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Determination and use of straight-line calibration functions

Détermination et utilisation des fonctions d'étalonnage linéaire

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Foreword

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ISO/TS 28037:2010 was prepared by Technical Committee ISO/TC 69, *Applications of statistical methods*, Subcommittee SC 6, *Measurement methods and results*.

Introduction

Calibration is an essential part of many measurement procedures and often involves fitting to measured data a calibration function that best describes the relationship of one variable to another. This Technical Specification considers straight-line calibration functions that describe a dependent variable Y as a function of an independent variable X. The straight-line relationship depends on the intercept A and the slope B of the line. A and B are referred to as the parameters of the line. The purpose of a calibration procedure is to determine estimates a and b of A and B for a particular measuring system under consideration on the basis of measurement data $(x_i,\ y_i)$, $i = 1, \ldots, m$, provided by the measuring system. The measurement data have associated uncertainty, which means there will be uncertainty associated with a and b. This Technical Specification describes how a and b can be determined given the data and the associated uncertainty information. It also provides a means for evaluating the uncertainties associated with these estimates. The treatment of uncertainty in this Technical Specification is carried out in a manner consistent with ISO/IEC Guide 98-3:2008, "Guide to the expression of uncertainty in measurement" (GUM).

Given the uncertainty information associated with the measurement data, an appropriate method can be specified to determine estimates of the calibration function parameters. This uncertainty information may include quantified covariance effects, relating to dependencies among some or all of the quantities involved.

Once the straight-line model has been fitted to the data, it is necessary to determine whether or not the model and data are consistent with each other. In cases of consistency, the model so obtained can validly be used to predict a value x of the variable X corresponding to a measured value y of the variable Y provided by the same measuring system. It can also be used to evaluate the uncertainties associated with the calibration function parameters and the uncertainty associated with the predicted value x.

The determination and use of a straight-line calibration function can therefore be considered to consist of five steps:

1 Obtaining uncertainty and covariance information associated with the measurement data – although dependent on the particular area of measurement, examples are provided within this Technical Specification;

2 Providing best estimates of the straight-line parameters;

3 Validating the model, both in terms of the functional form (does the data reflect a straight-line relationship?) and statistically (is the spread of the data consistent with their associated uncertainties?) using a chi-squared test;

4 Obtaining the standard uncertainties and covariance associated with the estimate of the straight-line parameters.

5 Using the calibration function for prediction, that is, determining an estimate x of the X-variable and its associated uncertainty corresponding to a measured value y of the Y-variable and its associated uncertainty.

The above steps are shown diagrammatically in Figure 1.

The main aim of this Technical Specification is to consider steps 2 to 5. Therefore, as part of step 1, before using this Technical Specification, the user will need to provide standard uncertainties, and covariances if relevant, associated with the measured Y-values and, as appropriate, those associated with the measured X-values. Account should be taken of the principles of the GUM in evaluating these uncertainties on the basis of a measurement model that is specific to the area of concern.

ISO 11095:1996 [14] is concerned with linear calibration using reference materials. It differs from this Technical Specification in the ways given in Table 1.

The numerical methods given are based on reference [6].

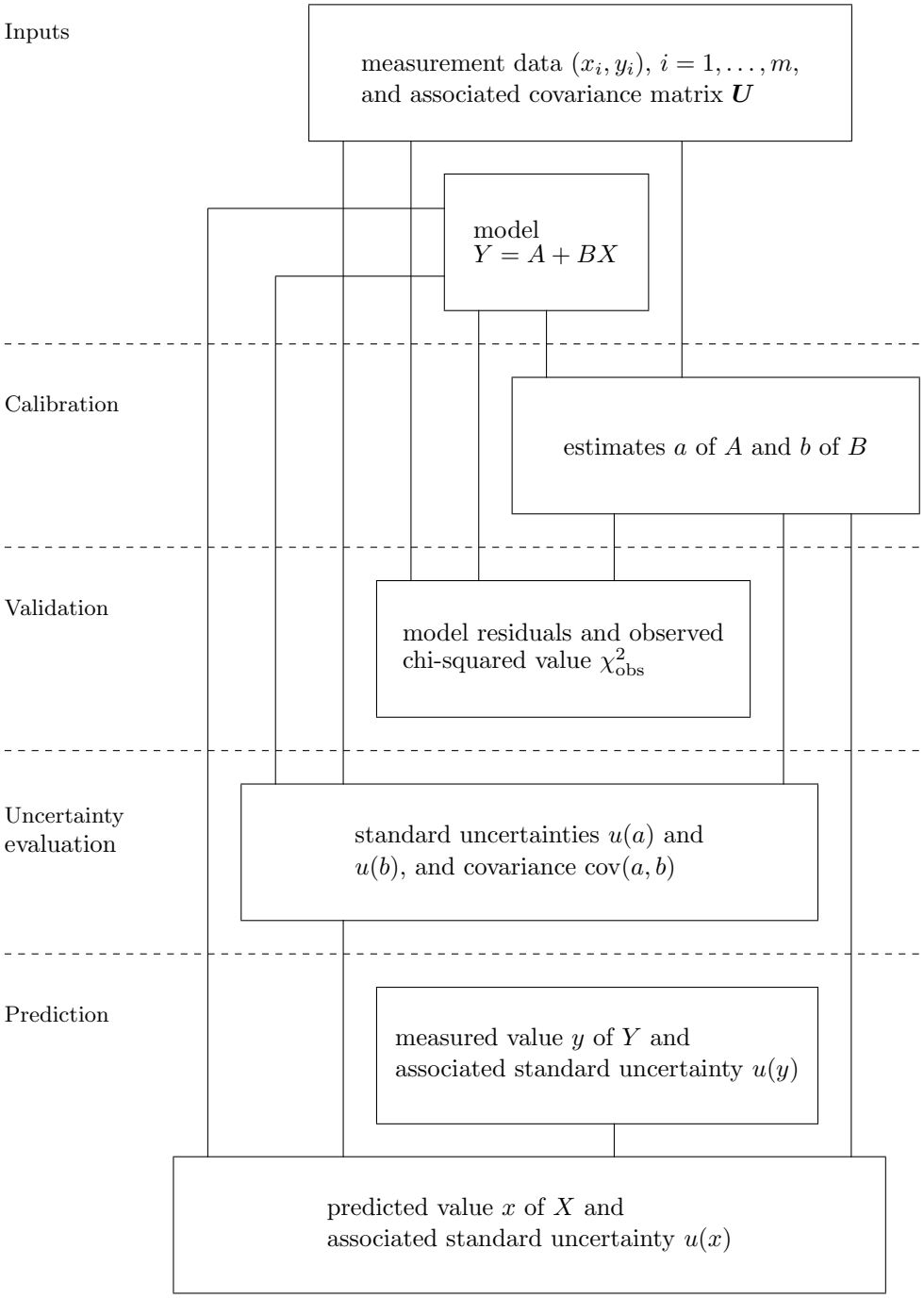

Figure 1 — Summary of the steps in the determination and use of straight-line calibration functions

Table 1 — Differences between ISO 11095:1996 and ISO/TS 28037:2010

Feature	ISO 11095:1996	ISO/TS 28037:2010
Specifically addresses reference materials	Yes	More general
X-values assumed to be known exactly	Yes	More general uncertainty information
All measured values obtained independently	Yes	More general uncertainty information
Terminology aligned with GUM	No	Yes
Types of uncertainty structure treated	Two	Five, including the most general case
Only uncertainty associated with random errors	Yes	More general uncertainty information
Consistency test	ANOVA	Chi-squared
Uncertainty associated with predictions	Ad hoc	GUM compatible

Determination and use of straight-line calibration functions

1 Scope

This Technical Specification is concerned with linear, that is, straight-line, calibration functions that describe the relationship between two variables X and Y, namely, functions of the form $Y = A + BX$. Although many of the principles apply to more general types of calibration function, the approaches described exploit the simple form of the straight-line calibration function wherever possible.

Values of the parameters A and B, are determined on the basis of measured data points $(x_i,\ y_i)$, $i = 1, \ldots, m$. Various cases are considered relating to the nature of the uncertainties associated with these data. No assumption is made that the errors relating to the y_i are homoscedastic (having equal variance), and similarly for the x_i when the errors are not negligible.

Estimates of the parameters A and B are determined using least squares methods. The emphasis of this Technical Specification is on choosing the least squares method most appropriate for the type of measurement data, in particular methods that reflect the associated uncertainties. The most general type of covariance matrix associated with the measurement data is treated, but important special cases that lead to simpler calculations are described in detail.

For all cases considered, methods for validating the use of the straight-line calibration functions and for evaluating the uncertainties and covariance associated with the parameter estimates are given.

The Technical Specification also describes the use of the calibration function parameter estimates and their associated uncertainties and covariance to predict a value of X and its associated standard uncertainty given a measured value of Y and its associated standard uncertainty.

NOTE 1 The Technical Specification does not give a general treatment of outliers in measurement data, although the validation tests given can be used as a basis for identifying discrepant data.

NOTE 2 The Technical Specification describes a method to evaluate the uncertainties associated with the measurement data in the case that those uncertainties are known only up to a scale factor (Annex E).

2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO/IEC Guide 99:2007, *International vocabulary of metrology — Basic and general concepts and associated terms (VIM)*

ISO/IEC Guide 98-3:2008, *Uncertainty of measurement — Part 3: Guide to the expression of uncertainty in measurement (GUM:1995)*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO/IEC Guide 98-3:2008 and ISO/IEC Guide 99:2007 and the following apply.

A glossary of principal symbols is given in Annex G.

3.1
measured quantity value
quantity value representing a measurement result

[ISO/IEC Guide 99:2007 2.10]

3.2
measurement uncertainty
non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used

[ISO/IEC Guide 99:2007 2.26]

3.3
standard measurement uncertainty
measurement uncertainty expressed as a standard deviation

[ISO/IEC Guide 99:2007 2.30]

3.4
covariance associated with two quantity values
parameter characterizing the interdependence of the quantity values being attributed to two measurands, based on the information used

3.5
measurement covariance matrix
covariance matrix
matrix of dimension $N \times N$ associated with a vector estimate of a vector quantity of dimension $N \times 1$, containing on its diagonal the squares of the standard uncertainties associated with the respective components of the vector estimate of the vector quantity, and, in its off-diagonal positions, the covariances associated with pairs of components of the vector estimate of the vector quantity

NOTE 1 A covariance matrix $\boldsymbol{U}_{\boldsymbol{x}}$ of dimension $N \times N$ associated with the vector estimate $\boldsymbol{x}$ of a vector quantity $\boldsymbol{X}$ has the representation

$$\boldsymbol{U}_{\boldsymbol{x}} = \begin{bmatrix} \operatorname{cov}(x_1, x_1) & \cdots & \operatorname{cov}(x_1, x_N) \\ \vdots & \ddots & \vdots \\ \operatorname{cov}(x_N, x_1) & \cdots & \operatorname{cov}(x_N, x_N) \end{bmatrix},$$

where $\operatorname{cov}(x_i, x_i) = u^2(x_i)$ is the variance (squared standard uncertainty) associated with x_i and $\operatorname{cov}(x_i, x_j)$ is the covariance associated with x_i and x_j. $\operatorname{cov}(x_i, x_j) = 0$ if elements X_i and X_j of $\boldsymbol{X}$ are uncorrelated.

NOTE 2 Covariances are also known as mutual uncertainties.

NOTE 3 A covariance matrix is also known as a variance-covariance matrix.

NOTE 4 Definition adapted from ISO/IEC Guide 98-3:2008/Suppl. 1:2008, definition 3.11 [13].

3.6
measurement model
mathematical relation among all quantities known to be involved in a measurement

[ISO/IEC Guide 99:2007 2.48]

3.7
functional model
statistical model involving errors associated with the dependent variable

3.8
structural model
statistical model involving errors associated with the independent and dependent variables

3.9
calibration
operation that, under specified conditions, in a first step, establishes a relation between the quantity values with measurement uncertainties provided by measurement standards and corresponding indications with associated measurement uncertainties and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication

NOTE 1 A calibration may be expressed by a statement, calibration function, calibration diagram, calibration curve, or calibration table. In some cases, it may consist of an additive or multiplicative correction of the indication with associated measurement uncertainty.

NOTE 2 Calibration should not be confused with adjustment of a measuring system, often mistakenly called 'self-calibration', nor with verification of calibration.

NOTE 3 Often the first step alone in the above definition is perceived as being calibration.

[ISO/IEC Guide 99:2007 2.39]

3.10
probability distribution
⟨random variable⟩ function giving the probability that a random variable takes any given value or belongs to a given set of values

NOTE 1 The probability on the whole set of values of the random variable equals 1.

NOTE 2 A probability distribution is termed univariate when it relates to a single (scalar) random variable, and multivariate when it relates to a vector of random variables. A multivariate probability distribution is also described as a joint distribution.

NOTE 3 A probability distribution can take the form of a distribution function or a probability density function.

NOTE 4 Definition and note 1 adapted from ISO 3534-1:1993, definition 1.3 and ISO/IEC Guide 98-3:2008, definition C.2.3; notes 2 and 3 adapted from ISO/IEC Guide 98-3:2008/Suppl. 1:2008, definition 3.1 [13].

3.11
normal distribution
probability distribution of a continuous random variable X having the probability density function

$$g_x(\xi) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\xi-\mu}{\sigma}\right)^2\right],$$

for $-\infty < \xi < +\infty$

NOTE 1 μ is the expectation and σ is the standard deviation of X.

NOTE 2 The normal distribution is also known as the Gaussian distribution.

NOTE 3 Definition and note 1 adapted from ISO 3534-1:1993, definition 1.37; note 2 adapted from ISO/IEC Guide 98-3:2008, definition C.2.14.

3.12
***t*-distribution**
probability distribution of a continuous random variable X having the probability density function

$$g_x(\xi) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\pi\nu}\Gamma(\nu/2)}\left(1+\frac{\xi^2}{\nu}\right)^{-(\nu+1)/2},$$

for $-\infty < \xi < +\infty$, with parameter ν, a positive integer, the degrees of freedom of the distribution, where

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t}\,\mathrm{d}t, \qquad z > 0,$$

is the gamma function

[ISO/IEC Guide 98-3:2008/Suppl. 1:2008 3.5]

3.13
chi-squared distribution
χ^2 distribution
probability distribution of a continuous random variable X having the probability density function

$$g_X(\xi) = \frac{\xi^{(\nu/2)-1}}{2^{\nu/2}\Gamma(\nu/2)} \exp\left(-\frac{\xi}{2}\right),$$

for $0 \leq \xi < \infty$, with parameter ν, a positive integer, where Γ is the gamma function

NOTE The sum of the squares of ν independent standardized normal variables is a χ^2 random variable with parameter ν; ν is then called the degrees of freedom.

3.14
positive definite matrix
matrix $\boldsymbol{M}$ of dimension $n \times n$ having the property $\boldsymbol{z}^\top \boldsymbol{M} \boldsymbol{z} > 0$ for all non-zero vectors $\boldsymbol{z}$ of dimension $n \times 1$

3.15
positive semi-definite matrix
matrix $\boldsymbol{M}$ of dimension $n \times n$ having the property $\boldsymbol{z}^\top \boldsymbol{M} \boldsymbol{z} \geq 0$ for all non-zero vectors $\boldsymbol{z}$ of dimension $n \times 1$

4 Conventions and notation

For the purpose of this Technical Specification the following conventions and notations are adopted.

4.1 X is termed the independent variable and Y the dependent variable even when the knowledge of X and Y is 'interchangeable', as in Clause 7, for example.

4.2 The quantities A and B are termed the parameters of the straight-line calibration function $Y = A + BX$. A and B are also used to denote (dummy) variables in expressions involving the calibration function parameters.

4.3 The quantities X_i and Y_i are used as (dummy) variables to denote the co-ordinates of the ith data point.

4.4 The constants A^* and B^* are (unknown) values of A and B that specify the straight-line calibration function $Y = A^* + B^* X$ for a particular measuring system under consideration.

4.5 The constants X_i^* and Y_i^* are the (unknown) co-ordinates of the ith data point provided by the measuring system satisfying $Y_i^* = A^* + B^* X_i^*$.

4.6 x_i and y_i are the measured values of the co-ordinates of the ith data point.

4.7 a and b are estimates of the calibration function parameters for the measuring system.

4.8 x_i^* and y_i^* are estimates of the co-ordinates of the ith data point satisying $y_i^* = a + bx_i^*$.

4.9 A vector of dimension $m \times 1$ is denoted thus:

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}, \qquad \boldsymbol{x}^\top = \begin{bmatrix} x_1 & \dots & x_m \end{bmatrix},$$

and a matrix of dimension $m \times n$ is denoted thus:

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix}, \qquad \boldsymbol{A}^\top = \begin{bmatrix} a_{11} & \dots & a_{m1} \\ \vdots & \ddots & \vdots \\ a_{1n} & \dots & a_{mn} \end{bmatrix}.$$

The dimension of the vector or matrix is always specified to avoid possible confusion.

4.10 $\top$ denotes transpose.

4.11 The zero matrix is denoted by $\mathbf{0}$ and the unit vector is denoted by $\mathbf{1}$.

4.12 Some symbols have more than one meaning. The context clarifies the usage.

4.13 Numbers displayed in tables to a fixed number of decimal places are correctly rounded representations of numbers stored to higher precision, as would be the case in a spreadsheet, for example. Therefore, minor inconsistencies may be perceived between displayed column sums and the column sums of the displayed numbers.

4.14 In some tables, a subclause number above a column or columns indicates where the formula is given for determining the values below.

4.15 In the examples, while data values are provided to a given precision, the results of calculations are provided to a higher precision to allow the user to compare results when undertaking the calculations.

5 Principles of straight-line calibration

5.1 General

5.1.1 This clause considers how a relationship $Y = A + BX$ describing the dependent variable Y (also called 'response') as a function of the independent variable X (also called 'stimulus') can be determined from measurement data. In the context of calibration, the measurement data arise when a measuring instrument specified by (unknown) values A^* and B^* of the calibration function parameters is 'stimulated' by artefacts with calibrated values of X_i given in standard units, of a property of the artefacts, and the corresponding 'responses' or indications Y_i of the instrument are recorded. The relationship provides the response Y of the system given an artefact with calibrated quantity X. This process is termed 'forward evaluation'. More useful in practice, the relationship allows a measured response y of Y to be converted to an estimate x, in standard units, of the property X of an artefact. This process is termed 'inverse evaluation' or 'prediction'.

5.1.2 The calibration of a measuring system should take into account measurement uncertainties, and, if present, covariances associated with the measurement data. The output of a calibration procedure is a calibration function to be used for prediction (and, if required, forward evaluation). The output also includes the standard uncertainties and covariance associated with the estimates a and b of the parameters describing the calibration function, which are used to evaluate the standard uncertainties associated with prediction (and forward evaluation).

5.2 Inputs to determining the calibration function

5.2.1 Measurement data

The information required to determine the straight-line calibration function are the measurement data and their associated standard uncertainties and covariances. In this Technical Specification, the measurement data are denoted

by (x_i, y_i), $i = 1, \ldots, m$, that is, m pairs of measured values of X and Y. It is assumed that m is at least two and that the values of x_i are not all equal to each other.

NOTE The uncertainties associated with the estimates a and b generally decrease as m increases. Therefore, calibration should aim to use as many measured data points as is economically viable.

5.2.2 Associated uncertainties and covariances

The standard uncertainties associated with x_i and y_i are denoted by $u(x_i)$ and $u(y_i)$ respectively. The covariance associated with x_i and x_j is denoted by $\mathrm{cov}(x_i, x_j)$. Similarly, those associated with y_i and y_j, and with x_i and y_j, are denoted by $\mathrm{cov}(y_i, y_j)$ and $\mathrm{cov}(x_i, y_j)$, respectively. Annex D indicates how the uncertainties and covariances associated with the measured response and stimulus variables can be evaluated and gives an interpretation of that uncertainty information. The complete uncertainty information is represented by an array of elements (matrix) $\boldsymbol{U}$ of dimension $2m \times 2m$ holding the variances (squared standard uncertainties) $u^2(x_i)$ and $u^2(y_i)$ and the covariances:

$$\boldsymbol{U} = \begin{bmatrix} u^2(x_1) & \ldots & \mathrm{cov}(x_1, x_m) & \mathrm{cov}(x_1, y_1) & \ldots & \mathrm{cov}(x_1, y_m) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \mathrm{cov}(x_m, x_1) & \ldots & u^2(x_m) & \mathrm{cov}(x_m, y_1) & \ldots & \mathrm{cov}(x_m, y_m) \\ \mathrm{cov}(y_1, x_1) & \ldots & \mathrm{cov}(y_1, x_m) & u^2(y_1) & \ldots & \mathrm{cov}(y_1, y_m) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \mathrm{cov}(y_m, x_1) & \ldots & \mathrm{cov}(y_m, x_m) & \mathrm{cov}(y_m, y_1) & \ldots & u^2(y_m) \end{bmatrix}.$$

For many applications, some or all covariances are taken as zero (see 5.3).

NOTE This Technical Specification is concerned with problems in which the $u(x_i)$ or the $u(y_i)$ are generally different.

5.3 Determining the calibration function

5.3.1 The inputs to determining the calibration function are the measurement data and their associated uncertainties and possibly covariances. Given parameters A and B, the inputs can be used to provide a measure of the departure of the ith data point (x_i, y_i) from the line $Y = A + BX$. The estimates a and b are determined by minimizing a sum of squares of these departures, or a more general measure when any covariances are non-zero. How this is achieved depends on the 'uncertainty structure' associated with the measurement data. This uncertainty structure relates to the answers to the following questions:

i) Are the uncertainties associated with the measured values x_i negligible?

ii) Are the covariances associated with pairs of measured values negligible?

5.3.2 The following cases, given in increasing order of complexity and depending on the answers to the questions in 5.3.1, are considered in this Technical Specification:

a) The only uncertainties are associated with the measured values y_i and all covariances associated with the data are regarded as negligible (Clause 6);

b) Uncertainties are associated with the measured values x_i and y_i and all covariances associated with the data are regarded as negligible (Clause 7);

c) Uncertainties are associated with the measured values x_i and y_i and the only covariances are associated with the pairs (x_i, y_i) (Clause 8);

d) The only uncertainties are associated with the measured values y_i and the only covariances are associated with the y_i and the y_j $(i \neq j)$ (Clause 9);

e) The most general case in which there are uncertainties associated with the measured values x_i and y_i and covariances associated with all pairs of values of the x_i, the x_j, the y_k and the y_ℓ (Clause 10).

5.3.3 For each case in 5.3.2 are given

a) the prescribed measurement data and uncertainty structure,

b) the corresponding statistical model,

c) the least squares problem addressed,

d) the calculation steps,

e) properties of the statistical model,

f) validation of the model,

g) organization of the calculations for the computer, where appropriate,

h) a numerical algorithm, where appropriate, and

i) one or more worked examples.

5.4 Numerical treatment

In Annex C, a general approach to the most general case e) in 5.3.2 is given. It can be used to treat all the other cases and uses sophisticated, numerically stable methods. The cases a) to c) in 5.3.2 can, however, be treated using elementary operations, which can be implemented in a spreadsheet, for example. The cases d) and e) in 5.3.2 require some matrix operations, which are straightforward to implement in a computer language supporting matrix arithmetic, but are not well suited to spreadsheet calculations.

5.5 Uncertainties and covariance associated with the calibration function parameters

5.5.1 For all cases considered, estimates of the calibration function parameters can be expressed (explicitly or implicitly) as functions of the measurement data. The principles of the GUM [ISO/IEC Guide 98-3:2008] can be applied to propagate the uncertainties and covariances associated with the measurement data through these functions to obtain those associated with these parameter estimates. In this way, the measurement data are used to provide estimates a and b of the calibration function parameters, and to evaluate standard uncertainties $u(a)$ and $u(b)$ and the covariance $\mathrm{cov}(a, b)$ associated with these estimates. For the cases a) and d) in 5.3.2, the propagation is exact since the parameter estimates can be expressed as linear combinations of the inputs y_i. For the other cases, in which the parameter estimates cannot be so expressed, the propagation is approximate, based on a linearization about the parameter estimates. For many purposes, the approximation incurred by the linearization will be sufficiently accurate.

NOTE When the propagation of uncertainty is approximate, and particularly if the uncertainties involved are large (for example, in some areas of biological measurement), an approach based on the propagation of distributions can be employed. This approach [ISO/IEC Guide 98-3:2008/Suppl. 1:2008] uses a Monte Carlo method (not treated in this Technical Specification).

5.5.2 The primary outputs in describing the straight-line calibration function are the parameter estimate vector $\boldsymbol{a}$ of dimension 2×1 and the covariance matrix $\boldsymbol{U}_{\boldsymbol{a}}$ of dimension 2×2 given by

$$\boldsymbol{a} = \begin{bmatrix} a \\ b \end{bmatrix}, \qquad \boldsymbol{U}_{\boldsymbol{a}} = \begin{bmatrix} u^2(a) & \mathrm{cov}(a, b) \\ \mathrm{cov}(b, a) & u^2(b) \end{bmatrix}, \tag{1}$$

where $u(a)$ and $u(b)$ are the standard uncertainties associated with a and b, respectively, and $\mathrm{cov}(a, b) = \mathrm{cov}(b, a)$ is the covariance associated with a and b.

5.6 Validation of the model

5.6.1 In determining the estimates a and b of the straight-line calibration function parameters, it is assumed that the model $Y = A + BX$ is valid and that the uncertainties associated with the measurement data give a credible measure of the departure of the measurement data from a straight line. Once a and b have been determined, the actual departure of the data points from the best-fit calibration function can be assessed against a predicted departure. This comparison involves an aggregate measure of departure expressed in terms of the sum of squares χ^2_{obs} of m weighted residuals, the ith weighted residual being a measure of the departure of the ith data point from the line, or, when the covariance associated with the ith data point (x_i, y_i) is non-zero, a more general form. If χ^2_{obs} is much bigger than expected, on statistical grounds there is reason to call into question the validity of the model assumptions.

5.6.2 From a statistical viewpoint, the measurement data can be regarded as realizations of random variables. If the probability distributions characterizing these random variables were known, it would be possible in principle to determine the probability distribution for the aggregate measure of departure in 5.6.1. Then the probability could be calculated that χ^2_{obs}, regarded as a draw from this aggregate distribution, exceeded any particular quantile of the distribution. However, as the information about these quantities is often limited to the measured values themselves and their associated variances (taken to be the expectations and variances, respectively, of the random variables characterized by these distributions), there is insufficient information to determine the distribution for this measure. Instead, the assessment of validity is performed assuming that the distributions for these quantities are normal. With this assumption, which is henceforth taken to hold, at least for validation purposes, the distribution for this measure is χ^2_ν with $\nu = m - 2$ degrees of freedom. Accordingly, the probability that χ^2_{obs} exceeds any particular quantile of χ^2_ν can be determined (see 6.3, 7.3, 9.3, 10.3). The 95 % quantile is used.

NOTE 1 If χ^2_{obs} exceeds the 95 % quantile of χ^2_ν, the straight-line calibration function can be regarded as not explaining the data sufficiently well for practical purposes. In such a case, the data and associated uncertainties should be checked for possible mistakes. A calibration function consisting of a polynomial in X of degree 2 or higher or some other mathematical form can be entertained; such a consideration is beyond the scope of this Technical Specification.

NOTE 2 There is a possibility that the model is 'too good' in that the observed value χ^2_{obs} is significantly smaller than the expected value. This possibility typically corresponds to the uncertainties associated with the measurement data being quoted as too large, and is not considered further in this Technical Specification.

5.6.3 In order to obtain as much value as possible from a calibration, it is desirable that input uncertainties are derived prior to determining the calibration function parameters, rather than being evaluated once a fit to the data has been determined, with associated uncertainties estimated from the data or known up to a scale factor. The latter case is considered in Annex E.

5.6.4 If, in any particular case, the validation of the model fails, that is, χ^2_{obs} exceeds the 95 % quantile of χ^2_ν (see 5.6.2), the calculated standard uncertainties $u(a)$ and $u(b)$ and covariance $\text{cov}(a, b)$ (see 5.5.2) should be regarded as unreliable, as should the uncertainty associated with a predicted value (see 5.7).

5.7 Use of the calibration function

5.7.1 The calibration function is typically used for prediction (inverse evaluation) where, given an estimate of Y and its associated standard uncertainty, the corresponding value of X is estimated and its associated standard uncertainty is evaluated. Evaluation of the latter uncertainty makes use of the standard uncertainties associated with the estimates a and b as well as their associated covariance. See 11.1.

5.7.2 Forward evaluation where, given an estimate of X and its associated uncertainty, the corresponding value of Y is obtained together with its associated standard uncertainty, is sometimes required, for example, when comparing the calibrations of a set of similar instruments. See 11.2.

NOTE It is assumed that the conditions of measurement that held during the calibration hold at the time the calibration function is subsequently used. Otherwise, either a new calibration would be necessary or an appropriate adjustment should be made to take account of any change such as drift that might have occurred (and that any associated uncertainty is also handled). Control charts can be useful for this purpose.

5.8 Determining the ordinary least squares best-fit straight line to data

5.8.1 The ordinary (unweighted) least squares best-fit straight line to the data is defined by the values a and b of the parameters A and B that minimize

$$\sum_{i=1}^{m}(y_i - A - Bx_i)^2. \tag{2}$$

These values satisfy the equations given by equating to zero the partial derivatives of first order of expression (2) with respect to A and B.

5.8.2 a and b can be calculated in the following steps:

1 Set $x_0 = \dfrac{1}{m}\sum_{i=1}^{m} x_i$ and $y_0 = \dfrac{1}{m}\sum_{i=1}^{m} y_i$;

2 Set $\widetilde{x}_i = x_i - x_0$ and $\widetilde{y}_i = y_i - y_0$, $i = 1, \ldots, m$;

3 Set $b = \dfrac{\sum_{i=1}^{m} \widetilde{x}_i \widetilde{y}_i}{\sum_{i=1}^{m} \widetilde{x}_i^2}$ and $a = y_0 - bx_0$.

5.8.3 The values x_0 and y_0 are such that the best-fit line to the translated data points $(\widetilde{x}_i, \widetilde{y}_i)$ passes through the origin and has the same slope as the best-fit line to the original data points (x_i, y_i).

NOTE Mathematically, the best-fit parameters are determined by solving a pair of linear equations involving a matrix of dimension 2×2. For the transformed data points, this matrix is diagonal, allowing the solution parameters to be determined easily. Translating the data also has a beneficial effect in terms of numerical accuracy of the computed solution [4, page 33].

5.8.4 The methods described in the Clauses 6 to 10 below constitute extensions of the calculations in 5.8.2 that take into account the prescribed uncertainty information.

6 Model for uncertainties associated with the y_i

6.1 General

6.1.1 This clause considers the case 5.3.2 a), namely when the following information is provided for $i = 1, \ldots, m$:

a) measurement data (x_i, y_i), and

b) standard uncertainty $u(y_i)$ associated with y_i.

Annex D provides guidance on obtaining these uncertainties. All other uncertainties and covariances associated with the data are regarded as negligible.

6.1.2 The case 5.3.2 a) corresponds to that described by the statistical model

$$y_i = A^* + B^* x_i + e_i, \qquad i = 1, \ldots, m, \tag{3}$$

where the e_i are realizations of independent random variables with expectations zero and variances $u^2(y_i)$ [9, page 1]. A^* and B^* are the (unknown) values of the calibration function parameters for the measuring system for which a calibration is required and which provides the measurement data. This model, having no uncertainty associated with the x_i, is known as a functional model.

6.1.3 Let $w_i = 1/u(y_i)$, $i = 1, \ldots, m$. The estimates a and b are those that minimize the weighted sum of squares

$$\sum_{i=1}^{m} R_i^2 \equiv \sum_{i=1}^{m} w_i^2 (y_i - A - Bx_i)^2 \tag{4}$$

with respect to A and B. This minimization problem is known as a weighted least squares (WLS) problem. These estimates satisfy the equations given by equating to zero the partial derivatives of first order of expression (4) with respect to A and B.

6.2 Calibration parameter estimates and associated standard uncertainties and covariance

6.2.1 Estimates a and b are calculated in steps 1 to 5; the standard uncertainties $u(a)$ and $u(b)$ and covariance $\mathrm{cov}(a, b)$ are evaluated in step 6:

1 Set $w_i = \dfrac{1}{u(y_i)}$, $i = 1, \ldots, m$, and $F^2 = \displaystyle\sum_{i=1}^{m} w_i^2$;

2 Set $g_0 = \dfrac{1}{F^2} \displaystyle\sum_{i=1}^{m} w_i^2 x_i$ and $h_0 = \dfrac{1}{F^2} \displaystyle\sum_{i=1}^{m} w_i^2 y_i$;

3 Set $g_i = w_i(x_i - g_0)$ and $h_i = w_i(y_i - h_0)$, $i = 1, \ldots, m$;

4 Set $G^2 = \displaystyle\sum_{i=1}^{m} g_i^2$;

5 Set $b = \dfrac{1}{G^2} \displaystyle\sum_{i=1}^{m} g_i h_i$ and $a = h_0 - b g_0$;

6 Set $u^2(a) = \dfrac{1}{F^2} + \dfrac{g_0^2}{G^2}$, $u^2(b) = \dfrac{1}{G^2}$ and $\mathrm{cov}(a, b) = -\dfrac{g_0}{G^2}$.

NOTE 1 Steps 1 to 5 are equivalent to the steps:

i) Set $w_i = \dfrac{1}{u(y_i)}$, $i = 1, \ldots, m$, $x_0 = \dfrac{\sum_{i=1}^{m} w_i^2 x_i}{\sum_{i=1}^{m} w_i^2}$ and $y_0 = \dfrac{\sum_{i=1}^{m} w_i^2 y_i}{\sum_{i=1}^{m} w_i^2}$;

ii) Set $\widetilde{x}_i = x_i - x_0$ and $\widetilde{y}_i = y_i - y_0$, $i = 1, \ldots, m$;

iii) Set $b = \dfrac{\sum_{i=1}^{m} w_i^2 \widetilde{x}_i \widetilde{y}_i}{\sum_{i=1}^{m} w_i^2 \widetilde{x}_i^2}$ and $a = y_0 - b x_0$.

NOTE 2 Steps 1 to 5 determine the least squares solution to the system of equations

$$w_i a + w_i x_i b = w_i y_i, \qquad i = 1, \ldots, m.$$

NOTE 3 If the $u(y_i)$ are identical, so that the w_i are identical, a and b are the same as those given by the ordinary least squares best-fit line in 5.8.2.

NOTE 4 $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$ in step 6 are obtained by applying the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008 to a and b as provided by steps 1 to 5.

6.2.2 The estimates a and b determined in 6.1.3 have the following properties [15] for data y_i according to the model (3):

i) The estimates a and b are given by linear combinations of the data y_i.

ii) The estimates a and b can be regarded as realizations of random variables whose expectations are A^* and B^*, respectively.

iii) The covariance matrix for the random variables in ii) is specified by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$ calculated in 6.2.1.

Property i) states that a and b are derived using a linear estimation method. Property ii) states that the linear estimation method is unbiased. Properties ii) and iii) jointly show that the estimation method is consistent in the sense that as the number m of data points is increased, the estimates a and b converge to A^* and B^*, respectively.

The estimation method of 6.1.3 has the following optimal property for data y_i according to the model (3):

iv) The estimates $\breve{a}$ and $\breve{b}$ provided by any unbiased, linear estimation method can be regarded as realizations of random variables whose variances are at least as large as those associated with the WLS estimation method.

Property iv) can be interpreted as follows. For constants c and d, the standard uncertainty $u(c\breve{a} + d\breve{b})$ associated with a linear combination of the estimates $\breve{a}$ and $\breve{b}$ provided by any unbiased, linear estimation method is at least as great as $u(ca+db)$. Properties i) to iv) justify the use of least squares methods for data compatible with the model (3). Note that in the use of this model statements are only made about the expectations and variances associated with the e_i; the associated distributions are not further specified. If the additional assumption is made that the e_i are realizations of normally distributed random variables, then further properties associated with the WLS estimation method can be made:

v) The random variables in ii) are characterized by a bivariate normal distribution centred on A^* and B^* with covariance matrix specified by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$.

vi) The estimates a and b are maximum likelihood estimates, corresponding to the most likely values of A and B that could have given rise to the observed measurement data y_i.

vii) In the context of Bayesian inference, the state-of-knowledge distribution for A and B, given the observed measurement data y_i, is a bivariate normal distribution centred on a and b with covariance matrix specified by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$.

6.3 Validation of the model

If $m > 2$, the validity of the model can be partially tested using the weighted residuals r_i (continued from 6.2.1):

7 Form $r_i = w_i(y_i - a - bx_i)$, $i = 1, \ldots, m$;

8 Form the observed chi-squared value $\chi^2_{\mathrm{obs}} = \sum_{i=1}^{m} r_i^2$ and degrees of freedom $\nu = m - 2$;

9 Check whether χ^2_{obs} exceeds the 95 % quantile of χ^2_ν, and if it does reject the straight-line model.

NOTE The chi-squared test is based on an assumption that the e_i in model (3) are realizations of independent normal random variables.

6.4 Organization of the calculations

The calculations in 6.2.1 and 6.3 can be organized into one or two tableaux for implementation in a spreadsheet as in Tables 2 and 3, which can be amalgamated into a single table or spreadsheet.

Table 2 — Data for the weighted least squares straight-line calibration function

x_1	y_1	$u(y_1)$
x_2	y_2	$u(y_2)$
$\vdots$	$\vdots$	$\vdots$
x_m	y_m	$u(y_m)$

Table 3 — Organization of the calculations to determine the weighted least squares straight-line calibration function

				6.2.1 steps 2, 3				6.2.1 step 5 6.3 step 7	6.3 step 8
				g_0	h_0			a	
w_1	w_1^2	$w_1^2 x_1$	$w_1^2 y_1$	g_1	h_1	g_1^2	$g_1 h_1$	r_1	r_1^2
w_2	w_2^2	$w_2^2 x_2$	$w_2^2 y_2$	g_2	h_2	g_2^2	$g_2 h_2$	r_2	r_2^2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
w_m	w_m^2	$w_m^2 x_m$	$w_m^2 y_m$	g_m	h_m	g_m^2	$g_m h_m$	r_m	r_m^2
	$F^2 = \sum w_i^2$	$\sum w_i^2 x_i$	$\sum w_i^2 y_i$			$G^2 = \sum g_i^2$	$\sum g_i h_i$	b	$\chi^2_{\text{obs}} = \sum r_i^2$

EXAMPLE (EQUAL WEIGHTS) Table 4 gives six data points and their associated standard uncertainties. The measured values x_i are taken to be exact and the standard uncertainty associated with the measured values y_i is $u(y_i) = 0{,}5$. The weights are therefore taken to be $w_i = 1/u(y_i) = 2{,}0,\ i = 1, \ldots, 6$.

Table 4 — Data representing six measurement points, equal weights

x_i	y_i	$u(y_i)$
1,0	3,3	0,5
2,0	5,6	0,5
3,0	7,1	0,5
4,0	9,3	0,5
5,0	10,7	0,5
6,0	12,1	0,5

The best fit straight-line parameters are calculated as in Table 5. From the table, $g_0 = 84{,}000/24{,}000 = 3{,}500$, $h_0 = 192{,}400/24{,}000 = 8{,}017$, $b = 123{,}000/70{,}000 = 1{,}757$ and $a = 8{,}017 - (1{,}757)(3{,}500) = 1{,}867$.

Table 5 — Calculation tableau associated with the data in Table 4

w_i	w_i^2	$w_i^2 x_i$	$w_i^2 y_i$	g_i	h_i	g_i^2	$g_i h_i$	r_i	r_i^2
				3,500	8,017			$a = 1{,}867$	
2,000	4,000	4,000	13,200	−5,000	−9,433	25,000	47,167	−0,648	0,419
2,000	4,000	8,000	22,400	−3,000	−4,833	9,000	14,500	0,438	0,192
2,000	4,000	12,000	28,400	−1,000	−1,833	1,000	1,833	−0,076	0,006
2,000	4,000	16,000	37,200	1,000	2,567	1,000	2,567	0,810	0,655
2,000	4,000	20,000	42,800	3,000	5,367	9,000	16,100	0,095	0,009
2,000	4,000	24,000	48,400	5,000	8,167	25,000	40,833	−0,619	0,383
	24,000	84,000	192,400			70,000	123,000	$b = 1{,}757$	1,665

The standard uncertainties and covariance associated with the fitted parameters can also be evaluated, using the formulæ in 6.2.1, from information in Table 5:

$$u^2(a) = 1/24{,}000 + (3{,}500)^2/70{,}000, \text{ so that } u(a) = 0{,}465;$$
$$u^2(b) = 1/70{,}000, \text{ so that } u(b) = 0{,}120;$$
$$u(a, b) = -3{,}500/70{,}000 = -0{,}050.$$

The observed chi-squared value is $\chi^2_{\text{obs}} = 1{,}665$ with $\nu = 4$ degrees of freedom, as calculated in Table 5 using 6.3. Since χ^2_{obs} does not exceed the 95 % quantile of χ^2_ν, namely 9,488, this is no reason to doubt the consistency of the straight-line model and the data.

The data and fitted straight-line calibration function are displayed in Figure 2. Standard uncertainties associated with the y_i are illustrated (and in subsequent figures) by vertical lines, centred on y_i and having extremities $y_i - u(y_i)$ and $y_i + u(y_i)$. The weighted residuals are shown in Figure 3.

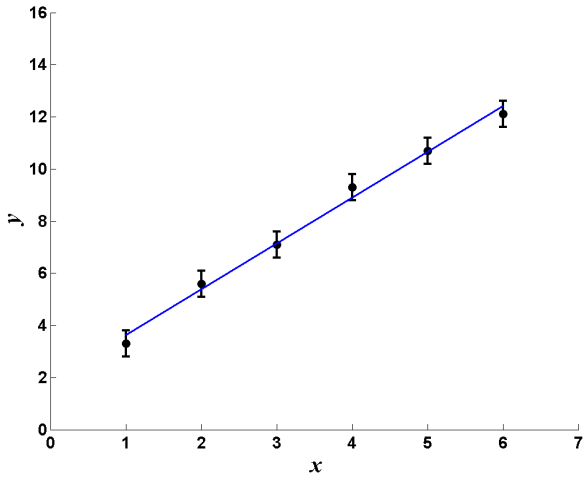

Figure 2 — Data in Table 4 and fitted straight-line calibration function obtained in Table 5

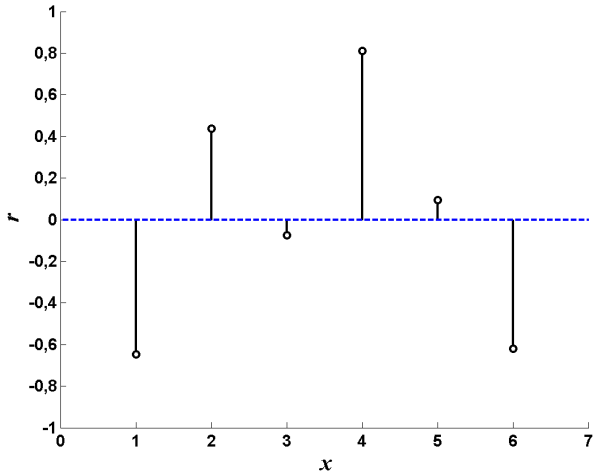

Figure 3 — Weighted residuals r_i obtained in Table 5

EXAMPLE (UNEQUAL WEIGHTS) Table 6 gives six data points and their associated standard uncertainties. The x_i are taken to be exact. The y_i were obtained using two instrument settings, so that for larger values of X, the y_i are less accurate.

Table 6 — Data representing six measurement points, unequal weights

x_i	y_i	$u(y_i)$
1,0	3,2	0,5
2,0	4,3	0,5
3,0	7,6	0,5
4,0	8,6	1,0
5,0	11,7	1,0
6,0	12,8	1,0

The best fit straight-line parameters are calculated as in Table 7. From the table, $g_0 = 39{,}000/15{,}000 = 2{,}600$, $h_0 = 93{,}500/15{,}000 = 6{,}233$, $b = 65{,}000/31{,}600 = 2{,}057$ and $a = 6{,}233 - (2{,}057)(2{,}600) = 0{,}885$.

Table 7 — Calculation tableau associated with the data in Table 6

w_i	w_i^2	$w_i^2 x_i$	$w_i^2 y_i$	g_i	h_i	g_i^2	$g_i h_i$	r_i	r_i^2
				2,600	6,233			$a = 0{,}885$	
2,000	4,000	4,000	12,800	−3,200	−6,067	10,240	19,413	0,516	0,266
2,000	4,000	8,000	17,200	−1,200	−3,867	1,440	4,640	−1,398	1,955
2,000	4,000	12,000	30,400	0,800	2,733	0,640	2,187	1,088	1,183
1,000	1,000	4,000	8,600	1,400	2,367	1,960	3,313	−0,513	0,263
1,000	1,000	5,000	11,700	2,400	5,467	5,760	13,120	0,530	0,281
1,000	1,000	6,000	12,800	3,400	6,567	11,560	22,327	−0,427	0,182
	15,000	39,000	93,500			31,600	65,000	$b = 2{,}057$	4,131

The standard uncertainties and covariance associated with the fitted parameters can be evaluated, using the formulæ in 6.2.1, from information in Table 7:

$$u^2(a) = 1/15{,}000 + (2{,}600)^2/31{,}600, \text{ so that } u(a) = 0{,}530;$$
$$u^2(b) = 1/31{,}600, \text{ so that } u(b) = 0{,}178;$$
$$u(a,b) = -2{,}600/31{,}600 = -0{,}082.$$

The observed chi-squared value is $\chi^2_{\text{obs}} = 4{,}131$ with $\nu = 4$ degrees of freedom, as calculated in Table 7 using 6.3. Since χ^2_{obs} does not exceed the 95 % quantile of χ^2_ν, namely 9,488, this is no reason to doubt the consistency of the straight-line model and the data.

The data and fitted straight-line calibration function are displayed in Figure 4. The weighted residuals are shown in Figure 5.

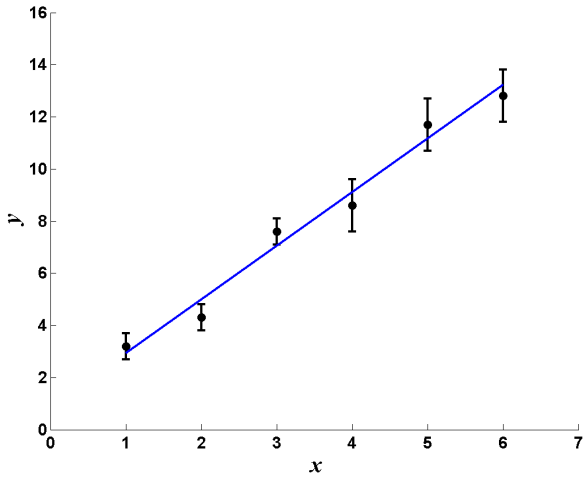

Figure 4 — Data in Table 6 and fitted straight-line calibration function obtained in Table 7

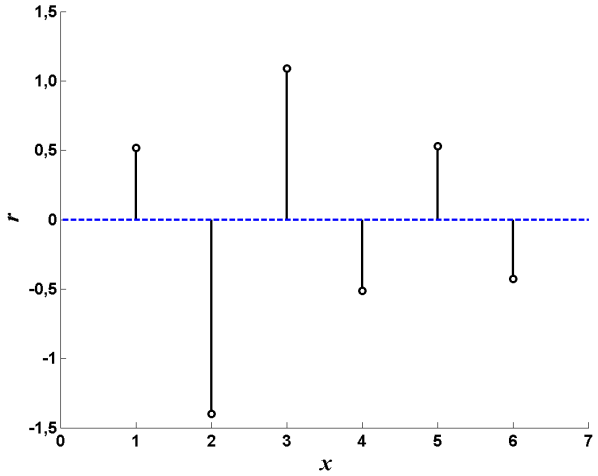

Figure 5 — Weighted residuals r_i obtained in Table 7

7 Model for uncertainties associated with the x_i and the y_i

7.1 General

7.1.1 This clause considers the case 5.3.2 b), namely when the following information is provided for $i = 1, \ldots, m$:

a) measurement data (x_i, y_i),

b) standard uncertainty $u(x_i)$ associated with x_i, and

c) standard uncertainty $u(y_i)$ associated with y_i.

Annex D provides guidance on obtaining these uncertainties. All covariances associated with the data are regarded as negligible.

7.1.2 The case 5.3.2 b) corresponds to that described by the statistical model

$$x_i = X_i^* + d_i, \qquad y_i = Y_i^* + e_i, \qquad Y_i^* = A^* + B^* X_i^*, \qquad i = 1, \ldots, m, \tag{5}$$

where the d_i and e_i are realizations of independent random variables with expectations zero and variances $u^2(x_i)$ and $u^2(y_i)$, respectively. This model is known as a structural model. In the model, (x_i, y_i) represent the measured co-ordinates of the (unobserved) point (X_i^*, Y_i^*) lying on the line $Y = A^* + B^* X$.

7.1.3 As the x_i (in addition to the y_i – see Clause 6) have associated uncertainties, account is also taken of them in determining a straight-line calibration function. The problem of determining a and b in this context is one of weighted orthogonal distance regression (weighted ODR) [3] or generalized distance regression (GDR) [2]. In the statistical literature it is referred to as an errors-in-variables model [7], [9, page 50], [17, page 189]. The estimates a and b are those that minimize the sum of squares

$$\sum_{i=1}^{m} \left[v_i^2 (x_i - X_i)^2 + w_i^2 (y_i - A - B X_i)^2 \right], \tag{6}$$

with respect to A, B, and X_i, $i = 1, \ldots, m$, for weights $v_i = 1/u(x_i)$ and $w_i = 1/u(y_i)$. Each solution estimate x_i^*, along with a and b, specifies the estimate (x_i^*, y_i^*), $y_i^* = a + b x_i^*$, of (X_i^*, Y_i^*) in model (5).

7.1.4 Given A and B, the values x_i^* that minimize the sum of squares (6) with respect to X_i are given by

$$x_i^* = x_i^*(A, B) = \left[u^2(y_i) x_i + (y_i - A) B u^2(x_i) \right] T_i, \qquad T_i = \frac{1}{u^2(y_i) + B^2 u^2(x_i)}. \tag{7}$$

Using expressions (7) the optimization problem can be posed in terms of parameters A and B alone by replacing X_i in expression (6) by $x_i^*(A, B)$ giving

$$\sum_{i=1}^{m} \left\{ v_i^2 \left[x_i - x_i^*(A, B) \right]^2 + w_i^2 \left[y_i - y_i^*(A, B) \right]^2 \right\}, \qquad y_i^*(A, B) = A + B x_i^*(A, B). \tag{8}$$

7.1.5 If

$$R_i = R_i(A, B) = \left\{ -B \left[x_i - x_i^*(A, B) \right] + \left[y_i - y_i^*(A, B) \right] \right\} T_i^{1/2}, \tag{9}$$

then the sum of squares (8) is equivalent to

$$\sum_{i=1}^{m} R_i^2.$$

The term R_i has the following geometric interpretation. The normal vector to the line $Y = A + BX$ is given by $(-B, 1)^\top / (1 + B^2)^{1/2}$ and R_i is a weighted multiple of the signed component of $(x_i - x_i^*(A, B), y_i - y_i^*(A, B))^\top$ in the direction of the normal vector.

NOTE 1 In ordinary least squares (see 5.8) and weighted least squares (see Clause 6), the distance to the line is measured 'vertically', that is, in the Y-direction, reflecting the fact that the deviation of the measured point (x_i, y_i) from the line can be accounted for in terms of an error e_i associated with y_i, since x_i is assumed to be known accurately. Weighted ODR addresses the case where there are also uncertainties associated with the x_i.

NOTE 2 Expressions (7) are given by equating to zero the partial derivatives of first order of expression (6) with respect to A, B and the X_i.

NOTE 3 If $u_i(x_i) = 0$ then, in expressions (7), $x_i^*(A, B) = x_i$ (so that $y_i^*(A, B) = A + Bx_i$) and $T_i = 1/u^2(y_i) = w_i^2$. Consequently, R_i in expression (9) is given by $R_i = w_i(y_i - A - Bx_i)$. Thus, if $u(x_i) = 0$ the term R_i is evaluated in the same way as in expression (4) in 6.1.3.

NOTE 4 If $u(x_i) = u(y_i) = u_i$, say, then $x_i^*(A, B)$ defines the point on the line $Y = A + BX$ closest to (x_i, y_i) and

$$T_i = \frac{1}{u_i^2}\frac{1}{1+B^2}, \qquad R_i = \frac{1}{u_i}\frac{1}{(1+B^2)^{1/2}}\left\{-B\left[x_i - x_i^*(A,B)\right] + \left[y_i - y_i^*(A,B)\right]\right\}.$$

Since the normal vector to the line is $(-B, 1)^\top/(1 + B^2)^{1/2}$, R_i is the weighted distance from the point (x_i, y_i) to the line $Y = A + BX$.

7.1.6 Subclause 7.1.3 involves A, B and the X_i, $i = 1, \ldots, m$, as variables in the minimization. The calculations given in 7.2.1 perform this minimization in a two-stage iteration [2]:

(i) from approximations to a and b, determine the corresponding optimal x_i^*, and

(ii) in terms of these x_i^*, determine new approximations to a and b that will reduce the sum of squares (6).

NOTE No notational distinction is made between x_i^* at a typical iteration and the final solution value.

7.2 Calibration parameter estimates and associated standard uncertainties and covariance

7.2.1 Estimates a and b are calculated in steps 1 to 6 below using the iterative scheme indicated in 7.1.6; the standard uncertainties $u(a)$ and $u(b)$ and covariance $\mathrm{cov}(a, b)$ are evaluated in step 7 (see Annex B):

1 Obtain initial approximations $\widetilde{a}$ and $\widetilde{b}$ to a and b, for example, by determining the weighted least squares best-fit line to the data (see 6.2.1 steps 1 to 5), ignoring the uncertainties associated with the x_i;

2 Set $t_i = \dfrac{1}{u^2(y_i) + \widetilde{b}^2 u^2(x_i)}$, $x_i^* = \left[x_i u^2(y_i) + (y_i - \widetilde{a})\widetilde{b}u^2(x_i)\right] t_i$ and $z_i = y_i - \widetilde{a} - \widetilde{b}x_i$, $i = 1, \ldots, m$;

3 Set $f_i = t_i^{1/2}$, $g_i = f_i x_i^*$ and $h_i = f_i z_i$, $i = 1, \ldots, m$;

4 Determine the (unweighted) least squares solution δa and δb to the system of equations

$$(\delta A) f_i + (\delta B) g_i = h_i, \qquad i = 1, \ldots, m,$$

that is

i) Set $F^2 = \sum_{i=1}^{m} f_i^2$;

ii) Set $g_0 = \dfrac{1}{F^2}\sum_{i=1}^{m} f_i g_i$ and $h_0 = \dfrac{1}{F^2}\sum_{i=1}^{m} f_i h_i$;

iii) Set $\widetilde{g}_i = g_i - g_0 f_i$ and $\widetilde{h}_i = h_i - h_0 f_i$, $i = 1, \ldots, m$;

iv) Set $\widetilde{G}^2 = \sum_{i=1}^{m} \widetilde{g}_i^2$;

v) Set $\delta b = \dfrac{1}{\widetilde{G}^2}\sum_{i=1}^{m}\widetilde{g}_i\widetilde{h}_i$ and $\delta a = h_0 - (\delta b)g_0$;

5 Update the current approximations to the parameters and residuals: $\widetilde{a} := \widetilde{a} + \delta a$, $\widetilde{b} := \widetilde{b} + \delta b$, $r_i = \tilde{h}_i - (\delta b)\tilde{g}_i, i = 1, \ldots, m$;

6 Repeat steps 2 to 5 until convergence has been achieved. Set $a = \widetilde{a}$, $b = \widetilde{b}$;

7 Set $u^2(a) = \dfrac{1}{F^2} + \dfrac{g_0^2}{\widetilde{G}^2}$, $u^2(b) = \dfrac{1}{\widetilde{G}^2}$ and $\mathrm{cov}(a,b) = -\dfrac{g_0}{\widetilde{G}^2}$, where g_0, h_0, etc., are the values calculated in step 4.

NOTE 1 The calculations in step 4 are similar to those in steps 1 to 5 in 6.2.1.

NOTE 2 In step 2, x_i^* defines the point $(x_i^*, a + bx_i^*)$ on the current approximation to the best-fit straight-line calibration function that is closest, as a weighted distance, to the measured data point (x_i, y_i).

NOTE 3 In step 3, the calculated h_i represents a value of the generalized distance R_i in expression (9) from the ith data point to the current estimate of the straight-line calibration function. The algorithm is designed to minimize the sum of squares of such distances.

NOTE 4 In step 4, the corrections δa and δb will generally decrease in magnitude by ultimately an approximately constant factor from iteration to iteration. The size of the reduction depends largely on the uncertainties associated with the data: the smaller these uncertainties are, the greater the reduction will be. The iterative scheme can be terminated when the magnitudes of the corrections are judged to be negligible.

NOTE 5 The residuals calculated in step 5 are associated with the solution of the system of equations solved in step 4. At convergence, the r_i calculated in step 5 is the same as the h_i calculated in step 3.

NOTE 6 Strictly only the residuals calculated in step 5 at the final iteration are required. However, for ease of presentation in tableau format (Table 9 in 7.4), the residuals are calculated at each iteration.

NOTE 7 $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a,b)$ in step 7 are obtained by applying the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008 to a and b as provided by steps 1 to 6.

7.2.2 While it is possible to derive the properties in 6.2.2 for the WLS estimation method, the fact that the estimates a and b determined by minimizing the sum of squares (6) depend non-linearly on the data x_i and y_i means that the corresponding properties for weighted ODR cannot be straightforwardly stated. The estimates a and b determined in 7.1.3 have the following properties for data x_i and y_i according to the model (5):

i) The estimates a and b are given by non-linear functions of the data x_i and y_i.

ii) The estimates a and b can be regarded as realizations of random variables whose expectations are approximately A^* and B^*, respectively.

iii) The elements of the covariance matrix for the random variables in ii) are approximated by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a,b)$ calculated in 7.2.1.

The approximations in ii) and iii) will be more accurate for data having smaller associated uncertainties. However, the estimation method has the following consistency property:

iv) For data satisfying the model (5), as the number m of data points increases, the estimates a and b converge to A^* and B^*, respectively [16].

By contrast, the WLS estimation method will generally underestimate the magnitude of the slope parameter [5] for data generated according to the model (5).

If the additional assumption is made that the d_i and e_i are realizations of normally distributed random variables, then further properties associated with the weighted ODR estimation method can be stated:

v) The random variables in ii) are characterized approximately by a bivariate normal distribution centred on A^* and B^* with covariance matrix specified by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$.

vi) The estimates a and b are maximum likelihood estimates, corresponding to the most likely values of A and B that could have given rise to the observed measurement data x_i and y_i.

vii) In the context of Bayesian inference, the state-of-knowledge distribution for A and B, given the observed measurement data x_i and y_i, is approximated by a bivariate normal distribution centred on a and b with covariance matrix specified by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$.

7.3 Validation of the model

If $m > 2$, the validity of the model can be partially tested using the weighted residuals r_i calculated in step 5 in 7.2.1 at the final iteration, that is, at convergence (continued from 7.2.1):

8 Form the observed chi-squared value $\chi^2_{\mathrm{obs}} = \sum_{i=1}^{m} r_i^2$ and degrees of freedom $\nu = m - 2$;

9 Check whether χ^2_{obs} exceeds the 95 % quantile of χ^2_ν, and if it does reject the straight-line model.

NOTE The chi-squared test is based on an assumption that the d_i and e_i in model (5) are realizations of independent normal random variables and on a first order approximation.

7.4 Organization of the calculations

The calculations in 7.2.1 and 7.3 can be organized into two sequences of tableaux, suitable for implementation in a spreadsheet. The first tableau (Table 8), given approximations $\widetilde{a}$ and $\widetilde{b}$ (see 7.2.1 step 1), calculates the f_i, g_i and h_i (see 7.2.1 step 3). The second tableau (Table 9) uses these f_i, g_i and h_i to calculate corrections δa and δb (see 7.2.1 step 4).

Table 8 — Calculations for determining the straight-line calibration function, given approximations $\widetilde{a}$ and $\widetilde{b}$ to the line parameter estimates a and b

				7.2.1 step 1 or step 5	7.2.1 step 2	7.2.1 step 2	7.2.1 step 3		
				$\widetilde{a}$	$\widetilde{b}$				
x_1	$u(x_1)$	y_1	$u(y_1)$	t_1	x_1^*	z_1	f_1	g_1	h_1
x_2	$u(x_2)$	y_2	$u(y_2)$	t_2	x_2^*	z_2	f_2	g_2	h_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
x_m	$u(x_m)$	y_m	$u(y_m)$	t_m	x_m^*	z_m	f_m	g_m	h_m

Table 9 — Organization of the calculations to determine corrections δa and δb for the GDR straight-line calibration function

			7.2.1 steps 4 ii), 4 iii)				7.2.1 steps 4 v), 5	7.3 step 8
			g_0	h_0			δa	
f_1^2	$f_1 g_1$	$f_1 h_1$	$\widetilde{g}_1$	$\widetilde{h}_1$	$\widetilde{g}_1^2$	$\widetilde{g}_1\widetilde{h}_1$	r_1	r_1^2
f_2^2	$f_2 g_2$	$f_2 h_2$	$\widetilde{g}_2$	$\widetilde{h}_2$	$\widetilde{g}_2^2$	$\widetilde{g}_2\widetilde{h}_2$	r_2	r_2^2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
f_m^2	$f_m g_m$	$f_m h_m$	$\widetilde{g}_m$	$\widetilde{h}_m$	$\widetilde{g}_m^2$	$\widetilde{g}_m\widetilde{h}_m$	r_m	r_m^2
$F^2 = \sum f_i^2$	$\sum f_i g_i$	$\sum f_i h_i$			$\widetilde{G}^2 = \sum \widetilde{g}_i^2$	$\sum \widetilde{g}_i\widetilde{h}_i$	δb	$\sum r_i^2$

EXAMPLE Table 10 gives six measured data points and their associated standard uncertainties.

Table 10 — Six measured data points and corresponding uncertainties

x_i	$u(x_i)$	y_i	$u(y_i)$
1,2	0,2	3,4	0,2
1,9	0,2	4,4	0,2
2,9	0,2	7,2	0,2
4,0	0,2	8,5	0,4
4,7	0,2	10,8	0,4
5,9	0,2	13,5	0,4

In order to determine initial approximations $\widetilde{a}$ and $\widetilde{b}$ (7.2.1 step 1), a weighted least squares straight-line calibration function is determined. Following the scheme described in 6.2, the tableaux given in Tables 11 and 12 are obtained.

Table 11 — Data representing six measurement points

x_i	y_i	$u(y_i)$
1,2	3,4	0,2
1,9	4,4	0,2
2,9	7,2	0,2
4,0	8,5	0,4
4,7	10,8	0,4
5,9	13,5	0,4

Table 12 — Calculation tableau associated with the data in Table 11 to determine initial approximations $\widetilde{a}$ and $\widetilde{b}$

w_i	w_i^2	$w_i^2 x_i$	$w_i^2 y_i$	g_i	h_i	g_i^2	$g_i h_i$	r_i	r_i^2
				2,573 3	6,186 7			$a = 0{,}658\,3$	
5,000 0	25,000 0	30,000 0	85,000 0	−6,866 7	−13,933 3	47,151 1	95,675 6	0,818 6	0,670 1
5,000 0	25,000 0	47,500 0	110,000 0	−3,366 7	−8,933 3	11,334 4	30,075 6	−1,700 6	2,892 0
5,000 0	25,000 0	72,500 0	180,000 0	1,633 3	5,066 7	2,667 8	8,275 6	1,557 7	2,426 4
2,500 0	6,250 0	25,000 0	53,125 0	3,566 7	5,783 3	12,721 1	20,627 2	−1,879 1	3,531 0
2,500 0	6,250 0	29,375 0	67,500 0	5,316 7	11,533 3	28,266 9	61,318 9	0,111 3	0,012 4
2,500 0	6,250 0	36,875 0	84,375 0	8,316 7	18,283 3	69,166 9	152,056 4	0,416 3	0,173 3
	93,750 0	241,250 0	580,000 0			171,308 3	368,029 2	$b = 2{,}148\,3$	9,705 2

The initial approximations are $\widetilde{a} = 0{,}658\,3$ and $\widetilde{b} = 2{,}148\,3$. Given these approximations, the first tableau (Table 13) of the form in Table 8 can be calculated to obtain f_i, g_i and h_i. The second tableau (Table 14) of the form in Table 9 then calculates increments $\delta a = -0{,}078\,4$ and $\delta b = 0{,}011\,1$ (7.2.1 step 4). At the end of the iteration, the approximations $\widetilde{a}$ and $\widetilde{b}$ are updated (7.2.1 step 5):

$$\widetilde{a} := \widetilde{a} + \delta a = 0{,}658\,3 - 0{,}078\,4 = 0{,}579\,9;$$
$$\widetilde{b} := \widetilde{b} + \delta b = 2{,}148\,3 + 0{,}011\,1 = 2{,}159\,4;$$

With these updated values of $\widetilde{a}$ and $\widetilde{b}$, two new tableaux are formed (Tables 15 and 16) to determine further corrections $\delta a = -0{,}001\,0$ and $\delta b = 0{,}000\,2$. The process is repeated a third time (Tables 17 and 18). In this case, the magnitudes of the corrections are less than 0,000 05, which is judged to be negligible for the purpose, and the final approximations to the parameter estimates are $a = 0{,}578\,8$ and $b = 2{,}159\,7$.

The standard uncertainties and covariance (7.2.1 step 7) associated with the fitted parameters can also be evaluated from information in the final tableau (Table 18):

$$u^2(a) = 1/21{,}897\,7 + (3{,}141\,4)^2/54{,}427\,1 \text{ so that } u(a) = 0{,}476\,4;$$
$$u^2(b) = 1/54{,}427\,1, \text{ so that } u(b) = 0{,}135\,5;$$
$$u(a,b) = -3{,}141\,4/54{,}427\,1 = -0{,}057\,7.$$

The observed chi-squared value is $\chi^2_{\text{obs}} = 2{,}743$ with $\nu = 4$ degrees of freedom, as calculated in Table 18 using 7.3. Since χ^2_{obs} does not exceed the 95 % quantile of χ^2_ν, namely 9,488, this is no reason to doubt the consistency of the straight-line model and the data.

The data points and weighted ODR straight-line calibration function are graphed in Figure 6. The graph also gives, for each i, the location of (x_i^*, y_i^*), the point on the line closest in probabilistic terms to the data point (x_i, y_i). The weighted residuals are illustrated in Figure 7.

Table 13 — First iteration to determine f_i, g_i and h_i, given $\widetilde{a}$ and $\widetilde{b}$

x_i	$u(x_i)$	y_i	$u(y_i)$	t_i	x_i^*	z_i	f_i	g_i	h_i
				0,658 3	2,148 3				
1,200 0	0,200 0	3,400 0	0,200 0	4,452 2	1,262 6	0,163 7	2,110 0	2,664 2	0,345 5
1,900 0	0,200 0	4,400 0	0,200 0	4,452 2	1,769 9	−0,340 1	2,110 0	3,734 5	−0,717 6
2,900 0	0,200 0	7,200 0	0,200 0	4,452 2	3,019 2	0,311 6	2,110 0	6,370 6	0,657 5
4,000 0	0,200 0	8,500 0	0,400 0	2,901 9	3,812 6	−0,751 5	1,703 5	6,494 7	−1,280 2
4,700 0	0,200 0	10,800 0	0,400 0	2,901 9	4,711 1	0,044 7	1,703 5	8,025 3	0,076 1
5,900 0	0,200 0	13,500 0	0,400 0	2,901 9	5,941 6	0,166 7	1,703 5	10,121 4	0,284 0

Table 14 — First iteration to determine corrections δa and δb, given f_i, g_i and h_i

f_i^2	$f_i g_i$	$f_i h_i$	$\widetilde{g}_i$	$\widetilde{h}_i$	$\widetilde{g}_i^2$	$\widetilde{g}_i\widetilde{h}_i$	r_i	r_i^2
			3,123 9	−0,043 7			$\delta a = -0{,}078\ 4$	
4,452 2	5,621 6	0,729 0	−3,927 3	0,437 8	15,423 6	−1,719 3	0,481 4	0,231 8
4,452 2	7,879 9	−1,514 1	−2,857 0	−0,625 3	8,162 3	1,786 4	−0,593 5	0,352 3
4,452 2	13,442 2	1,387 4	−0,220 9	0,749 8	0,048 8	−0,165 6	0,752 3	0,565 9
2,901 9	11,063 6	−2,180 7	1,173 2	−1,205 7	1,376 4	−1,414 5	−1,218 7	1,485 2
2,901 9	13,671 0	0,129 7	2,703 8	0,150 6	7,310 8	0,407 3	0,120 6	0,014 5
2,901 9	17,241 6	0,483 8	4,799 9	0,358 5	23,038 7	1,720 8	0,305 2	0,093 1
22,062 2	68,919 9	−0,964 8			55,360 6	0,615 2	$\delta b = 0{,}011\ 1$	2,742 9

Table 15 — As Table 13 but for the second iteration

x_i	$u(x_i)$	y_i	$u(y_i)$	t_i	x_i^*	z_i	f_i	g_i	h_i
				0,579 9	2,159 4				
1,200 0	0,200 0	3,400 0	0,200 0	4,414 6	1,287 3	0,228 9	2,101 1	2,704 7	0,480 8
1,900 0	0,200 0	4,400 0	0,200 0	4,414 6	1,792 2	−0,282 7	2,101 1	3,765 5	−0,594 1
2,900 0	0,200 0	7,200 0	0,200 0	4,414 6	3,036 5	0,357 9	2,101 1	6,379 9	0,751 9
4,000 0	0,200 0	8,500 0	0,400 0	2,885 8	3,821 2	−0,717 5	1,698 8	6,491 3	−1,218 9
4,700 0	0,200 0	10,800 0	0,400 0	2,885 8	4,717 7	0,070 9	1,698 8	8,014 2	0,120 5
5,900 0	0,200 0	13,500 0	0,400 0	2,885 8	5,944 8	0,179 6	1,698 8	10,098 8	0,305 1

Table 16 — As Table 14 but for the second iteration

f_i^2	$f_i g_i$	$f_i h_i$	$\widetilde{g}_i$	$\widetilde{h}_i$	$\widetilde{g}_i^2$	$\widetilde{g}_i\widetilde{h}_i$	r_i	r_i^2
			3,141 2	−0,000 3			$\delta a = -0{,}001\ 0$	
4,414 6	5,682 7	1,010 3	−3,895 3	0,481 4	15,173 4	−1,875 1	0,482 3	0,232 6
4,414 6	7,911 7	−1,248 2	−2,834 4	−0,593 5	8,033 9	1,682 2	−0,592 8	0,351 4
4,414 6	13,404 7	1,579 8	−0,220 1	0,752 4	0,048 4	−0,165 6	0,752 5	0,566 2
2,885 8	11,027 1	−2,070 6	1,155 1	−1,218 4	1,334 2	−1,407 4	−1,218 7	1,485 2
2,885 8	13,614 3	0,204 6	2,678 1	0,120 9	7,172 0	0,323 8	0,120 3	0,014 5
2,885 8	17,155 5	0,518 3	4,762 6	0,305 6	22,682 4	1,455 3	0,304 4	0,092 7
21,901 2	68,796 1	−0,005 7			54,444 3	0,013 2	$\delta b = 0{,}000\ 2$	2,742 7

Table 17 — As Table 13 but for the third iteration

x_i	$u(x_i)$	y_i	$u(y_i)$	t_i	x_i^*	z_i	f_i	g_i	h_i
				0,578 8	2,159 7				
1,200 0	0,200 0	3,400 0	0,200 0	4,413 8	1,287 5	0,229 6	2,100 9	2,705 0	0,482 3
1,900 0	0,200 0	4,400 0	0,200 0	4,413 8	1,792 4	−0,282 2	2,100 9	3,765 7	−0,592 8
2,900 0	0,200 0	7,200 0	0,200 0	4,413 8	3,036 6	0,358 2	2,100 9	6,379 5	0,752 5
4,000 0	0,200 0	8,500 0	0,400 0	2,885 5	3,821 2	−0,717 4	1,698 7	6,490 9	−1,218 7
4,700 0	0,200 0	10,800 0	0,400 0	2,885 5	4,717 6	0,070 8	1,698 7	8,013 7	0,120 3
5,900 0	0,200 0	13,500 0	0,400 0	2,885 5	5,944 7	0,179 2	1,698 7	10,098 0	0,304 4

Table 18 — As Table 14 but for the third iteration

f_i^2	$f_i g_i$	$f_i h_i$	$\widetilde{g}_i$	$\widetilde{h}_i$	$\widetilde{g}_i^2$	$\widetilde{g}_i \widetilde{h}_i$	r_i	r_i^2
			3,141 4	0,000 0			$\delta a = 0{,}000\,0$	
4,413 8	5,682 9	1,013 3	−3,894 7	0,482 3	15,168 5	−1,878 5	0,482 3	0,232 7
4,413 8	7,911 3	−1,245 4	−2,834 0	−0,592 8	8,031 5	1,680 0	−0,592 8	0,351 4
4,413 8	13,402 7	1,580 9	−0,220 2	0,752 5	0,048 5	−0,165 7	0,752 5	0,566 2
2,885 5	11,025 8	−2,070 2	1,154 8	−1,218 7	1,333 5	−1,407 3	−1,218 7	1,485 2
2,885 5	13,612 6	0,204 3	2,677 6	0,120 3	7,169 5	0,322 0	0,120 3	0,014 5
2,885 5	17,153 1	0,517 1	4,761 9	0,304 4	22,675 6	1,449 6	0,304 4	0,092 7
21,897 7	68,788 4	0,000 0			54,427 1	0,000 1	$\delta b = 0{,}000\,0$	2,742 7

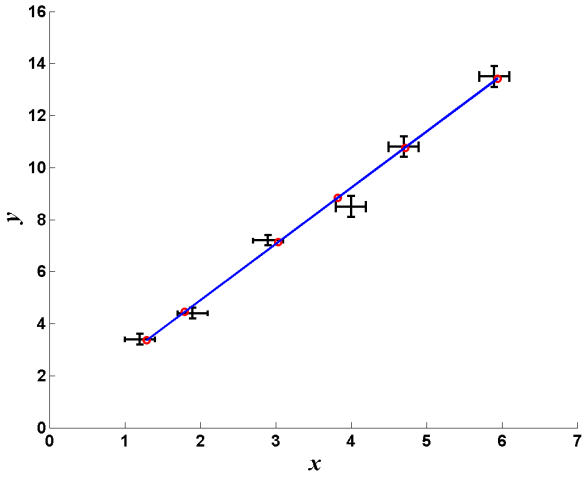

Figure 6 — Data in Table 10 and fitted straight-line calibration function obtained in Tables 11 to 18

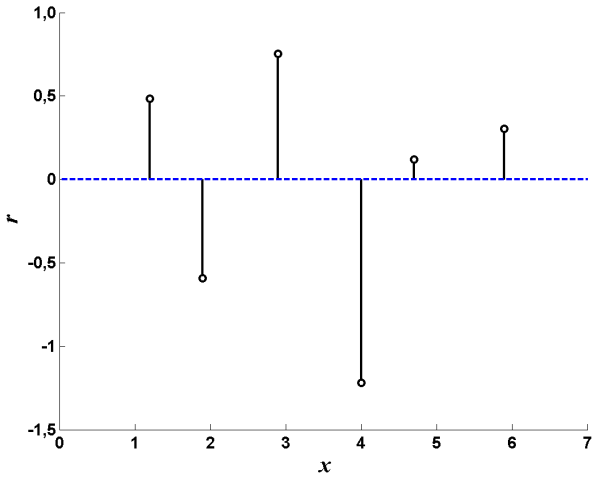

Figure 7 — Weighted distances obtained in Table 18

8 Model for uncertainties associated with the x_i and the y_i and covariances associated with the pairs (x_i, y_i)

8.1 General

8.1.1 This clause considers the case 5.3.2 c), namely when the following information is provided for $i = 1, \ldots, m$:

a) measurement data (x_i, y_i),

b) standard uncertainty $u(x_i)$ associated with x_i,

c) standard uncertainty $u(y_i)$ associated with y_i, and

d) covariance $\mathrm{cov}(x_i, y_i)$ associated with x_i and y_i.

Annex D provides guidance on obtaining these uncertainties and covariances. All other covariances associated with the data are regarded as negligible.

8.1.2 The case 5.3.2 c) corresponds to that of the statistical model

$$x_i = X_i^* + d_i, \qquad y_i = Y_i^* + e_i, \qquad Y_i^* = A^* + B^* X_i^*, \qquad i = 1, \ldots, m, \tag{10}$$

where each pair (d_i, e_i) is a realization of a bivariate random variable with expectation $(0, 0)^\top$ and covariance matrix having diagonal elements $u^2(x_i)$ and $u^2(y_i)$ and off-diagonal elements $\mathrm{cov}(x_i, y_i) = \mathrm{cov}(y_i, x_i)$, namely

$$\begin{bmatrix} u^2(x_i) & \mathrm{cov}(x_i, y_i) \\ \mathrm{cov}(y_i, x_i) & u^2(y_i) \end{bmatrix},$$

that is independent of the other such random variables.

NOTE The assumption that the (d_i, e_i) are realizations of bivariate normal random variables is only needed for the validation of the model (10).

8.2 Calibration parameter estimates and associated standard uncertainties and covariance

8.2.1 Algorithmically, this case can be handled by an extension (see Annex B) of the treatment in Clause 7. The calculations are identical to those in that clause, except step 2 in 7.2.1 is replaced by

2 Set $t_i = \dfrac{1}{u^2(y_i) - 2\widetilde{b}\mathrm{cov}(x_i, y_i) + \widetilde{b}^2 u^2(x_i)}$,

$x_i^* = \left\{ [u^2(y_i) - \widetilde{b}\mathrm{cov}(x_i, y_i)]x_i - [\mathrm{cov}(x_i, y_i) - \widetilde{b}u^2(x_i)](y_i - \widetilde{a}) \right\} t_i$ and

$z_i = y_i - \widetilde{a} - \widetilde{b}x_i$, $i = 1, \ldots, m$;

8.2.2 All the properties stated in 7.2.2 apply for data generated according to the model (10) and the remainder of Clause 7 follows analogously.

9 Model for uncertainties and covariances associated with the y_i

9.1 General

9.1.1 This clause considers the case 5.3.2 d), namely when the following information is provided for $i = 1, \ldots, m$:

a) measurement data (x_i, y_i),

b) standard uncertainty $u(y_i)$ associated with y_i, and

c) covariances $\mathrm{cov}(y_i, y_j)$ associated with the pair (y_i, y_j), $j = 1, \ldots, m$, $j \neq i$.

9.1.2 The squared standard uncertainties and covariances comprise the covariance matrix

$$\boldsymbol{U_y} = \begin{bmatrix} u^2(y_1) & \mathrm{cov}(y_1, y_2) & \ldots & \mathrm{cov}(y_1, y_{m-1}) & \mathrm{cov}(y_1, y_m) \\ \mathrm{cov}(y_2, y_1) & u^2(y_2) & \ldots & \mathrm{cov}(y_2, y_{m-1}) & \mathrm{cov}(y_2, y_m) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathrm{cov}(y_{m-1}, y_1) & \mathrm{cov}(y_{m-1}, y_2) & \ldots & u^2(y_{m-1}) & \mathrm{cov}(y_{m-1}, y_m) \\ \mathrm{cov}(y_m, y_1) & \mathrm{cov}(y_m, y_2) & \ldots & \mathrm{cov}(y_m, y_{m-1}) & u^2(y_m) \end{bmatrix}$$

of dimension $m \times m$ associated with $\boldsymbol{y} = (y_1, \ldots, y_m)^\top$. Annex D provides guidance on obtaining these uncertainties and covariances. All other uncertainties and covariances associated with the data are regarded as negligible.

9.1.3 The case 5.3.2 d) corresponds to that of the statistical model

$$y_i = A^* + B^* x_i + e_i, \qquad i = 1, \ldots, m, \tag{11}$$

where $\boldsymbol{e} = (e_1, \ldots, e_m)^\top$ is a realization of a multivariate random variable with vector expectation equal to the zero vector of dimension $m \times 1$ and covariance matrix of dimension $m \times m$ equal to $\boldsymbol{U_y}$ [21].

9.1.4 Estimates a and b are those that minimize the generalized sum of squares [8]

$$\begin{bmatrix} y_1 - (A + Bx_1) \\ \vdots \\ y_m - (A + Bx_m) \end{bmatrix}^\top \boldsymbol{U_y}^{-1} \begin{bmatrix} y_1 - (A + Bx_1) \\ \vdots \\ y_m - (A + Bx_m) \end{bmatrix} = \boldsymbol{e}^\top \boldsymbol{U_y}^{-1} \boldsymbol{e}, \tag{12}$$

where $\boldsymbol{e} = \boldsymbol{y} - A\boldsymbol{1} - B\boldsymbol{x}$, with respect to A and B. The problem of determining a and b in this context is known as one of Gauss-Markov regression (GMR) [2].

NOTE For the case where $\boldsymbol{U_y}$ is diagonal, the generalized sum of squares (12) simplifies to expression (4) in 6.1.3 leading to a WLS problem.

9.2 Calibration parameter estimates and associated standard uncertainties and covariance

9.2.1 If $\boldsymbol{U_y}$ is positive definite, so that the lower-triangular Cholesky factor $\boldsymbol{L_y}$ of dimension $m \times m$ of $\boldsymbol{U_y} = \boldsymbol{L_y}\boldsymbol{L_y}^\top$ exists [10] (see also A.4), estimates a and b of A and B can be calculated directly using the same general scheme as in 6.2.1 after some preliminary calculations using matrix-vector operations. Otherwise more involved numerical methods would be required. These operations transform the generalized sum of squares (12) into an ordinary sum of squares (2) as in 5.8.1, that is, the problem becomes an unweighted least squares problem with no covariance.

9.2.2 Parameter estimates a and b are calculated in steps 1 to 7 below; the standard uncertainties $u(a)$ and $u(b)$ and covariance $\mathrm{cov}(a, b)$ are evaluated in step 8:

1 Calculate the Cholesky factor $\boldsymbol{L_y}$ of dimension $m \times m$ of $\boldsymbol{U_y} = \boldsymbol{L_y}\boldsymbol{L_y}^\top$; see A.4.1;

2 Let $\boldsymbol{1}$ be the vector of ones of dimension $m \times 1$. Solve the three lower-triangular systems of equations $\boldsymbol{L_y f} = \boldsymbol{1}$, $\boldsymbol{L_y g} = \boldsymbol{x}$ and $\boldsymbol{L_y h} = \boldsymbol{y}$, where $\boldsymbol{f} = (f_1, \ldots, f_m)^\top$, etc. for $\boldsymbol{f}$, $\boldsymbol{g}$ and $\boldsymbol{h}$; see A.4.3;

3 Set $F^2 = \sum_{i=1}^{m} f_i^2$;

4 Set $g_0 = \frac{1}{F^2}\sum_{i=1}^{m} f_i g_i$ and $h_0 = \frac{1}{F^2}\sum_{i=1}^{m} f_i h_i$;

5 Set $\widetilde{g}_i = g_i - g_0 f_i$ and $\widetilde{h}_i = h_i - h_0 f_i$, $i = 1, \ldots, m$;

6 Set $\widetilde{G}^2 = \sum_{i=1}^{m} \widetilde{g}_i^2$;

7 Set $b = \frac{1}{\widetilde{G}^2}\sum_{i=1}^{m} \widetilde{g}_i \widetilde{h}_i$ and $a = h_0 - b g_0$;

8 Set $u^2(a) = \frac{1}{F^2} + \frac{g_0^2}{\widetilde{G}^2}$, $u^2(b) = \frac{1}{\widetilde{G}^2}$ and $\mathrm{cov}(a, b) = -\frac{g_0}{\widetilde{G}^2}$.

9.2.3 The estimates a and b determined in 9.1.4 have the following properties [15] for data y_i according to the model (11):

i) The estimates a and b are given by linear combinations of the data y_i.

ii) The estimates a and b can be regarded as realizations of random variables whose expectations are A^* and B^*, respectively.

iii) The covariance matrix for the random variables in ii) is specified by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$ calculated in 9.2.2.

Property i) states that a and b are derived using a linear estimation method. Property ii) states that the linear estimation method is unbiased. Properties ii) and iii) jointly show that the estimation method is consistent in the sense that as the number m of data points is increased, the estimates a and b converge to A^* and B^*, respectively.

The estimation method of 9.1.4 has the following optimal property for data y_i according to the model (11):

iv) The estimates $\breve{a}$ and $\breve{b}$ provided by any unbiased, linear estimation method can be regarded as realizations of random variables whose variances are at least as large as those associated with the GMR estimation method.

Property iv) can be interpreted as follows. For constants c and d, the standard uncertainty $u(c\breve{a} + d\breve{b})$ associated with a linear combination of the estimates $\breve{a}$ and $\breve{b}$ provided by any unbiased, linear estimation method is at least as great as $u(ca + db)$. Properties i) to iv) justify the use of least squares methods for data compatible with the model (11). Note that in the use of this model statements are only made about the expectations and variances associated with the e_i; the associated distributions are not further specified. If the additional assumption is made that the e_i are realizations of random variables characterized by a multivariate normal distribution, then further properties associated with the GMR estimation method can be made:

v) The random variables in ii) are characterized by a bivariate normal distribution centred on A^* and B^* with covariance matrix specified by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$.

vi) The estimates a and b are maximum likelihood estimates, corresponding to the most likely values of A and B that could have given rise to the observed measurement data y_i.

vii) In the context of Bayesian inference, the state-of-knowledge distribution for A and B, given the observed measurement data y_i, is a bivariate normal distribution centred on a and b with covariance matrix specified by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$.

NOTE 1 The properties listed above are the same as those for the WLS estimation method of 6.1.3 for data generated according to the model (3).

NOTE 2 $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$ in step 8 are obtained by applying the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008 to a and b as provided by steps 1 to 7.

9.3 Validation of the model

If $m > 2$, the validity of the model can be partially tested using the weighted residuals r_i (continued from 9.2.2):

9 Form $r_i = \widetilde{h}_i - b\widetilde{g}_i$, $i = 1, \ldots, m$;

10 Form the observed chi-squared value $\chi^2_{\mathrm{obs}} = \sum_{i=1}^{m} r_i^2$ and degrees of freedom $\nu = m - 2$;

11 Check whether χ^2_{obs} exceeds the 95 % quantile of χ^2_ν, and if it does reject the straight-line model.

NOTE The chi-squared test is based on an assumption that the e_i in model (11) are realizations of random variables characterized by a multivariate normal distribution.

9.4 Organization of the calculations

The calculations in 9.2.2 and 9.3 can be organized into a number of tableaux as in Tables 19 to 21. Table 20 contains the f_i, g_i and h_i calculated in steps 1 and 2 in 9.2.2 in terms of the Cholesky factorization $\boldsymbol{L_y}$ of the covariance matrix $\boldsymbol{U_y}$. Table 21 uses these f_i, g_i and h_i to calculate estimates a and b of the parameters of the straight-line calibration function.

Table 19 — Data for the Gauss-Markov straight-line calibration function

x_1	y_1
x_2	y_2
$\vdots$	$\vdots$
x_m	y_m

Table 20 — Initial calculations to determine the Gauss-Markov straight-line calibration function

9.2.2 steps 1, 2		
f_1	g_1	h_1
f_2	g_2	h_2
$\vdots$	$\vdots$	$\vdots$
f_m	g_m	h_m

Table 21 — Organization of the calculations to determine the Gauss-Markov straight-line calibration function

			9.2.2 steps 4, 5				9.2.2 step 7 9.3 step 9	9.3 step 10
			g_0	h_0			a	
f_1^2	$f_1 g_1$	$f_1 h_1$	$\widetilde{g}_1$	$\widetilde{h}_1$	$\widetilde{g}_1^2$	$\widetilde{g}_1\widetilde{h}_1$	r_1	r_1^2
f_2^2	$f_2 g_2$	$f_2 h_2$	$\widetilde{g}_2$	$\widetilde{h}_2$	$\widetilde{g}_2^2$	$\widetilde{g}_2\widetilde{h}_2$	r_2	r_2^2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
f_m^2	$f_m g_m$	$f_m h_m$	$\widetilde{g}_m$	$\widetilde{h}_m$	$\widetilde{g}_m^2$	$\widetilde{g}_m\widetilde{h}_m$	r_m	r_m^2
$F^2 = \sum f_i^2$	$\sum f_i g_i$	$\sum f_i h_i$			$\widetilde{G}^2 = \sum \widetilde{g}_i^2$	$\sum \widetilde{g}_i\widetilde{h}_i$	b	$\chi^2_{\mathrm{obs}} = \sum r_i^2$

EXAMPLE Table 22 gives ten measured data points (x_i, y_i) and the standard uncertainties associated with the y_i.

The data are obtained using the model described in D.2.2 with $u_{\mathrm{R}} = 1{,}0$, $u_{\mathrm{S},1} = 1{,}0$ and $u_{\mathrm{S},2} = 2{,}0$.

Table 22 — Data representing ten measurement points, the y_i having an associated covariance matrix

x_i	y_i
1,0	1,3
2,0	4,1
3,0	6,9
4,0	7,5
5,0	10,2
6,0	12,0
7,0	14,5
8,0	17,1
9,0	19,5
10,0	21,0

The covariance matrix $\boldsymbol{U_y}$ of dimension 10×10 associated with the y_i is

$$\boldsymbol{U_y} = \begin{bmatrix} 2{,}0 & 1{,}0 & 1{,}0 & 1{,}0 & 1{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 \\ 1{,}0 & 2{,}0 & 1{,}0 & 1{,}0 & 1{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 \\ 1{,}0 & 1{,}0 & 2{,}0 & 1{,}0 & 1{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 \\ 1{,}0 & 1{,}0 & 1{,}0 & 2{,}0 & 1{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 \\ 1{,}0 & 1{,}0 & 1{,}0 & 1{,}0 & 2{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 5{,}0 & 4{,}0 & 4{,}0 & 4{,}0 & 4{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 4{,}0 & 5{,}0 & 4{,}0 & 4{,}0 & 4{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 4{,}0 & 4{,}0 & 5{,}0 & 4{,}0 & 4{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 4{,}0 & 4{,}0 & 4{,}0 & 5{,}0 & 4{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 4{,}0 & 4{,}0 & 4{,}0 & 4{,}0 & 5{,}0 \end{bmatrix}.$$

The Cholesky factor $\boldsymbol{L_y}$ of dimension 10×10 of $\boldsymbol{U_y} = \boldsymbol{L_y}\boldsymbol{L_y}^{\top}$, calculated using either algorithm described in A.4.1, is

$$\boldsymbol{L_y} = \begin{bmatrix} 1{,}414\,2 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}707\,1 & 1{,}224\,7 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}707\,1 & 0{,}408\,2 & 1{,}154\,7 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}707\,1 & 0{,}408\,2 & 0{,}288\,7 & 1{,}118\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}707\,1 & 0{,}408\,2 & 0{,}288\,7 & 0{,}223\,6 & 1{,}095\,4 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 2{,}236\,1 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 1{,}788\,9 & 1{,}341\,6 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 1{,}788\,9 & 0{,}596\,3 & 1{,}201\,9 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 1{,}788\,9 & 0{,}596\,3 & 0{,}369\,8 & 1{,}143\,5 & 0{,}000\,0 \\ 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 1{,}788\,9 & 0{,}596\,3 & 0{,}369\,8 & 0{,}269\,1 & 1{,}111\,4 \end{bmatrix}.$$

The vectors $\boldsymbol{f}$, $\boldsymbol{g}$ and $\boldsymbol{h}$ in Table 23 are calculated according to step 2 in 9.2.2.

Table 23 — Initial calculation tableau associated with the data in Table 22

f_i	g_i	h_i
0,707 1	0,707 1	0,919 2
0,408 2	1,224 7	2,816 9
0,288 7	1,732 1	4,416 7
0,223 6	2,236 1	3,957 8
0,182 6	2,738 6	5,696 3
0,447 2	2,683 3	5,366 6
0,149 1	1,639 8	3,652 2
0,092 5	1,849 0	4,428 4
0,067 3	2,219 8	5,320 8
0,052 9	2,646 3	5,536 0

The best fit straight-line parameters in Table 24 are calculated according to Table 21. From Table 24, $g_0 = 4{,}404\,8/1{,}071\,4 = 4{,}111\,1$, $h_0 = 9{,}004\,8/1{,}071\,4 = 8{,}404\,4$, $b = 54{,}218\,5/24{,}629\,6 = 2{,}201\,4$ and $a = 8{,}404\,4 - (2{,}201\,4)(4{,}111\,1) = -0{,}645\,6$.

Table 24 — Calculation tableau associated with the data in Table 22

f_i^2	$f_i g_i$	$f_i h_i$	$\widetilde{g}_i$	$\widetilde{h}_i$	$\widetilde{g}_i^2$	$\widetilde{g}_i \widetilde{h}_i$	r_i	r_i^2
			4,111 1	8,404 4			$a = -0{,}645\,6$	
0,500 0	0,500 0	0,650 0	−2,199 9	−5,023 6	4,839 5	11,051 4	−0,180 9	0,032 7
0,166 7	0,500 0	1,150 0	−0,453 6	−0,614 2	0,205 8	0,278 6	0,384 4	0,147 7
0,083 3	0,500 0	1,275 0	0,545 3	1,990 6	0,297 3	1,085 4	0,790 2	0,624 5
0,050 0	0,500 0	0,885 0	1,316 8	2,078 5	1,734 0	2,737 0	−0,820 2	0,672 7
0,033 3	0,500 0	1,040 0	1,988 0	4,161 9	3,952 3	8,273 9	−0,214 5	0,046 0
0,200 0	1,200 0	2,400 0	0,844 7	1,608 0	0,713 6	1,358 3	−0,251 6	0,063 3
0,022 2	0,244 4	0,544 4	1,026 9	2,399 4	1,054 6	2,464 0	0,138 7	0,019 2
0,008 5	0,170 9	0,409 4	1,468 9	3,651 4	2,157 8	5,363 6	0,417 7	0,174 5
0,004 5	0,149 3	0,357 9	1,943 3	4,755 5	3,776 3	9,241 2	0,477 7	0,228 2
0,002 8	0,140 1	0,293 0	2,428 7	5,091 2	5,898 6	12,365 0	−0,255 2	0,065 1
1,071 4	4,404 8	9,004 8			24,629 6	54,218 5	$b = 2{,}201\,4$	2,074 0

The standard uncertainties and covariance associated with a and b are evaluated from Table 24 using step 8 in 9.2.2:

$$u^2(a) = 1/1{,}071\,4 + (4{,}111\,1)^2/24{,}629\,6, \text{ so that } u(a) = 1{,}272\,6;$$
$$u^2(b) = 1/24{,}629\,6, \text{ so that } u(b) = 0{,}201\,5;$$
$$u(a,b) = -4{,}111\,1/24{,}629\,6 = -0{,}166\,9.$$

The observed chi-squared value is $\chi^2_{\text{obs}} = 2{,}074$ with 8 degrees of freedom, as calculated in Table 24 using 9.3. Since χ^2_{obs} does not exceed the 95 % quantile of χ^2_ν, namely 15,507, this is no reason to doubt the consistency of the straight-line model and the data.

The data points and fitted straight-line calibration function are shown in Figure 8. The weighted residuals are illustrated in Figure 9.

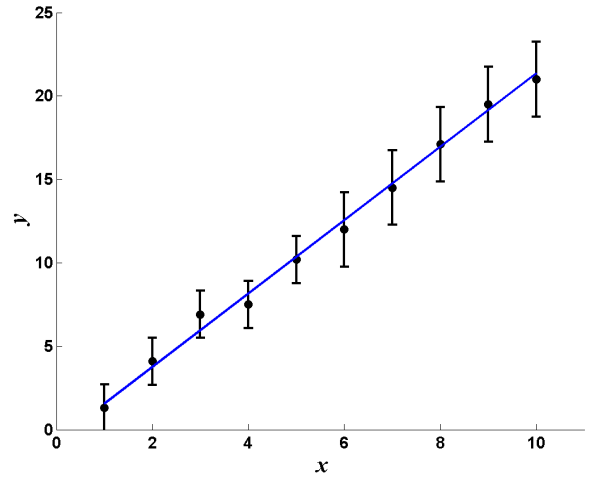

Figure 8 — Data in Table 22 and fitted straight-line calibration function obtained in Table 24

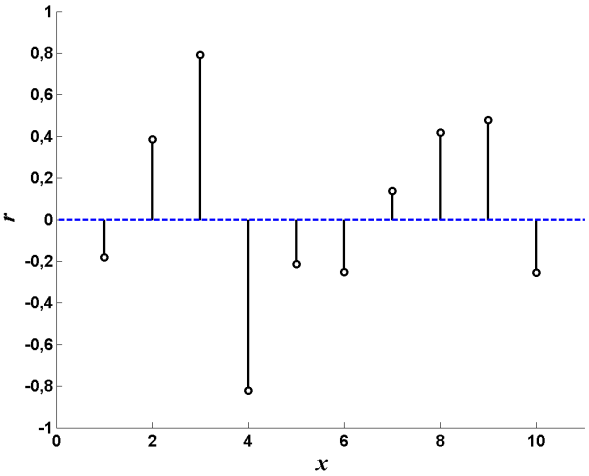

Figure 9 — Weighted residuals r_i calculated in Table 24

10 Model for uncertainties and covariances associated with the x_i and the y_i

10.1 General

10.1.1 This clause considers the case 5.3.2 e), namely the most general case in which all measurement data have associated uncertainties and covariances. Annex D provides guidance on obtaining these uncertainties and covariances.

10.1.2 The standard uncertainties and covariances comprise the covariance matrix

$$\boldsymbol{U} = \begin{bmatrix} u^2(x_1) & \dots & \mathrm{cov}(x_1, x_m) & \mathrm{cov}(x_1, y_1) & \dots & \mathrm{cov}(x_1, y_m) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \mathrm{cov}(x_m, x_1) & \dots & u^2(x_m) & \mathrm{cov}(x_m, y_1) & \dots & \mathrm{cov}(x_m, y_m) \\ \mathrm{cov}(y_1, x_1) & \dots & \mathrm{cov}(y_1, x_m) & u^2(y_1) & \dots & \mathrm{cov}(y_1, y_m) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \mathrm{cov}(y_m, x_1) & \dots & \mathrm{cov}(y_m, x_m) & \mathrm{cov}(y_m, y_1) & \dots & u^2(y_m) \end{bmatrix}$$

of dimension $2m \times 2m$ associated with the vector $(x_1, \dots, x_m, y_1, \dots, y_m)^\top$ of measurement data of dimension $2m \times 1$.

10.1.3 The case 5.3.2 e) corresponds to that of the statistical model

$$x_i = X_i^* + d_i, \qquad y_i = Y_i^* + e_i, \qquad Y_i^* = A^* + B^* X_i^*, \qquad i = 1, \dots, m, \tag{13}$$

where the vector $(d_1, \dots, d_m, e_1, \dots, e_m)^\top$ of dimension $2m \times 1$ is a realization of a multivariate random variable with vector expectation equal to the zero vector of dimension $2m \times 1$ and covariance matrix of dimension $2m \times 2m$ equal to $\boldsymbol{U}$ [21].

10.1.4 Estimates a and b are those that minimize the generalized sum of squares

$$\begin{bmatrix} x_1 - X_1 \\ \vdots \\ x_m - X_m \\ y_1 - (A + BX_1) \\ \vdots \\ y_m - (A + BX_m) \end{bmatrix}^\top \boldsymbol{U}^{-1} \begin{bmatrix} x_1 - X_1 \\ \vdots \\ x_m - X_m \\ y_1 - (A + BX_1) \\ \vdots \\ y_m - (A + BX_m) \end{bmatrix} = \begin{bmatrix} \boldsymbol{d} \\ \boldsymbol{e} \end{bmatrix}^\top \boldsymbol{U}^{-1} \begin{bmatrix} \boldsymbol{d} \\ \boldsymbol{e} \end{bmatrix}, \tag{14}$$

where $\boldsymbol{d} = \boldsymbol{x} - \boldsymbol{X}$ and $\boldsymbol{e} = \boldsymbol{y} - A\boldsymbol{1} - B\boldsymbol{x}$, with respect to A, B and X_i, $i = 1, \dots, m$. The problem of determining a and b in this context is known as one of generalized Gauss-Markov regression (GGMR) [2].

10.2 Calibration parameter estimates and associated standard uncertainties and covariance

10.2.1 If $\boldsymbol{U}$ is positive definite, so that the lower-triangular Cholesky factor $\boldsymbol{L}$ of dimension $2m \times 2m$ of $\boldsymbol{U} = \boldsymbol{L}\boldsymbol{L}^\top$ exists [10] (also see A.4), estimates a and b of A and B can be calculated in an iterative scheme using matrix-vector operations. Otherwise, more involved numerical methods would be required. These operations transform the generalized sum of squares (14) into an ordinary sum of squares (2) as in 5.8.1, that is, the problem becomes an unweighted least squares problem with no covariance. The iterative scheme also involves approximations x_i^*, which define the points $(x_i^*, A + Bx_i^*)$ on the line closest to the measured data points (x_i, y_i), where closeness is measured in terms of weighted distance, taking into account the uncertainty information specified by $\boldsymbol{U}$.

10.2.2 Estimates a and b are calculated in steps 1 to 10 below using an iterative scheme based on that in 6.2.1; the standard uncertainties $u(a)$ and $u(b)$ and covariance $\mathrm{cov}(a, b)$ are evaluated in step 11:

1 Obtain initial approximations $\widetilde{\boldsymbol{t}} = (\widetilde{x}_1, \dots, \widetilde{x}_m,\ \widetilde{a},\ \widetilde{b})^\top$ to the parameters;

2 Calculate the vector of dimension $2m \times 1$,

$$\boldsymbol{f} = \begin{bmatrix} x_1 - \widetilde{x}_1 \\ \vdots \\ x_m - \widetilde{x}_m \\ y_1 - \left(\widetilde{a} + \widetilde{b}\widetilde{x}_1\right) \\ \vdots \\ y_m - \left(\widetilde{a} + \widetilde{b}\widetilde{x}_m\right) \end{bmatrix} = \begin{bmatrix} \boldsymbol{x} - \widetilde{\boldsymbol{x}} \\ \boldsymbol{y} - \widetilde{a}\mathbf{1} - \widetilde{b}\widetilde{\boldsymbol{x}} \end{bmatrix},$$

and the (Jacobian) matrix of dimension $2m \times (m+2)$,

$$\boldsymbol{J} = \begin{bmatrix} -1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -1 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & -1 & 0 & 0 \\ -\widetilde{b} & 0 & \cdots & 0 & 0 & -1 & -\widetilde{x}_1 \\ 0 & -\widetilde{b} & \cdots & 0 & 0 & -1 & -\widetilde{x}_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -\widetilde{b} & 0 & -1 & -\widetilde{x}_{m-1} \\ 0 & 0 & \cdots & 0 & -\widetilde{b} & -1 & -\widetilde{x}_m \end{bmatrix} = \begin{bmatrix} -\boldsymbol{I} & \mathbf{0} & \mathbf{0} \\ -\widetilde{b}\boldsymbol{I} & -\mathbf{1} & -\widetilde{\boldsymbol{x}} \end{bmatrix},$$

where $\widetilde{\boldsymbol{x}} = (\widetilde{x}_1, \ldots, \widetilde{x}_m)^\top$, $\widetilde{a}$ and $\widetilde{b}$ are extracted from the current estimate $\widetilde{\boldsymbol{t}}$ of the parameter vector;

3 Calculate the Cholesky factor $\boldsymbol{L}$ of dimension $2m \times 2m$ of $\boldsymbol{U} = \boldsymbol{L}\boldsymbol{L}^\top$ [10]; see A.4.1;

4 Solve the lower-triangular systems

$$\boldsymbol{L}\widetilde{\boldsymbol{f}} = \boldsymbol{f} \qquad \text{and} \qquad \boldsymbol{L}\widetilde{\boldsymbol{J}} = \boldsymbol{J},$$

to determine the transformed vector $\widetilde{\boldsymbol{f}}$ of dimension $2m \times 1$ and transformed matrix $\widetilde{\boldsymbol{J}}$ of dimension $2m \times (m+2)$; see A.4.3;

5 Form the vector $\boldsymbol{g} = \widetilde{\boldsymbol{J}}^\top \widetilde{\boldsymbol{f}}$ of dimension $(m+2) \times 1$ and matrix $\boldsymbol{H} = \widetilde{\boldsymbol{J}}^\top \widetilde{\boldsymbol{J}}$ of dimension $(m+2) \times (m+2)$;

6 Determine the Cholesky factor $\boldsymbol{M}$, a lower-triangular matrix of dimension $(m+2) \times (m+2)$ in $\boldsymbol{H} = \boldsymbol{M}\boldsymbol{M}^\top$; see A.4.1;

7 Solve the lower-triangular system $\boldsymbol{M}\boldsymbol{q} = -\boldsymbol{g}$ to determine the vector $\boldsymbol{q}$ of dimension $(m+2) \times 1$; see A.4.3;

8 Solve the upper-triangular system $\boldsymbol{M}^\top \delta\boldsymbol{t} = \boldsymbol{q}$ to determine the correction vector $\delta\boldsymbol{t}$ of dimension $(m+2) \times 1$; see A.4.4;

9 Update the current approximations to the parameters: $\widetilde{\boldsymbol{t}} := \widetilde{\boldsymbol{t}} + \delta\boldsymbol{t}$;

10 Repeat steps 2 to 9 until convergence has been achieved. Set $a = \widetilde{a}$ and $b = \widetilde{b}$ (elements $m+1$ and $m+2$ of $\widetilde{\boldsymbol{t}}$);

11 Partition $\boldsymbol{M}$ obtained in step 6 as

$$\boldsymbol{M} = \begin{bmatrix} \boldsymbol{M}_{11} & \mathbf{0} \\ \boldsymbol{M}_{21} & \boldsymbol{M}_{22} \end{bmatrix},$$

where

$$\boldsymbol{M}_{22} = \begin{bmatrix} m_{11} & 0 \\ m_{21} & m_{22} \end{bmatrix}$$

is the lower right lower-triangular submatrix of dimension 2×2 of $\boldsymbol{M}$. Then

$$u^2(a) = \frac{m_{22}^2 + m_{21}^2}{m_{11}^2 m_{22}^2}, \qquad u^2(b) = \frac{m_{11}^2}{m_{11}^2 m_{22}^2} = \frac{1}{m_{22}^2} \qquad \text{and} \qquad \operatorname{cov}(a,b) = -\frac{m_{21}}{m_{11} m_{22}^2}.$$

NOTE 1 In step 1, initial approximations are provided by $\widetilde{\boldsymbol{t}} = (x_1, \ldots, x_m, a_0, b_0)^\top$, where a_0 and b_0 are the straight-line parameter values determined by a weighted least squares fit to the data; see 6.2.1.

NOTE 2 In step 8, the correction vector $\delta\boldsymbol{t}$ will generally decrease in magnitude by ultimately an approximately constant factor from iteration to iteration. The size of the reduction depends largely on the uncertainties associated with the data: the smaller the uncertainties are, the greater the reduction will be. The iterative scheme can be terminated when the magnitude of the correction is judged to be negligible.

NOTE 3 In step 8, the correction $\delta\boldsymbol{t}$ is given by the least squares solution of the matrix equation

$$\widetilde{\boldsymbol{J}}\delta\boldsymbol{t} = \widetilde{\boldsymbol{f}},$$

the solution of which is defined by the normal equations

$$\boldsymbol{H} = \widetilde{\boldsymbol{J}}^\top\widetilde{\boldsymbol{J}}\delta\boldsymbol{t} = -\widetilde{\boldsymbol{J}}\widetilde{\boldsymbol{f}} = -\boldsymbol{g}.$$

NOTE 4 Steps 5 to 8 solve the normal equations using Cholesky factorization. A numerically more stable approach is to use a QR factorization [10] of $\widetilde{\boldsymbol{J}}$ (see A.5.1). The scheme described in C.2 employs a QR factorization and avoids calculations involving the inverse of $\boldsymbol{L}$ such as those in step 4.

NOTE 5 In matrix terms, the covariance matrix associated with the estimates a and b is

$$\boldsymbol{U_a} = \boldsymbol{M}_{22}^{-\top}\boldsymbol{M}_{22}^{-1}.$$

NOTE 6 A more general and numerically more stable approach to solving the generalized Gauss-Markov regression problem is outlined in C.2. The above approach assumes that the matrix $\boldsymbol{U}$ is positive definite and does not represent any strong correlation.

NOTE 7 $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$ in step 11 are obtained by applying the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008 to a and b as provided by steps 1 to 10.

10.2.3 The fact that the estimates a and b determined by minimizing the sum of squares (14) depend non-linearly on the data x_i and y_i means that the properties for GGMR cannot be straightforwardly stated. The estimates a and b determined in 10.1.4 have the following properties for data x_i and y_i according to the model (13):

i) The estimates a and b are given by non-linear functions of the data x_i and y_i.

ii) The estimates a and b can be regarded as realizations of random variables whose expectations are approximately A^* and B^*, respectively.

iii) The elements of the covariance matrix for the random variables in ii) are approximated by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$ calculated in 10.2.2.

The approximations above will be more accurate for data having smaller associated uncertainties. However, the estimation method has the following consistency property:

iv) For data satisfying the model (13), as the number m of data points increases, the estimates a and b converge to A^* and B^*, respectively [16].

If the additional assumption is made that the d_i and e_i are realizations of random variables characterized by a multivariate normal distribution, then further properties associated with the GGMR estimation method can be stated:

v) The random variables in ii) are characterized approximately by a bivariate normal distribution centred on A^* and B^* with covariance matrix specified by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$.

vi) The estimates a and b are maximum likelihood estimates giving the most likely values of A and B that could have given rise to the observed measurement data x_i and y_i.

vii) In the context of Bayesian inference, the state-of-knowledge distribution for A and B, given the observed measurement data x_i and y_i, is approximated by a bivariate normal distribution centred on a and b with covariance matrix specified by $u^2(a)$, $u^2(b)$ and $\mathrm{cov}(a, b)$.

10.3 Validation of the model

If $m > 2$, the validity of the model can be partially tested using the weighted residuals $\widetilde{f}_i$ (continued from 10.2.2):

12 Form the observed chi-squared value $\chi^2_{\text{obs}} = \sum_{i=1}^{2m} \widetilde{f}_i^2$ and degrees of freedom $\nu = m - 2$;

13 Check whether χ^2_{obs} exceeds the 95 % quantile of χ^2_ν, and if it does reject the straight-line model.

NOTE The chi-squared test is based on an assumption that the d_i and e_i in model (13) are realizations of random variables characterized by a multivariate normal distribution and on a first order approximation.

EXAMPLE Table 25 gives seven measured data points (x_i, y_i) obtained using the measurement models described in D.2 and D.4.

The covariance matrix associated with the y_i is derived using the measurement model (D.1) with $u_S = 2{,}0$ and $u_R = 1{,}0$.

The data x_i and associated covariance matrix are derived using the measurement model (D.2) with $z_1 = 50$, $z_2 = 100$, $z_3 = 200$, $u(z_1) = 0{,}5$, $u(z_2) = u(z_3) = 1{,}0$, and $u_{D,i} = 0{,}5$.

Table 25 — Data representing seven measurement points, the x_i and y_i having associated covariance matrices

x_i	y_i
50,4	52,3
99,0	97,8
149,9	149,7
200,4	200,1
248,5	250,4
299,7	300,9
349,1	349,2

The covariance matrix $\boldsymbol{U_x}$ of dimension 7×7 associated with the x_i is

$$\boldsymbol{U_x} = \begin{bmatrix} 0{,}50 & 0{,}00 & 0{,}25 & 0{,}00 & 0{,}25 & 0{,}00 & 0{,}25 \\ 0{,}00 & 1{,}25 & 1{,}00 & 0{,}00 & 0{,}00 & 1{,}00 & 1{,}00 \\ 0{,}25 & 1{,}00 & 1{,}50 & 0{,}00 & 0{,}25 & 1{,}00 & 1{,}25 \\ 0{,}00 & 0{,}00 & 0{,}00 & 1{,}25 & 1{,}00 & 1{,}00 & 1{,}00 \\ 0{,}25 & 0{,}00 & 0{,}25 & 1{,}00 & 1{,}50 & 1{,}00 & 1{,}25 \\ 0{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 2{,}25 & 2{,}00 \\ 0{,}25 & 1{,}00 & 1{,}25 & 1{,}00 & 1{,}25 & 2{,}00 & 2{,}50 \end{bmatrix}.$$

The Cholesky factor $\boldsymbol{L_x}$ of dimension 7×7 of $\boldsymbol{U_x} = \boldsymbol{L_x}\boldsymbol{L_x}^{\top}$, as calculated using either algorithm described in A.4.1, is

$$\boldsymbol{L_x} = \begin{bmatrix} 0{,}707\,1 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}000\,0 & 1{,}118\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}353\,6 & 0{,}894\,4 & 0{,}758\,3 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 1{,}118\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}353\,6 & 0{,}000\,0 & 0{,}164\,8 & 0{,}894\,4 & 0{,}740\,2 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}000\,0 & 0{,}894\,4 & 0{,}263\,8 & 0{,}894\,4 & 0{,}211\,5 & 0{,}731\,9 & 0{,}000\,0 \\ 0{,}353\,6 & 0{,}894\,4 & 0{,}428\,6 & 0{,}894\,4 & 0{,}343\,6 & 0{,}292\,8 & 0{,}622\,5 \end{bmatrix}.$$

The covariance matrix $\boldsymbol{U_y}$ of dimension 7×7 associated with the y_i is

$$\boldsymbol{U_y} = \begin{bmatrix} 5{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 \\ 1{,}00 & 5{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 \\ 1{,}00 & 1{,}00 & 5{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 \\ 1{,}00 & 1{,}00 & 1{,}00 & 5{,}00 & 1{,}00 & 1{,}00 & 1{,}00 \\ 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 5{,}00 & 1{,}00 & 1{,}00 \\ 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 5{,}00 & 1{,}00 \\ 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 1{,}00 & 5{,}00 \end{bmatrix}.$$

The Cholesky factor $\boldsymbol{L_y}$ of dimension 7×7 of $\boldsymbol{U_y} = \boldsymbol{L_y}\boldsymbol{L_y}^{\top}$, as calculated using either algorithm described in A.4.1, is

$$\boldsymbol{L_y} = \begin{bmatrix} 2{,}236\,1 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}447\,2 & 2{,}190\,9 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}447\,2 & 0{,}365\,1 & 2{,}160\,2 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}447\,2 & 0{,}365\,1 & 0{,}308\,6 & 2{,}138\,1 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}447\,2 & 0{,}365\,1 & 0{,}308\,6 & 0{,}267\,3 & 2{,}121\,3 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}447\,2 & 0{,}365\,1 & 0{,}308\,6 & 0{,}267\,3 & 0{,}235\,7 & 2{,}108\,2 & 0{,}000\,0 \\ 0{,}447\,2 & 0{,}365\,1 & 0{,}308\,6 & 0{,}267\,3 & 0{,}235\,7 & 0{,}210\,8 & 2{,}097\,6 \end{bmatrix}.$$

The covariance matrix $\boldsymbol{U}$ of dimension 14×14 is given by

$$\boldsymbol{U} = \begin{bmatrix} \boldsymbol{U_x} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{U_y} \end{bmatrix}.$$

NOTE For this example, there is correlation associated with each pair x_i and x_j and each pair y_i and y_j but no correlation associated with the pair x_i and y_j, that is, $\mathrm{cov}(x_i, y_j) = 0$ for all i and j.

The Cholesky factor $\boldsymbol{L}$ of dimension 14×14 of $\boldsymbol{U} = \boldsymbol{L}\boldsymbol{L}^{\top}$ is given by

$$\boldsymbol{L} = \begin{bmatrix} \boldsymbol{L}_x & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{L}_y \end{bmatrix}.$$

The weighted least squares fit to the data (6.2.1 steps 1 to 5) gives approximations $\widetilde{a} = 0{,}270\,7$ and $\widetilde{b} = 1{,}001\,1$. The iterative scheme is started with $\widetilde{\boldsymbol{t}} = (x_1, \ldots, x_7, \widetilde{a}, \widetilde{b})^{\top}$.

Table 26 gives the initial vector $\widetilde{\boldsymbol{t}}_0$, the corrections $\delta\boldsymbol{t}_k$ for the kth iteration, $k = 1, \ldots, 4$, and the final estimate $\widetilde{\boldsymbol{t}} = \widetilde{\boldsymbol{t}}_4$.

Table 26 — Change in parameter vector $\widetilde{t}$

$\widetilde{\boldsymbol{t}}_0$	$\delta\boldsymbol{t}_1 \times 10^{-2}$	$\delta\boldsymbol{t}_2 \times 10^{-4}$	$\delta\boldsymbol{t}_3 \times 10^{-6}$	$\delta\boldsymbol{t}_4 \times 10^{-8}$	$\widetilde{\boldsymbol{t}}_4$
50,400 0	17,253 1	1,258 0	3,078 2	0,290 4	50,572 7
99,000 0	−43,150 1	−3,214 5	−6,320 1	−0,710 1	98,568 2
149,900 0	−29,164 1	−3,960 4	−3,888 9	−0,756 4	149,608 0
200,400 0	2,967 7	−10,762 9	−0,602 4	−1,716 5	200,428 6
248,500 0	24,039 4	−11,406 4	3,237 8	−1,706 4	248,739 3
299,700 0	−22,251 0	−15,776 7	−3,358 1	−2,611 0	299,475 9
349,100 0	−20,619 2	−16,621 7	−3,380 5	−2,742 9	348,892 1
0,270 7	7,504 0	−33,395 7	0,100 6	−5,301 9	0,342 4
1,001 1	0,011 0	0,211 3	0,007 6	0,033 7	1,001 2

The best estimates of A and B are $a = 0{,}342\,4$ and $b = 1{,}001\,2$.

At the final iteration the matrix $\boldsymbol{M}$ of dimension 9×9 is

$$\boldsymbol{M} = \begin{bmatrix} 1{,}775\,5 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}181\,0 & 1{,}695\,9 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ -0{,}424\,6 & -0{,}543\,0 & 1{,}430\,6 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}181\,0 & 0{,}237\,8 & 0{,}689\,3 & 1{,}531\,2 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ -0{,}424\,6 & 0{,}505\,3 & 0{,}099\,9 & -0{,}724\,9 & 1{,}245\,3 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}374\,8 & -0{,}560\,7 & -0{,}237\,7 & -0{,}426\,9 & -0{,}030\,6 & 1{,}346\,5 & 0{,}000\,0 & 0{,}000\,0 & 0{,}000\,0 \\ -0{,}230\,8 & -0{,}293\,1 & -0{,}827\,1 & 0{,}093\,2 & -0{,}582\,8 & -0{,}971\,1 & 0{,}832\,9 & 0{,}000\,0 & 0{,}000\,0 \\ 0{,}051\,3 & 0{,}048\,2 & 0{,}097\,1 & 0{,}002\,2 & 0{,}064\,5 & 0{,}092\,7 & 0{,}389\,9 & 0{,}676\,2 & 0{,}000\,0 \\ -10{,}765\,2 & -3{,}038\,1 & -0{,}381\,5 & 13{,}930\,2 & 30{,}184\,4 & 38{,}841\,2 & 127{,}115\,5 & 107{,}270\,6 & 110{,}967\,7 \end{bmatrix},$$

so that $\boldsymbol{M}_{22}$ (10.2.2 step 11) is

$$\boldsymbol{M}_{22} = \begin{bmatrix} 0{,}676\,2 & 0{,}000\,0 \\ 107{,}270\,6 & 110{,}967\,7 \end{bmatrix}.$$

The standard uncertainties and covariance associated with a and b as evaluated in step 11 in 10.2.2 are

$$u^2(a) = \frac{(110{,}967\,7)^2 + (107{,}270\,6)^2}{(0{,}676\,2)^2(110{,}967\,7)^2}, \text{ so that } u(a) = 2{,}056\,9;$$

$$u^2(b) = \frac{1}{(110{,}967\,7)^2}, \text{ so that } u(b) = 0{,}009\,0;$$

$$\operatorname{cov}(a, b) = -\frac{107{,}270\,6}{(0{,}676\,2)(110{,}967\,7)^2} = -0{,}012\,9.$$

The observed chi-squared value is $\chi^2_{\text{obs}} = 1{,}772$ with $\nu = 5$ degrees of freedom, as calculated in step 12 in 10.3. Since χ^2_{obs} does not exceed the 95 % quantile of χ^2_{ν}, namely 11,070, this is no reason to doubt the consistency of the straight-line model and the data.

11 Use of the calibration function

The use of the calibration function for prediction and forward evaluation is independent of the method used to obtain estimates of the calibration function parameters and evaluate their associated standard uncertainties and covariance.

11.1 Prediction

11.1.1 Consider the following are prescribed, following an application of one of Clauses 6 to 10:

a) straight-line parameters estimates a and b, and standard uncertainties $u(a)$ and $u(b)$ and covariance $\mathrm{cov}(a, b)$ associated with a and b, and

b) measured value y of Y and associated standard uncertainty $u(y)$.

Consider that y has been obtained independently of the measurement data used to establish the calibration function.

11.1.2 The estimate x of X corresponding to y is

$$x = \frac{y - a}{b}. \tag{15}$$

11.1.3 The standard uncertainty $u(x)$ associated with x is given by

$$c(a) = -\frac{1}{b}, \qquad c(b) = -\frac{y - a}{b^2}, \qquad c(y) = \frac{1}{b},$$
$$u^2(x) = c^2(a)u^2(a) + c^2(b)u^2(b) + 2c(a)c(b)\mathrm{cov}(a, b) + c^2(y)u^2(y).$$

NOTE 1 The formula for $u^2(x)$ is established using the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008. It is approximate, being based on a linearization of the formula (15). $c(a)$, $c(b)$ and $c(y)$ represent sensitivity coefficients.

NOTE 2 For computational purposes, a matrix formulation may be advantageous:

$$u^2(x) = \boldsymbol{c}^\top \begin{bmatrix} u^2(a) & \mathrm{cov}(a, b) & 0 \\ \mathrm{cov}(b, a) & u^2(b) & 0 \\ 0 & 0 & u^2(y) \end{bmatrix} \boldsymbol{c}, \qquad \boldsymbol{c} = \begin{bmatrix} c(a) \\ c(b) \\ c(y) \end{bmatrix}.$$

NOTE 3 In the case $b = 0$, that is, the best-fit line is $y = a$, which corresponds to an inadmissible calibration function, prediction cannot be carried out.

NOTE 4 The validity of the standard uncertainty $u(x)$ depends on the satisfaction of the relevant chi-squared test given in Clauses 6 to 10.

EXAMPLE 1 Regarding the numerical example of weighted least squares (WLS) with *known equal weights* described in Clause 6, the best fit straight-line parameters and their associated standard uncertainties and covariance are

$$a = 1{,}867, \quad b = 1{,}757, \quad u(a) = 0{,}465, \quad u(b) = 0{,}120, \quad \mathrm{cov}(a, b) = -0{,}050.$$

Let $y = 10{,}5$ be an additional measured value of Y and $u(y) = 0{,}5$ its associated standard uncertainty.

From 11.1.2, an estimate of the value x of X corresponding to y is

$$x = (10{,}5 - 1{,}867)/1{,}757 = 4{,}913.$$

Using 11.1.3, the associated standard uncertainty $u(x)$ is given by

$$c(a) = -1/1{,}867 = -0{,}569,$$
$$c(b) = -(10{,}5 - 1{,}867)/(1{,}757)^2 = -2{,}796,$$
$$c(y) = 1/1{,}757 = 0{,}569,$$
$$u^2(x) = (-0{,}569)^2(0{,}217) + (-2{,}796)^2(0{,}014) + (2)(-0{,}569)(-2{,}796)(-0{,}050) + (-0{,}569)^2(0{,}5)^2 = 0{,}104,$$

so that $u(x) = 0{,}322$.

EXAMPLE 2 Regarding the numerical example of weighted least squares (WLS) with *known unequal weights* described in Clause 6, the best fit straight-line parameters and their associated standard uncertainties and covariance are

$$a = 0{,}885, \quad b = 2{,}057, \quad u(a) = 0{,}530, \quad u(b) = 0{,}178, \quad \mathrm{cov}(a, b) = -0{,}082.$$

Let $y = 10{,}5$ be an additional measured value of Y and $u(y) = 1{,}0$ its associated standard uncertainty.

From 11.1.2, an estimate of the value x of X corresponding to y is

$$x = (10{,}5 - 0{,}885)/2{,}057 = 4{,}674.$$

Using 11.1.3, the associated standard uncertainty $u(x)$ is given by

$$c(a) = -1/0{,}885 = -0{,}486,$$
$$c(b) = -(10{,}5 - 0{,}885)/(2{,}057)^2 = -2{,}272,$$
$$c(y) = 1/2{,}057 = 0{,}486,$$
$$u^2(x) = (-0{,}486)^2(0{,}281) + (-2{,}272)^2(0{,}032) + (2)(-0{,}486)(-2{,}272)(-0{,}082) + (-0{,}486)^2(1{,}0)^2 = 0{,}284,$$

so that $u(x) = 0{,}533$.

In this example and 11.1 EXAMPLE 1, the influence of the different uncertainties associated with the value of y can be seen in the corresponding uncertainties associated with the respective values of x.

11.2 Forward evaluation

Consider the following are prescribed, following an application of one of Clauses 6 to 10:

a) straight-line parameters estimates a and b, and standard uncertainties $u(a)$ and $u(b)$ and covariance $\mathrm{cov}(a, b)$ associated with a and b, and

b) measured value x of X and associated standard uncertainty $u(x)$.

Consider that x has been obtained independently of the measurement data used to establish the calibration function.

11.2.1 The estimate y of Y corresponding to x is

$$y = a + bx. \tag{16}$$

11.2.2 The standard uncertainty $u(y)$ associated with y is given by

$$c(a) = 1, \qquad c(b) = x, \qquad c(x) = b,$$
$$u^2(y) = c^2(a)u^2(a) + c^2(b)u^2(b) + 2c(a)c(b)\mathrm{cov}(a, b) + c^2(x)u^2(x).$$

NOTE 1 The formula for $u^2(y)$ is established using the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008. It is approximate, being based on a linearization of the formula (16). $c(a)$, $c(b)$ and $c(y)$ represent sensitivity coefficients.

NOTE 2 For computational purposes, a matrix formulation may be advantageous:

$$u^2(y) = \boldsymbol{c}^\top \begin{bmatrix} u^2(a) & \mathrm{cov}(a, b) & 0 \\ \mathrm{cov}(b, a) & u^2(b) & 0 \\ 0 & 0 & u^2(x) \end{bmatrix} \boldsymbol{c}, \qquad \boldsymbol{c} = \begin{bmatrix} c(a) \\ c(b) \\ c(x) \end{bmatrix}.$$

NOTE 3 The validity of the standard uncertainty $u(y)$ depends on the satisfaction of the relevant chi-squared test given in Clauses 6 to 10.

EXAMPLE Regarding the numerical example of weighted least squares (WLS) with *known equal weights* described in Clause 6, the best fit straight-line parameters and their associated standard uncertainties and covariance are

$$a = 1{,}867, \quad b = 1{,}757, \quad u(a) = 0{,}465, \quad u(b) = 0{,}120, \quad \mathrm{cov}(a, b) = -0{,}050.$$

Let $x = 3{,}5$ be an additional measured value of X and and $u(x) = 0{,}2$ its associated standard uncertainty, and assume that $\mathrm{cov}(x, a) = \mathrm{cov}(x, b) = 0$, that is, there is no correlation associated with x and a, and with x and b.

From 11.2.1, an estimate of the value y of Y corresponding to x is

$$y = 1{,}867 + (1{,}757)(3{,}5) = 8{,}017.$$

Using 11.2.2 the associated standard uncertainty $u(y)$ is given by

$$u^2(y) = 0{,}217 + (3{,}5)^2(0{,}014) + (2)(3{,}5)(-0{,}050) + (1{,}757)^2(0{,}2)^2 = 0{,}165,$$

so that $u(y) = 0{,}406$.

Annex A
(informative)

Matrix operations

A.1 General

This annex describes matrix operations that are used in this Technical Specification.

A.2 Elementary operations

In the following operations, $\boldsymbol{A}$ is a matrix of dimension $m \times n$ with element $\boldsymbol{A}(i,j) = a_{ij}$ in the ith row and jth column, $\boldsymbol{B}$ is a matrix of dimension $n \times k$, $\boldsymbol{C}$ is a (square) matrix of dimension $m \times m$ and $\boldsymbol{d}$ a vector of dimension $n \times 1$ with jth element d_j.

A.2.1 Matrix-vector multiplication

The matrix-vector product $\boldsymbol{Ad}$ is the vector $\boldsymbol{e}$ of dimension $m \times 1$ with ith element e_i defined by

$$e_i = \sum_{j=1}^{n} a_{ij} d_j = a_{i1} d_1 + a_{i2} d_2 + \cdots + a_{in} d_n.$$

A.2.2 Matrix-matrix multiplication

The matrix product $\boldsymbol{AB}$ is the matrix of dimension $m \times k$ whose jth column is the product of $\boldsymbol{A}$ and the jth column of $\boldsymbol{B}$.

A.2.3 Matrix transpose

The transpose $\boldsymbol{A}^\top$ of the matrix $\boldsymbol{A}$ is the matrix of dimension $n \times m$ with element $\boldsymbol{A}(j,i) = a_{ji}$ in the jth row and ith column.

A.2.4 Identity matrix

The identity matrix of order m is the matrix $\boldsymbol{I}$ of dimension $m \times m$ such that $\boldsymbol{I}(j,j) = 1, j = 1, \ldots, m$, and all other elements are zero.

A.2.5 Inverse of a square matrix

The inverse of $\boldsymbol{C}$, if it exists, is denoted by $\boldsymbol{C}^{-1}$ and is the matrix of dimension $m \times m$ such that

$$\boldsymbol{C}\boldsymbol{C}^{-1} = \boldsymbol{C}^{-1}\boldsymbol{C} = \boldsymbol{I}.$$

The transpose of $\boldsymbol{C}^{-1}$ is equal to the inverse of $\boldsymbol{C}^\top$ and is denoted by $\boldsymbol{C}^{-\top}$.

A.3 Elementary definitions

In the following definitions, $\boldsymbol{C}$ is a (square) matrix of dimension $m \times m$ with element $\boldsymbol{C}(i,j) = c_{ij}$ in the ith row and jth column.

A.3.1 Symmetric matrix

The matrix $\boldsymbol{C}$ is symmetric if $c_{ij} = c_{ji}$, $i = 1, \ldots, m$, $j = 1, \ldots, m$, that is, $\boldsymbol{C} = \boldsymbol{C}^\top$.

A.3.2 Invertible matrix

The matrix $\boldsymbol{C}$ is invertible if its inverse $\boldsymbol{C}^{-1}$ (see A.2.5) exists.

A.3.3 Lower-triangular and upper-triangular matrix

The matrix $\boldsymbol{C}$ is lower-triangular if $c_{ij} = 0$, $i < j$, and upper-triangular if $c_{ij} = 0$, $i > j$.

A.3.4 Orthogonal matrix

The matrix $\boldsymbol{C}$ is orthogonal if $\boldsymbol{C}^\top \boldsymbol{C} = \boldsymbol{I}$.

A.4 Cholesky factorization

The Cholesky factorization of the symmetric positive definite matrix $\boldsymbol{U}$ of dimension $m \times m$ is a lower-triangular matrix $\boldsymbol{L}$ of dimension $m \times m$ such that $\boldsymbol{U} = \boldsymbol{L}\boldsymbol{L}^\top$ [10].

A.4.1 Cholesky factorization algorithms

A.4.1.1 The following algorithm computes a lower-triangular matrix $\boldsymbol{L}$ such that $\boldsymbol{U} = \boldsymbol{L}\boldsymbol{L}^\top$.

Initialization

```
for k = 1 : m
    for j = k : m
        L(j,k) := U(j,k)
    end
end
for k = 2 : m
    for j = 1 : k − 1
        L(j,k) := 0
    end
end
```

Factorization

```
for k = 1 : m
    L(k,k) := √L(k,k)
    for j = k + 1 : m
        L(j,k) := L(j,k)/L(k,k)
    end
    for j = k + 1 : m
        for l = j : m
            L(l,j) := L(l,j) − L(l,k)L(j,k)
        end
    end
end
```

NOTE To overwrite the lower-triangular elements $\boldsymbol{U}(i,j), i \geq j$ of $\boldsymbol{U}$ with its Cholesky factorization, implement only the steps in the *Factorization* stage of the algorithm in A.4.1.1, using $\boldsymbol{U}$ instead of $\boldsymbol{L}$.

A.4.1.2 The calculations in A.4.1.1 can be re-organized to involve more vector-vector operations in order to improve execution speed in computer languages that support vector and array operations. For example,

Initialization

for $j = 1 : m$
  $\boldsymbol{L}(j, 1 : j) := \boldsymbol{U}(j, 1 : j)$
end
for $j = 1 : m - 1$
  $\boldsymbol{L}(j, j + 1 : m) := 0$
end

Factorization

for $j = 1 : m$
  if $j > 1$
    $\boldsymbol{L}(j : m, j) := \boldsymbol{L}(j : m, j) - \boldsymbol{L}(j : m, 1 : j - 1)\left(\boldsymbol{L}(j, 1 : j - 1)\right)^{\top}$
  end
  $\boldsymbol{L}(j : m, j) := \boldsymbol{L}(j : m, j)/\sqrt{\boldsymbol{L}(j, j)}$
end

NOTE To overwrite the lower-triangular elements $\boldsymbol{U}(i, j), i \geq j$ of $\boldsymbol{U}$ with its Cholesky factorization, implement only the steps in the *Factorization* stage of the algorithm in A.4.1.2, using $\boldsymbol{U}$ instead of $\boldsymbol{L}$.

A.4.2 Interpretation of the Cholesky factorization of a covariance matrix

A.4.2.1 Suppose E_i, $i = 1, \ldots, m$ are m independent random variables each with expectation zero and variance one and let e_i be realization of E_i. Let

$$y_1 = l_{11}e_1,$$
$$y_2 = l_{21}e_1 + l_{22}e_2.$$

Then $u^2(y_1) = l_{11}^2$ and $u^2(y_2) = l_{21}^2 + l_{22}^2$. The common dependence of y_1 and y_2 on e_1 means that y_1 and y_2 have associated correlation, with covariance $\mathrm{cov}(y_1, y_2) = l_{11}l_{21}$. Continuing, suppose

$$y_3 = l_{31}e_1 + l_{32}e_2 + l_{33}e_3,$$
$$\vdots$$
$$y_m = l_{m1}e_1 + l_{m2}e_2 + \cdots + l_{mm}e_m.$$

A.4.2.2 In matrix terms, $\boldsymbol{y} = \boldsymbol{L}\boldsymbol{e}$, with $\boldsymbol{L}$ lower-triangular. The common dependence of y_1 and y_3 on e_1 means that there is correlation associated with y_1 and y_3. Similarly, the common dependence of y_2 and y_3 on e_1 and e_2 means that there is correlation associated with y_2 and y_3, and so on.

A.4.2.3 Given a covariance matrix $\boldsymbol{U}$ associated with data y_i, the Cholesky factorization $\boldsymbol{U} = \boldsymbol{L}\boldsymbol{L}^{\top}$ calculates the coefficients l_{ij} such that the covariance matrix can be explained by assuming that the y_i are defined in A.4.2.1 as realizations of linear combinations defined by l_{ij} of independent random variables E_i. In practice, covariance matrices are often defined in terms of factorizations $\boldsymbol{U} = \boldsymbol{B}\boldsymbol{B}^{\top}$ and given $\boldsymbol{U}$ there are infinitely many factors $\boldsymbol{B}$ that can be used to construct $\boldsymbol{U}$. The Cholesky factorization, in which the linear combinations are represented by a lower-triangular matrix, is unique up to the numerical sign of the columns of $\boldsymbol{L}$.

A.4.3 Solution of a lower-triangular system

A.4.3.1 If $\boldsymbol{L}$ is a lower-triangular matrix of dimension $m \times m$ such that $\boldsymbol{L}(j, j) \neq 0$, $j = 1, \ldots, m$, and $\boldsymbol{x}$ is a vector of dimension $m \times 1$, the following algorithm computes the vector $\boldsymbol{y}$, where $\boldsymbol{y}$ is such that $\boldsymbol{L}\boldsymbol{y} = \boldsymbol{x}$, that is, $\boldsymbol{y} = \boldsymbol{L}^{-1}\boldsymbol{x}$.

Initialization

for $j = 1 : m$
  $y(j) := x(j)$
end

Solution

$y(1) := y(1)/\boldsymbol{L}(1,1)$
for $j = 2 : m$
  for $k = 1 : j - 1$
    $y(j) := y(j) - \boldsymbol{L}(j,k)y(k)$
  end
  $y(j) := y(j)/\boldsymbol{L}(j,j)$
end

NOTE To overwrite the vector $\boldsymbol{x}$ with the solution $\boldsymbol{y}$, implement only the steps in the *Solution* stage of the algorithm in A.4.3.1, using $\boldsymbol{x}$ instead of $\boldsymbol{y}$.

A.4.3.2 The algorithm in A.4.3.1 can be applied to solve the matrix equation $\boldsymbol{LY} = \boldsymbol{X}$ by successively applying it to each column of $\boldsymbol{X}$. The solution is mathematically given by $\boldsymbol{Y} = \boldsymbol{L}^{-1}\boldsymbol{X}$.

A.4.4 Solution of an upper-triangular system

A.4.4.1 The solution of an upper-triangular system can be determined in terms of the transpose of a lower-triangular matrix. If $\boldsymbol{L}$ is a lower-triangular matrix of dimension $m \times m$ such that $\boldsymbol{L}(j,j) \neq 0$, $j = 1,\ldots,m$, and $\boldsymbol{x}$ is a vector of dimension $m \times 1$, the following algorithm computes the vector $\boldsymbol{y}$, where $\boldsymbol{y}$ is such that $\boldsymbol{L}^{\top}\boldsymbol{y} = \boldsymbol{x}$, that is, $\boldsymbol{y} = \boldsymbol{L}^{-\top}\boldsymbol{x}$.

Initialization

for $j = 1 : m$
  $y(j) := x(j)$
end

Solution

$y(m) := y(m)/\boldsymbol{L}(m,m)$
for $j = j = m - 1 : -1 : 1$
  for $k = j + 1 : m$
    $y(j) := y(j) - \boldsymbol{L}(k,j)y(k)$
  end
  $y(j) := y(j)/\boldsymbol{L}(j,j)$
end

NOTE To overwrite the vector $\boldsymbol{x}$ with the solution $\boldsymbol{y}$, implement only the steps in the *Solution* stage of the algorithm in A.4.4.1, using $\boldsymbol{x}$ instead of $\boldsymbol{y}$.

A.4.4.2 The algorithm in A.4.4.1 can be applied to solve the matrix equation $\boldsymbol{L}^{\top}\boldsymbol{Y} = \boldsymbol{X}$ by successively applying it to each column of $\boldsymbol{X}$. The solution is mathematically given by $\boldsymbol{Y} = \boldsymbol{L}^{-\top}\boldsymbol{X}$.

A.5 Orthogonal factorization

Orthogonal matrices are combinations of rotations and reflections and have the property that pre-multiplication of a vector by an orthogonal matrix does not change the magnitude of that vector (the square root of the sum of squares of its elements). The columns of an orthogonal matrix can be regarded as defining a system of orthogonal axes. The importance of orthogonal factorization techniques is that they allow matrix equations to be solved in a numerically stable way. Algorithms for computing orthogonal factorizations of a matrix are described in references [1, 10, 20].

A.5.1 QR factorization

The QR factorization of a matrix $\boldsymbol{A}$ of dimension $m \times n$, with $m \geq n$, can be written as

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{R} = [\boldsymbol{Q}_1 \ \boldsymbol{Q}_2] \begin{bmatrix} \boldsymbol{R}_1 \\ \boldsymbol{0} \end{bmatrix} = \boldsymbol{Q}_1 \boldsymbol{R}_1,$$

where $\boldsymbol{Q} = [\boldsymbol{Q}_1 \ \boldsymbol{Q}_2]$ is an orthogonal matrix of dimension $m \times m$, $\boldsymbol{Q}_1$ is the matrix consisting of the first n columns of $\boldsymbol{Q}$, with $\boldsymbol{Q}_1^{\top}\boldsymbol{Q}_1 = \boldsymbol{I}$, and $\boldsymbol{R}_1$ is an upper-triangular matrix of dimension $n \times n$.

NOTE The QR factorization of a matrix $\boldsymbol{A}$ of dimension $m \times n$, with $m < n$, can also be obtained. In this Technical Specification, since all matrices for which the calculation of the QR factorization is required have $m \geq n$, the factorization is not provided.

A.5.2 RQ factorization

A.5.2.1 The RQ factorization of a matrix $\boldsymbol{B}$ of dimension $m \times n$, with $m \geq n$, can be written as

$$\boldsymbol{B} = \boldsymbol{T}\boldsymbol{Z} = \begin{bmatrix} \boldsymbol{T}_1 \\ \boldsymbol{T}_2 \end{bmatrix} \boldsymbol{Z},$$

where $\boldsymbol{Z}$ is orthogonal and $\boldsymbol{T}_2$ is upper-triangular.

A.5.2.2 The RQ factorization of a matrix $\boldsymbol{B}$ of dimension $m \times n$, with $m < n$, can be written as

$$\boldsymbol{B} = \boldsymbol{T}\boldsymbol{Z} = [\boldsymbol{0} \ \boldsymbol{T}_2] \begin{bmatrix} \boldsymbol{Z}_1 \\ \boldsymbol{Z}_2 \end{bmatrix} = \boldsymbol{T}_2 \boldsymbol{Z}_2,$$

where $\boldsymbol{Z}$ is orthogonal and $\boldsymbol{T}_2$ is upper-triangular.

Annex B
(informative)

Application of the Gauss-Newton algorithm to generalized distance regression

B.1 This annex derives the algorithms in 7.2.1 and 8.2.1 using the Gauss-Newton algorithm.

B.2 The algorithms in 7.2.1 and 8.2.1 are particular implementations of the iterative Gauss-Newton algorithm [10] for minimizing a sum of squares of non-linear functions:

$$F(\boldsymbol{A}) = \sum_{i=1}^{m} f_i^2(\boldsymbol{A}), \qquad \boldsymbol{A} = (A_1, \ldots, A_n)^\top, \qquad m \geq n.$$

B.3 Let $\widetilde{\boldsymbol{a}}$ be an approximation to the solution parameters $\boldsymbol{a}$ and

$$\boldsymbol{f} = \begin{bmatrix} f_1(\boldsymbol{A}) \\ \vdots \\ f_m(\boldsymbol{A}) \end{bmatrix} \qquad \text{and} \qquad \boldsymbol{J} = \begin{bmatrix} \dfrac{\partial f_1}{\partial A_1} & \cdots & \dfrac{\partial f_1}{\partial A_n} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_m}{\partial A_1} & \cdots & \dfrac{\partial f_m}{\partial A_n} \end{bmatrix}$$

be, respectively, the vector of dimension $m \times 1$ of function values and Jacobian matrix of dimension $m \times n$ of partial derivatives of first order with respect to the parameters, evaluated at the approximation $\widetilde{\boldsymbol{a}}$ to the parameters.

B.4 Let $\boldsymbol{p}$ solve

$$\boldsymbol{J}^\top \boldsymbol{J} \boldsymbol{p} = -\boldsymbol{J}^\top \boldsymbol{f}. \tag{B.1}$$

Then an updated estimate of the solution parameters is given by $\widetilde{\boldsymbol{a}} := \widetilde{\boldsymbol{a}} + \boldsymbol{p}$.

B.5 For the algorithms in 7.2.1 and 8.2.1, $\boldsymbol{A} = (A, B)^\top$ and the function $f_i(\boldsymbol{A})$ is a measure of the generalized distance from the ith data point (x_i, y_i) to the line $y = A + Bx$.

B.6 Let $\boldsymbol{U}_i$ be the covariance matrix associated with the ith data point:

$$\boldsymbol{U}_i = \begin{bmatrix} u^2(x_i) & \operatorname{cov}(x_i, y_i) \\ \operatorname{cov}(y_i, x_i) & u^2(y_i) \end{bmatrix},$$

and let $x_i^* \equiv x_i^*(A, B)$, known as the ith footpoint, solve

$$\min_x \quad d_i^2(x, A, B) = \begin{bmatrix} x_i - x \\ y_i - A - Bx \end{bmatrix}^\top \boldsymbol{U}_i^{-1} \begin{bmatrix} x_i - x \\ y_i - A - Bx \end{bmatrix}, \tag{B.2}$$

a function of A and B.

B.7 If $f_i^2(A, B)$ is defined by

$$f_i^2(A, B) = d_i^2(x_i^*(A, B), A, B),$$

i.e., $d_i^2(x, A, B)$ evaluated at the solution x_i^*, then the values of A and B that minimize

$$F(A, B) = \sum_{i=1}^{m} f_i^2(A, B)$$

determine the generalized distance regression best fit line. Implementation of the Gauss-Newton algorithm requires the determination of the partial derivatives of first order of $f_i(A, B)$ with respect to A and B to form the Jacobian matrix $\boldsymbol{J}$.

B.8 Let $\boldsymbol{n} = (-B, 1)^\top$ be a vector orthogonal to the line $y = A + Bx$ and suppose that x_i^* is a solution of the footpoint problem (B.2). Setting $\boldsymbol{x}_i = (x_i, y_i)^\top$, $\boldsymbol{x}_i^* = (x_i^*, A + Bx_i^*)^\top$ and

$$t_i = \boldsymbol{n}^\top \boldsymbol{U}_i \boldsymbol{n}, \tag{B.3}$$

then, expressing function values and derivatives in terms of U_i, A, B, x_i, y_i and x_i^*,

$$f_i(A, B) = t_i^{-1/2} \boldsymbol{n}^\top (\boldsymbol{x}_i - \boldsymbol{x}_i^*), \tag{B.4}$$

and

$$\frac{\partial f_i}{\partial A} = -t_i^{-1/2} \boldsymbol{n}^\top \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \qquad \frac{\partial f_i}{\partial B} = -t_i^{-1/2} \boldsymbol{n}^\top \begin{bmatrix} 0 \\ x_i^* \end{bmatrix}. \tag{B.5}$$

B.9 The solution x_i^* of the footpoint problem (B.2) is given by

$$\begin{bmatrix} p_i \\ q_i \end{bmatrix} = U_i \begin{bmatrix} -B \\ 1 \end{bmatrix}, \qquad x_i^* = \frac{-q_i x_i + p_i (y_i - A)}{-q_i + p_i B}. \tag{B.6}$$

NOTE Expressions (B.3), (B.4), (B.5) and (B.6) are defined in terms of $\boldsymbol{U}_i$ rather than its inverse $\boldsymbol{U}_i^{-1}$. There is no requirement for $\boldsymbol{U}_i$ to be invertible, but $\boldsymbol{n}^\top \boldsymbol{U}_i \boldsymbol{n}$ must be non-zero.

B.10 The algorithms in 7.2.1 and 8.2.1 implement the Gauss-Newton algorithm using explicit expressions for $f_i(A, B)$, $\partial f_i / \partial A$ and $\partial f_i / \partial B$. Solving for the update step $\boldsymbol{p}$ in expression (B.1) is formulated as a problem of determining the weighted least squares best fit straight-line (see 6.2.1 steps 1 to 5) for transformed data derived from the measurement data (x_i, y_i), associated covariance matrices $\boldsymbol{U}_i$ and the current approximations to A and B.

Annex C
(informative)

Orthogonal factorization approach to solving the generalized Gauss-Markov problem

C.1 General

The iterative algorithm described in 10.2.2 assumes that the covariance matrix $\boldsymbol{U}$ of dimension $2m \times 2m$ is positive definite and hence invertible. In particular, invertibility requires that all $u(x_i) > 0$ and $u(y_i) > 0$. In this annex a general algorithm is described that is appropriate for all valid (symmetric positive semi-definite) covariance matrices $\boldsymbol{U}$. All that is required is that the covariance matrix can be factorized as $\boldsymbol{U} = \boldsymbol{B}\boldsymbol{B}^\top$, where $\boldsymbol{B}$ is a matrix of dimension $2m \times p$ ($p \geq m$). Often covariance matrices are derived in terms of such a factorization. If $\boldsymbol{U}$ is invertible, $\boldsymbol{B}$ could be its Cholesky factor. The algorithm proceeds similarly to that described in 10.2.2 and requires the calculation of residuals $\boldsymbol{f}$ and Jacobian matrix $\boldsymbol{J}$, but the increment $\delta\boldsymbol{t}$ is determined using two orthogonal factorizations. Mathematically, $\delta\boldsymbol{t}$ minimizes

$$\boldsymbol{c}^\top \boldsymbol{c} = \sum_{i=1}^{p} c_i^2 \qquad \text{subject to the constraints} \qquad \boldsymbol{f} = -\boldsymbol{J}\delta\boldsymbol{t} + \boldsymbol{B}\boldsymbol{c}.$$

C.2 Calibration parameter estimates and associated standard uncertainties and covariance

Estimates a and b are calculated as in steps 1 to 9 below; the standard uncertainties $u(a)$ and $u(b)$ are evaluated in step 10:

1 Obtain initial approximations $\widetilde{\boldsymbol{t}} = (\widetilde{x}_1, \ldots, \widetilde{x}_m,\ \widetilde{a},\ \widetilde{b})^\top$ to the parameters;

2 Calculate the vector of dimension $2m \times 1$,

$$\boldsymbol{f} = \begin{bmatrix} x_1 - \widetilde{x}_1 \\ \vdots \\ x_m - \widetilde{x}_m \\ y_1 - \left(\widetilde{a} + \widetilde{b}\widetilde{x}_1\right) \\ \vdots \\ y_m - \left(\widetilde{a} + \widetilde{b}\widetilde{x}_m\right) \end{bmatrix} = \begin{bmatrix} \boldsymbol{x} - \widetilde{\boldsymbol{x}} \\ \boldsymbol{y} - \widetilde{a}\boldsymbol{1} - \widetilde{b}\widetilde{\boldsymbol{x}} \end{bmatrix},$$

and the (Jacobian) matrix of dimension $2m \times (m+2)$,

$$\boldsymbol{J} = \begin{bmatrix} -1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -1 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & -1 & 0 & 0 \\ -\widetilde{b} & 0 & \cdots & 0 & 0 & -1 & -\widetilde{x}_1 \\ 0 & -\widetilde{b} & \cdots & 0 & 0 & -1 & -\widetilde{x}_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -\widetilde{b} & 0 & -1 & -\widetilde{x}_{m-1} \\ 0 & 0 & \cdots & 0 & -\widetilde{b} & -1 & -\widetilde{x}_m \end{bmatrix} = \begin{bmatrix} -\boldsymbol{I} & \boldsymbol{0} & \boldsymbol{0} \\ -\widetilde{b}\boldsymbol{I} & -\boldsymbol{1} & -\widetilde{\boldsymbol{x}} \end{bmatrix},$$

where the $\widetilde{\boldsymbol{x}} = (\widetilde{x}_1, \ldots, \widetilde{x}_m)^\top$, $\widetilde{a}$ and $\widetilde{b}$ are extracted from the current estimate $\widetilde{\boldsymbol{t}}$ of the parameter vector;

3 Determine the QR factorization of $\boldsymbol{J}$:

$$\boldsymbol{J} = \boldsymbol{Q}\begin{bmatrix} \boldsymbol{R}_1 \\ \boldsymbol{0} \end{bmatrix},$$

where $\boldsymbol{Q}$ is an orthogonal matrix of dimension $2m \times 2m$ and $\boldsymbol{R}_1$ is an upper-triangular matrix of dimension $(m+2) \times (m+2)$; see A.5.1;

4 Form the matrix product $\boldsymbol{Q}^\top \boldsymbol{B}$ and determine its RQ factorization

$$\boldsymbol{Q}^\top \boldsymbol{B} = \boldsymbol{T}\boldsymbol{Z},$$

where $\boldsymbol{T}$ is a matrix of dimension $2m \times p$ and $\boldsymbol{Z}$ is an orthogonal matrix of dimension $p \times p$; see A.5.2;

5 Set $\widetilde{\boldsymbol{f}} = \boldsymbol{Q}^\top \boldsymbol{f}$ and partition $\widetilde{\boldsymbol{f}}$ and $\boldsymbol{T}$:

$$\widetilde{\boldsymbol{f}} = \begin{bmatrix} \widetilde{\boldsymbol{f}}_1 \\ \widetilde{\boldsymbol{f}}_2 \end{bmatrix}, \qquad \boldsymbol{T} = \begin{bmatrix} \boldsymbol{T}_{11} & \boldsymbol{T}_{12} \\ \boldsymbol{0} & \boldsymbol{T}_{22} \end{bmatrix},$$

where $\widetilde{\boldsymbol{f}}_1$ is a vector of dimension $(m+2) \times 1$, $\widetilde{\boldsymbol{f}}_2$ is a vector of dimension $(m-2) \times 1$, $\boldsymbol{T}_{11}$ is a matrix of dimension $(m+2) \times (p-m+2)$, $\boldsymbol{T}_{12}$ is a matrix of dimension $(m+2) \times (m-2)$ and $\boldsymbol{T}_{22}$ is an upper-triangular matrix of dimension $(m-2) \times (m-2)$;

6 Solve the upper-triangular system $\boldsymbol{T}_{22}\widetilde{\boldsymbol{e}}_2 = \widetilde{\boldsymbol{f}}_2$ to determine the vector $\widetilde{\boldsymbol{e}}_2 = (\widetilde{e}_{2,1}, \ldots, \widetilde{e}_{2,m-2})^\top$ of dimension $(m-2) \times 1$; see A.4.4;

7 Solve the upper-triangular system $\boldsymbol{R}_1 \delta\boldsymbol{t} = \boldsymbol{T}_{12}\widetilde{\boldsymbol{e}}_2 - \widetilde{\boldsymbol{f}}_1$ to determine the increment $\delta\boldsymbol{t}$; see A.4.4;

8 Update the current approximations to the parameters: $\widetilde{\boldsymbol{t}} := \widetilde{\boldsymbol{t}} + \delta\boldsymbol{t}$;

9 Repeat steps 2 to 8 until convergence has been achieved. Set $a = \widetilde{a}$ and $b = \widetilde{b}$ (elements $m+1$ and $m+2$ of $\widetilde{\boldsymbol{t}}$);

10 Let $\boldsymbol{R_a}$ be the lower right submatrix of dimension 2×2 of $\boldsymbol{R}_1$ and $\boldsymbol{T_a}$ the lower right submatrix of dimension 2×2 of $\boldsymbol{T}_{11}$. Solve the upper-triangular system

$$\boldsymbol{R_a}\boldsymbol{K_a} = \boldsymbol{T_a},$$

for the upper triangular matrix $\boldsymbol{K_a}$ of dimension 2×2 (see A.4.4) and set $\boldsymbol{U_a} = \boldsymbol{K_a}\boldsymbol{K_a}^\top$. Then

$$u^2(a) = \boldsymbol{U_a}(1,1), \qquad u^2(b) = \boldsymbol{U_a}(2,2) \qquad \text{and} \qquad \operatorname{cov}(a,b) = \boldsymbol{U_a}(1,2).$$

NOTE 1 The approach described in C.2 represents the most general solution to determining linear calibration functions using least squares methods. All other approaches described in this document can be solved as special cases.

NOTE 2 Steps 1, 2, 8 and 9 in C.2 are identical to, respectively, steps 1, 2, 9 and 10 in 10.2.2.

C.3 Validation of the model

If $m > 2$, the validity of the model can be partially tested using the elements of the vector $\widetilde{\boldsymbol{e}}_2$ (continued from C.2):

11 Form the observed chi-squared value $\chi^2_{\text{obs}} = \sum_{i=1}^{m-2} \widetilde{e}^2_{2,i}$ and degrees of freedom $\nu = m-2$;

12 Check whether χ^2_{obs} exceeds the 95 % quantile of χ^2_ν, and if it does reject the straight-line model.

NOTE The chi-squared test is based on an assumption that the d_i and e_i in model (13) are realizations of random variables characterized by a multivariate normal distribution and on a first order approximation. Under this assumption the vector $\widetilde{\boldsymbol{e}}_2$ of dimension $(m-2) \times 1$ is associated with a multivariate Gaussian distribution with covariance matrix equal to the identity matrix of dimension $(m-2) \times (m-2)$ so that χ^2_{obs} is associated with a χ^2 distribution with $m-2$ degrees of freedom.

EXAMPLE 1 The QR factorization approach can be applied to the numerical example described in Clause 10.

The covariance matrix $\boldsymbol{U_x}$ arises in factored form (see D.4) as

$$\boldsymbol{U_x} = \boldsymbol{B_x}\boldsymbol{B_x}^{\top},$$

where

$$\boldsymbol{B_x} = \begin{bmatrix} 0{,}5 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}5 & 0{,}0 & 0{,}0 \\ 0{,}0 & 0{,}5 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 1{,}0 & 0{,}0 \\ 0{,}0 & 0{,}0 & 0{,}5 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}5 & 1{,}0 & 0{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}5 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 1{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}5 & 0{,}0 & 0{,}0 & 0{,}5 & 0{,}0 & 1{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}5 & 0{,}0 & 0{,}0 & 1{,}0 & 1{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}5 & 0{,}5 & 1{,}0 & 1{,}0 \end{bmatrix}.$$

The covariance matrix $\boldsymbol{U_y} = \boldsymbol{B_y}\boldsymbol{B_y}^{\top}$ also arises in factored form with

$$\boldsymbol{B_y} = \begin{bmatrix} 2{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 1{,}0 \\ 0{,}0 & 2{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 1{,}0 \\ 0{,}0 & 0{,}0 & 2{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 1{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 2{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 1{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 2{,}0 & 0{,}0 & 0{,}0 & 1{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 2{,}0 & 0{,}0 & 1{,}0 \\ 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 0{,}0 & 2{,}0 & 1{,}0 \end{bmatrix}.$$

The complete covariance matrix $\boldsymbol{U}$ of dimension 14×14 is factorized as $\boldsymbol{U} = \boldsymbol{B}\boldsymbol{B}^{\top}$, where $\boldsymbol{B}$ is the matrix of dimension 14×18

$$\boldsymbol{B} = \begin{bmatrix} \boldsymbol{B_x} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B_y} \end{bmatrix}.$$

For this example, the algorithm in C.2 is mathematically equivalent to that in 10.2.2 and the two approaches give very similar numerical results.

EXAMPLE 2 Table C.1 gives seven measured data points (x_i, y_i) obtained using the measurement models described in D.2 and D.5.

The covariance matrix associated with the y_i is derived using the model (D.1) with $u_{\mathrm{S}} = 2{,}0$ and $u_{\mathrm{R}} = 1{,}0$, and is the same as in Annex C EXAMPLE 1.

The data x_i and associated covariance matrix are derived using the measurement model (D.3) with $z_1 = 50$, $z_2 = 100$, $z_3 = 200$, $u(z_1) = 0{,}5$ and $u(z_2) = u(z_3) = 1{,}0$, so that

$$\boldsymbol{U_x} = \boldsymbol{B_x}\boldsymbol{B_x}^{\top},$$

where

$$\boldsymbol{B_x} = \begin{bmatrix} 0{,}5 & 0{,}0 & 0{,}0 \\ 0{,}0 & 1{,}0 & 0{,}0 \\ 0{,}5 & 1{,}0 & 0{,}0 \\ 0{,}0 & 0{,}0 & 1{,}0 \\ 0{,}5 & 0{,}0 & 1{,}0 \\ 0{,}0 & 1{,}0 & 1{,}0 \\ 0{,}5 & 1{,}0 & 1{,}0 \end{bmatrix}.$$

The complete covariance matrix $\boldsymbol{U}$ of dimension 14×14 can be factorized as $\boldsymbol{U} = \boldsymbol{B}\boldsymbol{B}^{\top}$, where $\boldsymbol{B}$ is the matrix of dimension 14×11

$$\boldsymbol{B} = \begin{bmatrix} \boldsymbol{B_x} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B_y} \end{bmatrix}.$$

For this example, the algorithm in 10.2.2 cannot be applied since $\boldsymbol{U}$ is not positive definite. The algorithm described in C.2 can be used instead.

Table C.2 gives the initial vector $\widetilde{\boldsymbol{t}}_0$, the corrections $\delta\widetilde{\boldsymbol{t}}_k$ for the kth iteration, $k = 1, \ldots, 5$, and the final estimate $\widetilde{\boldsymbol{t}} = \widetilde{\boldsymbol{t}}_5$.

Table C.1 — Data representing seven measurement points, the x_i and y_i having associated covariance matrices

x_i	y_i
50,5	47,1
99,7	98,4
150,2	153,7
199,5	194,0
249,9	251,9
299,2	297,5
349,7	349,0

Table C.2 — Change in parameter vector $\widetilde{t}$

$\widetilde{t}_0$	$\delta t_1 \times 10^{-2}$	$\delta t_2 \times 10^{-4}$	$\delta t_3 \times 10^{-6}$	$\delta t_4 \times 10^{-8}$	$\delta t_5 \times 10^{-10}$	$\widetilde{t}_5$
50,500 0	30,822 9	3,187 4	23,295 7	8,112 4	16,423 1	50,808 6
99,700 0	55,831 3	−13,836 5	26,113 6	−0,206 3	15,677 0	100,257 0
150,200 0	86,654 2	−10,649 1	49,409 3	7,906 1	32,100 2	151,065 5
199,500 0	−59,071 1	−48,597 6	−49,584 9	−44,790 4	−43,047 0	198,904 4
249,900 0	−28,248 2	−45,410 2	−26,289 1	−36,678 0	−26,623 7	249,613 0
299,200 0	−3,239 8	−62,434 1	−23,471 3	−44,996 7	−27,369 8	299,161 3
349,700 0	27,583 1	−59,246 7	−0,175 5	−36,884 3	−10,946 8	349,969 9
−1,852 8	−50,620 3	−140,085 6	−63,931 6	−100,943 2	−68,134 5	−2,373 1
1,004 2	0,173 8	0,857 1	0,321 7	0,610 8	0,372 2	1,006 0

Annex D
(informative)

Provision of uncertainties and covariances associated with the measured x- and y-values

D.1 General

This annex indicates how the uncertainties and covariances associated with the measured response and stimulus measurement values can be obtained. The approach is based on the use of a measurement model of the processes underlying the determination of response and stimulus data, and the application of the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008. Illustrative examples are used for this purpose.

D.2 Response data 1

D.2.1 General

D.2.1.1 Suppose the quantity Y representing instrument response can be expressed by the measurement model

$$Y = Y_0 + E, \tag{D.1}$$

where Y_0 is a quantity realized by the indicated response and E a quantity representing a systematic effect. Suppose that the knowledge of Y_0 is encoded by a distribution with standard deviation u_{R}. This distribution is typically based on an analysis of a number of repeated indications of Y. Y_0 is estimated by the average of these indications and u_{R} is the standard uncertainty associated with this estimate. Suppose that the knowledge of E is such that E has expectation zero (that is, any necessary correction has been applied) and variance u_{S}^2 (obtained from an understanding dependent on the specific nature of the instrument).

D.2.1.2 It follows from expression (D.1) that, by applying the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008, the standard uncertainty $u(y_i)$ associated with a measured value y_i of Y is given by

$$u^2(y_i) = u_{\mathrm{S}}^2 + u_{\mathrm{R}}^2.$$

Moreover, the covariance associated with measured values y_i and y_j of Y is

$$\mathrm{cov}(y_i, y_j) = u_{\mathrm{S}}^2.$$

D.2.1.3 Thus the covariance matrix in this case is

$$\boldsymbol{U}_{\boldsymbol{y}} = \begin{bmatrix} u_{\mathrm{S}}^2 + u_{\mathrm{R}}^2 & u_{\mathrm{S}}^2 & \dots & u_{\mathrm{S}}^2 \\ u_{\mathrm{S}}^2 & u_{\mathrm{S}}^2 + u_{\mathrm{R}}^2 & \dots & u_{\mathrm{S}}^2 \\ \vdots & \vdots & \ddots & \vdots \\ u_{\mathrm{S}}^2 & u_{\mathrm{S}}^2 & \dots & u_{\mathrm{S}}^2 + u_{\mathrm{R}}^2 \end{bmatrix}.$$

D.2.2 Measurement model for uncertainties and covariances associated with the y_i

D.2.2.1 The data used in the example in Clause 9 are derived from a measuring system where two groups of measurements are made. Each group of measurements is subject to a different systematic effect with the two effects being uncorrelated, that is,

$$Y_i = \begin{cases} Y_{0,i} + E_1, & i = 1, \dots, m_1 < m, \\ Y_{0,i} + E_2, & i = m_1 + 1, \dots, m, \end{cases}$$

where $Y_{0,i}$ is a quantity realized by the ith indicated response and E_1 and E_2 quantities representing systematic effects. Suppose that the knowledge of $Y_{0,i}$ is such that $Y_{0,i}$ has variance u_{R}^2 and that the knowledge of E_k is such that E_k has expectation zero and variance $u_{\mathrm{S},k}^2$, for $k = 1, 2$.

D.2.2.2 The standard uncertainty $u(y_i)$ associated with a measured value y_i of Y_i is given by

$$u^2(y_i) = \begin{cases} u_{\mathrm{R}}^2 + u_{\mathrm{S},1}^2, & i = 1, \ldots, m_1, \\ u_{\mathrm{R}}^2 + u_{\mathrm{S},2}^2, & i = m_1 + 1, \ldots, m. \end{cases}$$

The covariances associated with measured values y_i and y_j are

$$\mathrm{cov}(y_i, y_j) = \begin{cases} u_{\mathrm{S},1}^2, & 1 \le i \le m_1, 1 \le j \le m_1, \\ u_{\mathrm{S},2}^2, & m_1 + 1 \le i \le m, m_1 + 1 \le j \le m, \\ 0, & \text{otherwise.} \end{cases}$$

D.2.2.3 The covariance matrix in this case is

$$\boldsymbol{U}_{\boldsymbol{y}} = \begin{bmatrix} u_{\mathrm{S},1}^2 + u_{\mathrm{R}}^2 & \cdots & u_{\mathrm{S},1}^2 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ u_{\mathrm{S},1}^2 & \cdots & u_{\mathrm{S},1}^2 + u_{\mathrm{R}}^2 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & u_{\mathrm{S},2}^2 + u_{\mathrm{R}}^2 & \cdots & u_{\mathrm{S},2}^2 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & u_{\mathrm{S},2}^2 & \cdots & u_{\mathrm{S},2}^2 + u_{\mathrm{R}}^2 \end{bmatrix}.$$

D.3 Response data 2

D.3.1 The measurement model is identical to that in expression (D.1) except that instead of the systematic effect E being absolute, D is a relative systematic effect:

$$Y = Y_0(1 + D).$$

D.3.2 The treatment is analogous to that of D.2 except that now, using u_{D} to denote the relative standard uncertainty associated with an estimate of Y_0,

$$\begin{aligned} u^2(y_i) &= y_i^2 u_{\mathrm{D}}^2 + u_{\mathrm{R}}^2, \\ \mathrm{cov}(y_i, y_j) &= y_i y_j u_{\mathrm{D}}^2. \end{aligned}$$

D.3.3 The covariance matrix in this case is

$$\boldsymbol{U}_{\boldsymbol{y}} = \begin{bmatrix} y_1^2 u_{\mathrm{D}}^2 + u_{\mathrm{R}}^2 & y_1 y_2 u_{\mathrm{D}}^2 & \cdots & y_1 y_m u_{\mathrm{D}}^2 \\ y_2 y_1 u_{\mathrm{D}}^2 & y_2^2 u_{\mathrm{D}}^2 + u_{\mathrm{R}}^2 & \cdots & y_2 y_m u_{\mathrm{D}}^2 \\ \vdots & \vdots & \ddots & \vdots \\ y_m y_1 u_{\mathrm{D}}^2 & y_m y_2 u_{\mathrm{D}}^2 & \cdots & y_m^2 u_{\mathrm{D}}^2 + u_{\mathrm{R}}^2 \end{bmatrix}.$$

D.4 Stimulus data 1

D.4.1 The data used in the example in Clause 10 are derived from the following measurement model, motivated by practice in mass metrology where a number of masses are used to generate multiple calibration values x_i. The stimulus data x_i are realizations of random variables X_i, $i = 1, \ldots, 7$, defined in terms of random variables Z_k, $k = 1, 2, 3$ and D_i, $i = 1, \ldots, 7$:

$$\begin{aligned} X_1 &= Z_1 + D_1, \\ X_2 &= Z_2 + D_2, \\ X_3 &= Z_1 + Z_2 + D_3, \\ X_4 &= Z_3 + D_4, \\ X_5 &= Z_1 + Z_3 + D_5, \\ X_6 &= Z_2 + Z_3 + D_6, \\ X_7 &= Z_1 + Z_2 + Z_3 + D_7. \end{aligned} \tag{D.2}$$

The random variables Z_k, $k = 1, 2, 3$, have expectations z_k and variances $u^2(z_k)$, while the D_i have expectations zero and variances $u^2_{D,i}$. (In mass calibration, the values z_k are the calibrated values for the masses and $u(z_k)$ the associated uncertainties.)

D.4.2 The uncertainties $u(z_k)$ and $u(d_i)$ are propagated through the measurement model in D.4.1 to those associated with estimates x_i of X_i using the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008. The common dependence of X_i on Z_k means that some of the covariances are nonzero. The propagation is most easily described in matrix terms. Let

$$\boldsymbol{C} = \left[\begin{array}{cc} \boldsymbol{C}_D & \boldsymbol{C}_Z \end{array} \right]$$

be the sensitivity matrix of dimension 7×10, where $\boldsymbol{C}_D = \boldsymbol{I}$ is the identity matrix of dimension 7×7 and

$$\boldsymbol{C}_Z = \left[\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{array} \right].$$

D.4.3 Let $\boldsymbol{S}_D$ be the diagonal matrix of dimension 7×7 with diagonal elements $\boldsymbol{S}_D(i, i) = u_{D,i}$, $i = 1, \ldots, 7$, and $\boldsymbol{S}_Z$ the diagonal matrix of dimension 3×3 with diagonal elements $\boldsymbol{S}_Z(k, k) = u(z_k)$, $k = 1, 2, 3$. Set

$$\boldsymbol{B}_{\boldsymbol{x}} = \left[\begin{array}{cc} \boldsymbol{C}_D & \boldsymbol{C}_Z \end{array} \right] \left[\begin{array}{cc} \boldsymbol{S}_D & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{S}_Z \end{array} \right] = \left[\begin{array}{cc} \boldsymbol{S}_D & \boldsymbol{C}_Z \boldsymbol{S}_Z \end{array} \right].$$

D.4.4 Then the best estimate of $\boldsymbol{X}$ is given by $\boldsymbol{x} = \boldsymbol{C}_Z \boldsymbol{z}$ of dimension 7×1 and the associated covariance matrix of dimension 7×7 is given by

$$\boldsymbol{U}_{\boldsymbol{x}} = \boldsymbol{B}_{\boldsymbol{x}} \boldsymbol{B}_{\boldsymbol{x}}{}^{\top} = \boldsymbol{S}_D^2 + \boldsymbol{C}_Z \boldsymbol{S}_Z^2 \boldsymbol{C}_Z^{\top}.$$

The term $\boldsymbol{S}_D^2$ is the variance contribution arising from the D_i while the second term is the contribution from the Z_k.

D.5 Stimulus data 2

D.5.1 The data used in Annex C EXAMPLE 2 are derived from the following measurement model related to that described in D.4. The stimulus data x_i are realizations of random variables X_i, $i = 1, \ldots, 7$, defined in terms of random variables Z_k, $k = 1, 2, 3$:

$$\begin{array}{rcl} X_1 & = & Z_1, \\ X_2 & = & Z_2, \\ X_3 & = & Z_1 + Z_2, \\ X_4 & = & Z_3, \\ X_5 & = & Z_1 + Z_3, \\ X_6 & = & Z_2 + Z_3, \\ X_7 & = & Z_1 + Z_2 + Z_3. \end{array} \qquad \text{(D.3)}$$

The random variables Z_k have expectations z_k and variances $u^2(z_k)$, $k = 1, 2, 3$.

D.5.2 The uncertainties $u(z_k)$ are propagated through the measurement model in D.5.1 to those associated with estimates x_i of X_i using the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008. Following the notation of D.4, the best estimate associated with X_i is given by $\boldsymbol{x} = \boldsymbol{C}_Z \boldsymbol{z}$ of dimension 7×1 and the associated covariance matrix of dimension 7×7 is given by

$$\boldsymbol{U}_{\boldsymbol{x}} = \boldsymbol{B}_{\boldsymbol{x}} \boldsymbol{B}_{\boldsymbol{x}}{}^{\top} = \boldsymbol{C}_Z \boldsymbol{S}_Z^2 \boldsymbol{C}_Z^{\top}, \qquad \boldsymbol{B}_{\boldsymbol{x}} = \boldsymbol{C}_Z \boldsymbol{S}_Z.$$

In this case $\boldsymbol{U}_{\boldsymbol{x}}$ is not invertible.

D.6 Stimulus and response data

D.6.1 Correlation, that is, non-zero covariances, associated with the measurement data x_i and y_i arises through the presence of effects that are common to both.

D.6.2 Suppose X and Y can be expressed by the measurement model

$$X = X_0 + T, \qquad Y = Y_0 + T, \tag{D.4}$$

where X_0, Y_0 and T are independent random variables with expectations x_0, y_0 and zero, and variances $u^2(x_0)$, $u^2(y_0)$ and $u^2(t)$, respectively.

D.6.3 It follows from expression (D.4) that, by applying the law of propagation of uncertainty in ISO/IEC Guide 98-3:2008, the standard uncertainties $u(x_i)$ and $u(y_i)$ associated with measured values x_i of X and y_i of Y are given by

$$u^2(x_i) = u^2(x_0) + u^2(t), \qquad u^2(y_i) = u^2(y_0) + u^2(t).$$

Moreover, the covariance associated with x_i and y_i is

$$\mathrm{cov}(x_i, y_i) = u^2(t).$$

D.6.4 If instead X and Y can be expressed by the measurement model

$$X = X_0 + T, \qquad Y = Y_0 - T,$$

the covariance associated with x_i and y_i is

$$\mathrm{cov}(x_i, y_i) = -u^2(t).$$

Annex E
(informative)

Uncertainties known up to a scale factor

E.1 This annex describes a method to evaluate the uncertainties associated with the measurement data in the case that those uncertainties are known only up to a scale factor.

E.2 This Technical Specification generally assumes that uncertainties associated with the measurement data are provided. This is the situation if the quantities (variables) involved have been characterized according to the principles of ISO/IEC Guide 98-3:2008 and ISO/IEC Guide 98-3:2008/Suppl. 1:2008 [13] in terms of probability distributions. The measurement value is given by the expectation of the variable and its associated variance by the variance of the variable.

NOTE In particular, regarding a measured value y as a realization of a variable characterized by a t-distribution with scale parameter s and ν degrees of freedom ($\nu > 2$), the standard uncertainty associated with y is given by $u(y) = [\nu/(\nu-2)]^{1/2}\, s$, the standard deviation of that distribution.

E.3 Since the calibration function is generally to be used in practical measurement, the evaluation of the uncertainties associated with the calibration data should be as complete and rigorous as possible. The estimates of the calibration function parameters and their associated uncertainties can then be used with confidence. A relaxation of this consideration addressed in this Technical Specification is the case in which uncertainties are known up to a multiplicative scaling constant. The commonest case [9, page 30] is that in which it is believed that the measured y-values have essentially identical uncertainty, but their common standard uncertainty σ is unknown. (This is an instance of the more general case where the covariance matrix $\boldsymbol{U} = \sigma^2 \boldsymbol{U}_0$, where $\boldsymbol{U}_0$ is given, but σ is unknown.) If $m > 2$, it is possible in this regard to provide an estimate $\widehat{\sigma}$ of σ on the basis of the dispersion of the data points about the fitted line. This estimate is known as the posterior estimate of σ, the qualification 'posterior' referring to the fact that it can only be determined after a best-fit line has been obtained for the data.

E.4 The posterior estimate is determined using the same concepts as those used in model validation. By making the further assumption that the input data are a realization of a multivariate normally distributed variable, the posterior estimate $\widehat{\sigma}$ is chosen so that χ^2_{obs} is equal to $m-2$, the expectation of the chi-squared distribution with $m-2$ degrees of freedom. No validation of the model and the data can be carried out in this case since the posterior estimate has been chosen so that the validation criterion is automatically satisfied.

E.5 This method should therefore only be used with extreme caution. For instance, if a plot of the data indicates that a straight-line calibration function is not appropriate, the method should not be used.

E.6 The parameter estimates a and b do not depend on the scale factor σ. An estimate of σ is only required to evaluate the standard uncertainties $u(a)$ and $u(b)$ and covariance $\text{cov}(a,b)$ associated with these estimates. For the case of $\boldsymbol{U}$ known completely, $u(a)$, $u(b)$ and $\text{cov}(a,b)$ can be evaluated from the data and $\boldsymbol{U}$ alone; no assumption about the distributions associated with the data is necessary. With an assumption of normality, the parameter estimates can be regarded as realizations of variables characterized by a certain bivariate distribution, as follows.

E.7 In the case where the data can be regarded as a realization of a multivariate normal distribution with known covariance matrix $\boldsymbol{U}$, the bivariate distribution in E.6 is normal with covariance matrix $\boldsymbol{U}_{\boldsymbol{a}}$ with elements $u^2(a)$, $u^2(b)$ and covariance $\text{cov}(a,b)$ as in expression (1).

E.8 For the case in E.4 where the multivariate normal distribution has covariance matrix $\boldsymbol{U} = \sigma^2 \boldsymbol{U}_0$, where $\boldsymbol{U}_0$ is known and σ is unknown, $\boldsymbol{U}_0$ is used in place of $\boldsymbol{U}$ in the calculations. The covariance matrix

$$\boldsymbol{U}_{\boldsymbol{a},0} = \begin{bmatrix} u_0^2(a) & \text{cov}_0(a,b) \\ \text{cov}_0(b,a) & u_0^2(b) \end{bmatrix}$$

associated with the estimates of the straight-line calibration parameters can be calculated. If $m > 2$, the observed chi-squared value (see 6.3) can be used to provide a posterior estimate of the scale factor associated with the input

uncertainties. Let χ^2_{obs} be calculated as in step 8 in 6.3, and set

$$\widehat{\sigma}^2 = \chi^2_{\text{obs}}/(m-2).$$

E.9 The scale-adjusted covariance matrix

$$\widehat{\boldsymbol{U}}_{\boldsymbol{a}} = \begin{bmatrix} \widehat{u}^2(a) & \widehat{\text{cov}}(a,b) \\ \widehat{\text{cov}}(b,a) & \widehat{u}^2(b) \end{bmatrix}$$

is then given by

$$\widehat{\boldsymbol{U}}_{\boldsymbol{a}} = \widehat{\sigma}^2 \boldsymbol{U}_{\boldsymbol{a},0},$$

that is, the scale-adjusted standard uncertainties $\widehat{u}(a)$ and $\widehat{u}(b)$ and covariance $\widehat{\text{cov}}(a,b)$ associated with the fitted parameters are given by

$$\widehat{u}^2(a) = \widehat{\sigma}^2 u_0^2(a), \qquad \widehat{u}^2(b) = \widehat{\sigma}^2 u_0^2(b), \qquad \widehat{\text{cov}}(a,b) = \widehat{\sigma}^2 \text{cov}_0(a,b). \tag{E.1}$$

E.10 The estimates (E.1) are based on the fit to a finite number m of data points and for small m will underestimate the variance of the distribution for the fitted parameters. For $m > 4$, a better estimate is determined [19, chapter 8] using

$$\widetilde{\sigma}^2 = \frac{m-2}{m-4}\frac{\chi^2_{\text{obs}}}{m-2} = \frac{\chi^2_{\text{obs}}}{m-4}.$$

NOTE Under the assumption of normality, the parameter estimates are then associated with a bivariate t-distribution with scale matrix $\widehat{\boldsymbol{U}}_{\boldsymbol{a}}$ and $m-2$ degrees of freedom. For $m > 4$, the covariance matrix of that distribution is given by

$$\widetilde{\boldsymbol{U}}_{\boldsymbol{a}} = \begin{bmatrix} \widetilde{u}^2(a) & \widetilde{\text{cov}}(a,b) \\ \widetilde{\text{cov}}(b,a) & \widetilde{u}^2(b) \end{bmatrix} = \frac{m-2}{m-4}\,\widehat{\boldsymbol{U}}_{\boldsymbol{a}} = \widetilde{\sigma}^2 \boldsymbol{U}_{\boldsymbol{a},0}, \tag{E.2}$$

where the inflating factor $(m-2)/(m-4)$ accounts for the fact that σ is being estimated rather than known in advance.

EXAMPLE (UNKNOWN WEIGHTS) In this example, the x_i are taken to be exact and the y_i to have equal but unknown standard uncertainties, and a posterior estimate of the uncertainties associated with the fitted parameters is evaluated from the residuals of the fit. The fit is determined by taking the weights equal to unity (implying that the standard uncertainties $u(y_i)$ are also nominally equal to unity). The data are given in Table E.1.

Table E.1 — Data representing six measurement points, with weights set to unity

x_i	y_i	$u(y_i)$
1,000	3,014	1
2,000	5,225	1
3,000	7,004	1
4,000	9,061	1
5,000	11,201	1
6,000	12,762	1

The best fit straight-line parameters are calculated as in Table E.2. From the table, $g_0 = 21{,}000/6{,}000 = 3{,}500$, $h_0 = 48{,}267/6{,}000 = 8{,}044$, $b = 34{,}363/17{,}500 = 1{,}964$ and $a = 8{,}044 - (1{,}964)(3{,}500) = 1{,}172$.

Table E.2 — Calculation tableau associated with the data in Table E.1

w_i	w_i^2	$w_i^2 x_i$	$w_i^2 y_i$	g_i	h_i	g_i^2	$g_i h_i$	r_i	r_i^2
				3,500	8,044			$a = 1{,}172$	
1,000	1,000	1,000	3,014	−2,500	−5,031	6,250	12,576	−0,122	0,015
1,000	1,000	2,000	5,225	−1,500	−2,819	2,250	4,229	0,126	0,016
1,000	1,000	3,000	7,004	−0,500	−1,040	0,250	0,520	−0,059	0,003
1,000	1,000	4,000	9,061	0,500	1,017	0,250	0,508	0,035	0,001
1,000	1,000	5,000	11,201	1,500	3,157	2,250	4,735	0,211	0,045
1,000	1,000	6,000	12,762	2,500	4,718	6,250	11,794	−0,191	0,037
	6,000	21,000	48,267			17,500	34,363	$b = 1{,}964$	0,116

The data and fitted straight-line calibration function are graphed in Figure E.1. The weighted residuals are illustrated in Figure E.2. Because the $u(y_i)$ are arbitrarily given the value unity, in this case the uncertainty bars greatly exceed the residuals in magnitude.

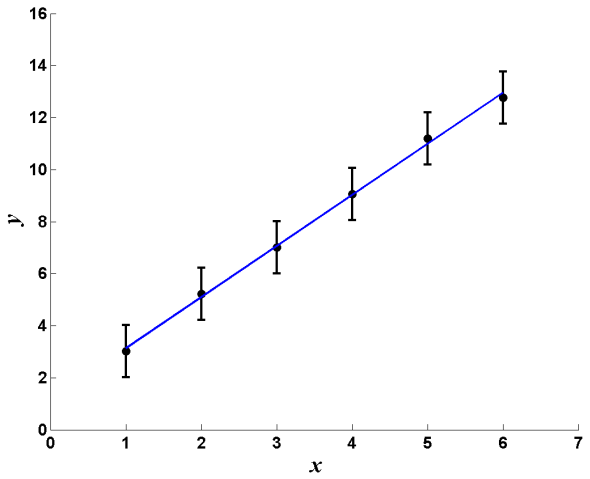

Figure E.1 — Data in Table E.1 and fitted straight-line calibration function obtained in Table E.2

If it were known a priori that $u(y_i) = 1$, $i = 1, \ldots, m$, then uncertainties associated with the fitted parameters would be calculated from the information in Table E.2:

$$u^2(a) = 1/6{,}000 + (3{,}500)^2/17{,}500, \text{ so that } u(a) = 0{,}931;$$
$$u^2(b) = 1/17{,}500, \text{ so that } u(b) = 0{,}239;$$
$$\text{cov}(a, b) = -3{,}500/17{,}500 = -0{,}200.$$

Because these calculations are based on the arbitrary assignment $u(y_i) = 1$, the posterior estimate $\widehat{\sigma}$ of $u(y_i)$ is required in

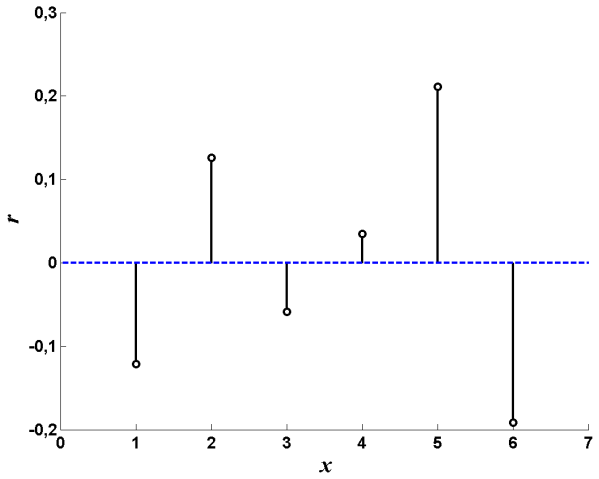

Figure E.2 — Weighted residuals calculated using the fitted straight-line calibration function obtained in Table E.2

order to evaluate the uncertainties associated with the fitted parameters. From the table,

$$\widehat{\sigma}^2 = \frac{\chi^2_{\text{obs}}}{m-2} = \frac{0{,}116}{4} = 0{,}029, \text{ or } \widehat{\sigma} = 0{,}171.$$

This value of $\widehat{\sigma}$ represents an estimate of the standard uncertainties $u(y_i)$ associated with the y_i based on the observed chi-squared value. Given this posterior estimate, the calculations can be repeated with $u(y_i) = 0{,}171$. The estimates for a and b would be unchanged, but the observed chi-squared value and uncertainties would be scaled as follows:

$$r_i = \frac{r_i}{\widehat{\sigma}},$$

so that $\chi^2_{\text{obs}}/\widehat{\sigma}^2 = m - 2 = 4$, the expectation of the chi-squared distribution with 4 degrees of freedom. Using formulæ (E.1),

$$\widehat{u}^2(a) = \widehat{\sigma}^2 u_0^2(a) = 0{,}867\widehat{\sigma}^2 = 0{,}025, \text{ so that } \widehat{u}(a) = 0{,}931\widehat{\sigma} = 0{,}159;$$
$$\widehat{u}^2(b) = \widehat{\sigma}^2 u_0^2(b) = 0{,}057\widehat{\sigma}^2 = 0{,}002, \text{ so that } \widehat{u}(b) = 0{,}239\widehat{\sigma} = 0{,}041;$$
$$\widehat{\text{cov}}(a,b) = \widehat{\sigma}^2 \text{cov}_0(a,b) = -0{,}200\widehat{\sigma}^2 = -0{,}006.$$

The elements of $\widehat{\boldsymbol{U}}_{\boldsymbol{a}}$ are those that would be evaluated if it were known, a priori, that $u(y_i) = \widehat{\sigma}$. However, $\widehat{\sigma}$ is an estimate of the standard uncertainties associated with the y_i. For $m > 4$, an inflation factor of $(m-2)/(m-4)$ can be incorporated into the covariance matrix to account for the additional uncertainty that arises from the fact that $\widehat{\sigma}$ is an estimate derived from m data points. Using formula (E.2),

$$\widetilde{\boldsymbol{U}}_{\boldsymbol{a}} = \frac{m-2}{m-4}\widehat{\boldsymbol{U}}_{\boldsymbol{a}} = 2\begin{bmatrix} 0{,}025 & -0{,}006 \\ -0{,}006 & 0{,}002 \end{bmatrix} = \begin{bmatrix} 0{,}050 & -0{,}012 \\ -0{,}012 & 0{,}003 \end{bmatrix},$$

so that $\widetilde{u}(a) = (0{,}050)^{1/2} = 0{,}225$, $\widetilde{u}(b) = (0{,}003)^{1/2} = 0{,}058$ and $\widetilde{\text{cov}}(a,b) = -0{,}012$.

Annex F
(informative)

Software implementation of described algorithms

F.1 Software implementing the algorithms described in this Technical Specification for determining and using straight-line calibration functions has been developed by the National Physical Laboratory (NPL) in the United Kingdom. The software is available as a compressed ZIP folder from the web sites of NPL at `www.npl.co.uk/mathematics-scientific-computing/software-support-for-metrology/software-downloads-(ssfm)` and the International Organization for Standardization at `standards.iso.org/iso/ts/28037/`.

F.2 Software, developed in the MATLAB programming language [18], is provided in the form of M-files and html files published using MATLAB Version 7.10.0 (R2010a). For users of MATLAB, the M-files may be run directly and also modified to run the algorithms for different measurement data. For users who do not have access to MATLAB, the software is best viewed as the provided html files. The software may be used as the basis for preparing implementations of the algorithms in other programming languages. Within the files, calls are made to a number of MATLAB functions that are also included with the software. For example, the function algm_gdr1_steps_2_to_5 implements steps 2 to 5 of the calculation procedure for the case 5.3.2 b) (uncertainties are associated with the measured values x_i and y_i and all covariances associated with the data are regarded as negligible) specified in 7.2.1. In addition, some use of MATLAB built-in functions is made, such as for obtaining the Cholesky factorization of a matrix. MATLAB scripts (having extension '.m') and html files ('.html') are provided as follows:

— TS28037_WLS1 runs the numerical example of weighted least squares (WLS) with *known equal weights* described in Clause 6, and performs the prediction described in 11.1 EXAMPLE 1 and forward evaluation described in 11.2;

— TS28037_WLS2 runs the numerical example of weighted least squares (WLS) with *known unequal weights* described in Clause 6 and performs the prediction described in 11.1 EXAMPLE 2;

— TS28037_WLS3 runs the numerical example of weighted least squares (WLS) with *unknown equal weights* described in Annex E;

— TS28037_GDR1 runs the numerical example of generalized distance regression (GDR) described in Clause 7;

— TS28037_GDR2 runs a numerical example to illustrate the algorithm for generalized distance regression (GDR) described in Clause 8;

— TS28037_GMR runs the numerical example of Gauss-Markov regression (GMR) described in Clause 9;

— TS28037_GGMR1 runs the numerical example of generalized Gauss-Markov regression (GGMR) described in Clause 10;

— TS28037_GGMR2 runs the numerical example of GGMR described in Clause 10 and Annex C EXAMPLE 1 using the orthogonal factorization approach described in C.2;

— TS28037_GGMR3 runs the numerical example of GGMR described in Annex C EXAMPLE 2 using the orthogonal factorization approach described in C.2.

While prediction and forward evaluation are implemented only in the scripts that solve WLS problems, the MATLAB code corresponding to these uses of the calibration function may be copied and pasted into any of the provided scripts.

F.3 The software should be used in conjunction with this Technical Specification. It is strongly recommended that users study this Technical Specification before running the software.

F.4 The software is provided with a software licence agreement (REF: MSC/L/10/001) and the use of the software is subject to the terms laid out in that agreement. By running the MATLAB code, the user accepts the terms of the agreement. Enquiries about the software should be directed to NPL at enquiries@npl.co.uk.

Annex G
(informative)

Glossary of principal symbols

A	intercept of the straight-line calibration function
A^*	unknown value of A for a particular measuring system
a	estimate of A
$\boldsymbol{a}$	vector $(a, b)^\top$ of parameter estimates
B	slope of the straight-line calibration function
B^*	unknown value of B for a particular measuring system
b	estimate of B
$\mathrm{cov}(a, b)$	covariance associated with a and b
d_i	$x_i - X_i^*$, a realization of a random variable with expectation zero and variance $u^2(x_i)$
e_i	$y_i - Y_i^*$, a realization of a random variable with expectation zero and variance $u^2(y_i)$
$\boldsymbol{L}$	lower-triangular matrix
m	number of measured points
r_i	weighted residual or weighted distance for the ith data point in terms of a and b
R_i	weighted residual or weighted distance for the ith data point expressed algebraically in terms of A and B
$\boldsymbol{U}$	covariance matrix of dimension $2m \times 2m$ associated with measurement data $(x_i, y_i),\ i = 1, \ldots, m$
$\boldsymbol{U_a}$	covariance matrix of dimension 2×2 associated with $\boldsymbol{a}$
$\boldsymbol{U_x}$	covariance matrix of dimension $m \times m$ associated with measurement data $x_i,\ i = 1, \ldots, m$
$\boldsymbol{U_y}$	covariance matrix of dimension $m \times m$ associated with measurement data $y_i,\ i = 1, \ldots, m$
u_R	standard deviation of random variable with distribution encoding knowledge of a random effect
u_S	standard deviation of random variable with distribution encoding knowledge of a systematic effect
$u(z)$	standard uncertainty associated with z, with z denoting a, b, x_i, y_i, etc.
v_i	reciprocal of $u(x_i)$
w_i	reciprocal of $u(y_i)$
X	independent (stimulus) variable
X_i	ith independent (stimulus) variable

X_i^*	unknown value of the ith independent (stimulus) variable provided by a measuring system
x	estimate of X (in the case of prediction) or measured value of X (forward evaluation)
x_i	ith measured value of X
x_i^*	estimate of ith independent (stimulus) variable
Y	dependent (response) variable
Y_i	ith dependent (response) variable
Y_i^*	unknown value of the ith dependent (response) variable provided by a measuring system
y	measured value of Y (in the case of prediction) or estimate of Y (forward evaluation)
y_i	ith measured value of Y
y_i^*	estimate of ith dependent (response) variable
ν	degrees of freedom of a model, a chi-squared distribution or a t-distribution
σ	standard deviation of a random variable characterized by a probability distribution
$\widehat{\sigma}$	posterior estimate of σ
χ^2_{obs}	observed chi-squared value
χ^2_ν	chi-squared distribution with ν degrees of freedom

Bibliography

[1] Anderson, E., Bai, Z., Bischof, C. H., Blackford, S., Demmel, J., Dongarra, J. J., Croz, J. D., l. A. Greenbaum, Hammarling, S., McKenney, A., and Sorensen, D. C. *LAPACK Users' Guide, 3rd ed.,* SIAM, Philadelphia, PA, 1999, http://www.netlib.org/lapack/lug/

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

[3] Boggs, P. T., Byrd, R. H., and Schnabel, R. B. A stable and efficient algorithm for nonlinear orthogonal distance regression, *SIAM J. Sci. Stat. Comput. 8*, 6 (1987), 1052–1078

[4] Butler, B. P., Cox, M. G., Ellison, S. L. R., and Hardcastle, W. A., Eds., *Statistics Software Qualification: Reference Data Sets*, Royal Society of Chemistry, Cambridge, 1996

[5] Carroll, R. J., Ruppert, D., and Stefanski, L. A. *Measurement error in nonlinear models*, Chapman& Hall/CRC, Boca Raton, 1995

[6] Cox, M. G., Forbes, A. B., Harris, P. M., and Smith, I. M. The classification and solution of regression problems for calibration, Tech. Rep. CMSC 24/03, National Physical Laboratory, Teddington, UK, 2003

[7] Draper, N. R., and Smith, H. *Applied Regression Analysis*, Wiley, New York, 1998, Third edition

[8] Forbes, A. B., Harris, P. M., and Smith, I. M. Generalised Gauss-Markov regression, In *Algorithms for Approximation IV* (Huddersfield, UK, 2002), J. Levesley, I. Anderson, and J. C. Mason, Eds., University of Huddersfield, pp. 270–277

[9] Fuller, W. A. *Measurement Error Models*, Wiley, New York, 1987

[10] Golub, G. H., and Van Loan, C. F. *Matrix Computations*, North Oxford Academic, Oxford, 1983

[11] ISO 3534-1:2006, *Statistics – Vocabulary and symbols – Part 1: General statistical terms and terms used in probability*

[12] ISO 3534-2:2006, *Statistics – Vocabulary and symbols – Part 2: Applied statistics*

[13] ISO/IEC Guide 98-3/Suppl. 1, *Uncertainty of measurement – Part 3: Guide to the expression of uncertainty in measurement (GUM:1995) – Supplement 1: Propagation of distributions using a Monte Carlo method*

[14] ISO 11095:1996, *Linear calibration using reference materials*

[15] Kendall, M. G., and Stuart, A. *The Advanced Theory of Statistics, Volume 2: Inference and Relationship.* Charles Griffin, London, 1961.

[16] Kukush, A., and Van Huffel, S. Consistency of elementwise-weighted total least squares estimator in a multivariate errors-in-variables model $AX = B$, *Metrika 59*, 1 (February 2004), 75–97

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

[18] MATLAB http://www.mathworks.com/products/matlab/

[19] Migon, H. S. and Gamerman, D. *Statistical Inference: An Integrated Approach*, Arnold, London, 1999

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

[21] Strang, G., and Borre, K. *Linear Algebra, Geodesy and GPS*, Wiley, Wellesley-Cambridge Press, 1997

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