisation of J can be evaluated efficiently as follows:

1. For each $i = 1, \ldots, m$, find the 2×2 orthogonal matrix

$$Q_i = \begin{bmatrix} Q_{i1} & Q_{i2} \end{bmatrix}$$

and the $2 \times (n+1)$ matrix

$$R_i = \begin{bmatrix} r_i & J_{i1} \\ \mathbf{0} & J_{i2} \end{bmatrix}$$

such that

$$Q_i R_i = \begin{bmatrix} Q_{i1} & Q_{i2} \end{bmatrix} \begin{bmatrix} r_i & J_{i1} \\ \mathbf{0} & J_{i2} \end{bmatrix} = \begin{bmatrix} K_i & J_i \end{bmatrix}.$$

2. Find the $m \times m$ orthogonal matrix

$$Q_0 = \begin{bmatrix} Q_{01} \\ \vdots \\ Q_{0m} \end{bmatrix}$$

and the $n \times n$ upper-triangular matrix R_0 such that

$$Q_0 \begin{bmatrix} R_0 \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} Q_{01} \\ \vdots \\ Q_{0m} \end{bmatrix} \begin{bmatrix} R_0 \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} J_{12} \\ \vdots \\ J_{m2} \end{bmatrix}.$$

3. The QR factorisation of J is then given by

$$J = QR,$$

where

$$Q = \begin{bmatrix} Q_{11} & & & Q_{12}Q_{01} \\ & \ddots & & \vdots \\ & & Q_{m1} & Q_{m2}Q_{0m} \end{bmatrix}$$

and

$$R = \begin{bmatrix} r1 & & & J_{11} \\ & \ddots & & \vdots \\ & & r_m & J_{m1} \\ & & & R_0 \end{bmatrix}.$$

$U_{\tilde{\zeta}}$, the uncertainty matrix associated with the solution parameters

$$\tilde{\zeta} = \begin{bmatrix} \mathbf{q} \\ \mathbf{a} \end{bmatrix}$$

is given by

$$U_{\tilde{\zeta}} = \left(\left(L^{-1} J \right)^{\mathrm{T}} \left(L^{-1} J \right) \right)^{-1}.$$

A similar analysis to that carried out in Section 4.2.2 yields

$$U_{\tilde{\zeta}} = U_1 U_1^{\mathrm{T}},$$

where U_1 is the solution of the upper-triangular system

$$R U_1 = T_{11}.$$

Partition R and T_{11} into rows $1 : m$ and $m + 1 : m + n$:

$$R_1 = \begin{bmatrix} R_{11} & R_{12} \\ \mathbf{0} & R_0 \end{bmatrix}, \quad T_{11} = \begin{bmatrix} W_{11} & W_{12} \\ \mathbf{0} & W_{22} \end{bmatrix},$$

where R_{11} and W_{11} are $m \times m$ upper-triangular, R_{12} and W_{12} are $m \times n$ and W_{22} is $n \times n$ upper-triangular.

Since R_1 is upper-triangular, R_1^{-1} is upper-triangular, i.e.,

$$R_1^{-1} = \begin{bmatrix} R_{11} & R_{12} \\ \mathbf{0} & R_0 \end{bmatrix}^{-1} = \begin{bmatrix} \tilde{R}_{11} & \tilde{R}_{12} \\ \mathbf{0} & \tilde{R}_0 \end{bmatrix},$$

where $\tilde{R}_{12}$ has dimensions $m \times n$ and $\tilde{R}_{11}$ and $\tilde{R}_0$ are respectively $m \times m$ and $n \times n$ upper-triangular.

Furthermore

$$\tilde{R}_{11} = R_{11}^{-1} \text{ and } \tilde{R}_0 = R_0^{-1}.$$

The matrix U_1 can be written as

$$\begin{aligned} U_1 &= R_1^{-1} W_{11} \\ &= \begin{bmatrix} R_{11}^{-1} & \tilde{R}_{12} \\ \mathbf{0} & R_0^{-1} \end{bmatrix} \begin{bmatrix} W_{11} & W_{12} \\ \mathbf{0} & W_{22} \end{bmatrix} \\ &= \begin{bmatrix} R_{11}^{-1} W_{11} & R_{11}^{-1} W_{12} + \tilde{R}_{12} W_{22} \\ \mathbf{0} & R_0^{-1} W_{22} \end{bmatrix}. \end{aligned}$$

$U_{\tilde{\mathbf{a}}}$, the uncertainty matrix of the solution parameters $\tilde{\mathbf{a}}$, is the lower-right $n \times n$ block of $U_{\tilde{\zeta}}$ and it is given by

$$U_{\tilde{\mathbf{a}}} = \left(R_0^{-1} W_{22}\right) \left(R_0^{-1} W_{22}\right)^{\mathrm{T}} = U U^{\mathrm{T}},$$

where U is the solution of the upper-triangular system

$$R_0 U = W_{22}.$$