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Introduction

This draft standard is based on national and international discussions. Your comments on this draft are invited and will assist in the preparation of the consequent standard.

For international standards, comments will be reviewed by the relevant UK national committee before sending the consensus UK vote and comments to the international committee, which will then decide appropriate action. If the international standard is approved, it is usual for the text to be published as a British Standard.

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Template for comments and secretariat observations

Date: xx/xx/20xx	Document: ISO/DIS xxxx
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1	2	(3)	4	5	(6)	7
MB	Clause No./ Subclause No./Annex (e.g. 3.1)	Paragraph/ Figure/Table/Note	Type of comment	Comment (justification for change) by the MB	Proposed change by the MB	Secretariat observations on each comment submitted
	3.1	Definition 1	ed	Definition is ambiguous and needs clarifying.	Amend to read '...so that the mains connector to which no connection...'	
	6.4	Paragraph 2	te	The use of the UV photometer as an alternative cannot be supported as serious problems have been encountered in its use in the UK.	Delete reference to UV photometer.	



DRAFT
International
Standard

ISO/DIS 28037

Determination and use of straight-line calibration functions

Détermination et utilisation des fonctions d'étalonnage linéaire

ICS: 03.120.30

ISO/TC 69/SC 6

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

ISO draws attention to the possibility that the implementation of this document may involve the use of (a) patent(s). ISO takes no position concerning the evidence, validity or applicability of any claimed patent rights in respect thereof. As of the date of publication of this document, ISO *had not* received notice of (a) patent(s) which may be required to implement this document. However, implementers are cautioned that this may not represent the latest information, which may be obtained from the patent database available at www.iso.org/patents. ISO shall not be held responsible for identifying any or all such patent rights.

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For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 69, *Application of statistical methods*, Subcommittee, Subcommittee SC 6, *Measurement methods and results*.

This second edition cancels and replaces the first edition (ISO/TS 28037:2010), which has been technically revised.

The main changes from ISO/TS 28037:2010 are as follows:

- Improved structuring has been implemented throughout and more user-friendly information incorporated.
- Some definitions have been deleted (functional model, structural model) and others have been added (correlation matrix, quotient).
- Some notation has been improved giving closer alignment with the normative references.
- The clause concerned with non-zero cross-covariances $u(x_i, y_j) (i \neq j)$ has been deleted since its occurrence seems not to arise in calibration problems.
- GUM-compliant solutions are provided in the main text for all uncertainty structures considered, with a calculation procedure added as an annex.
- Non-compliant solutions in the TS, which are valid for sufficiently small x -uncertainties, are retained, as annexes, for users who wish to continue to use procedures based on the TS.
- Real-life examples from physics and chemistry illustrating GUM-compliant solutions have added as an annex. Some existing examples in the TS are retained because of bullet 5.
- A few references have been added to support the updated material.
- The annex concerned with the Gauss-Newton algorithm has been removed because the information there can readily be obtained elsewhere (a reference is given).

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Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

Calibration is an essential part of many measurement procedures and often involves fitting to measured data a calibration function that describes the relationship of one variable to another. This document 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, referred to as the parameters of the line. A calibration procedure determines estimates a and b of A and B for a particular measuring system under consideration based on measured data $(x_i, y_i), i = 1, \dots, m$, provided by that system. The measured data have associated uncertainty, which means there will be uncertainty associated with a and b and covariance between them. This document describes how a and b can be estimated given the data and the associated uncertainty information using least-squares' regression methods accounting for that information. It also provides a means for evaluating the uncertainties and covariance associated with these estimates.

The treatment of uncertainty in this document is carried out in a manner compliant with ISO/IEC Guide 98-3:2008, 'Guide to the expression of uncertainty in measurement' (GUM) and other guides in the ISO/IEC Guide 98-3 series. 'GUM-compliance' in this document is described as follows. A characterization of the solution is the set of nonlinear equations given by equating to zero the partial derivatives of the least-squares objective function with respect to the parameters of the regression model. These equations constitute an implicit multivariate model: see Clause 6.3 of ISO Guide 98-3 Suppl. 2. Accordingly, estimates of the model parameters are given by solving those equations and their associated covariance matrix by expression (4) in that clause (also, see [25]).

Given the uncertainty information associated with the measured data, an appropriate method is used to estimate the calibration function parameters. This uncertainty information may include quantified covariance effects, relating to dependencies among some or all the quantities involved.

Once the straight-line model has been fitted to the data, it is necessary to determine whether the model and data are mutually consistent. 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, and to evaluate the uncertainty associated with x .

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

1. Obtaining measured data and associated uncertainty and covariance information.
2. Providing estimates of the straight-line parameters accounting for the information in Step 1.
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?).
4. Obtaining the standard uncertainties and covariance associated with the estimates of the straight-line parameters.
5. Using the calibration function for inverse evaluation (also sometimes known as '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. An estimate y of the Y -variable and its associated uncertainty given a value x of the X -variable, a process known as forward evaluation, and its associated uncertainty can also be determined.

Examples are provided, some from various areas of measurement and some synthetic.

[Figure 1](#) shows a related dependency chart.

Inputs

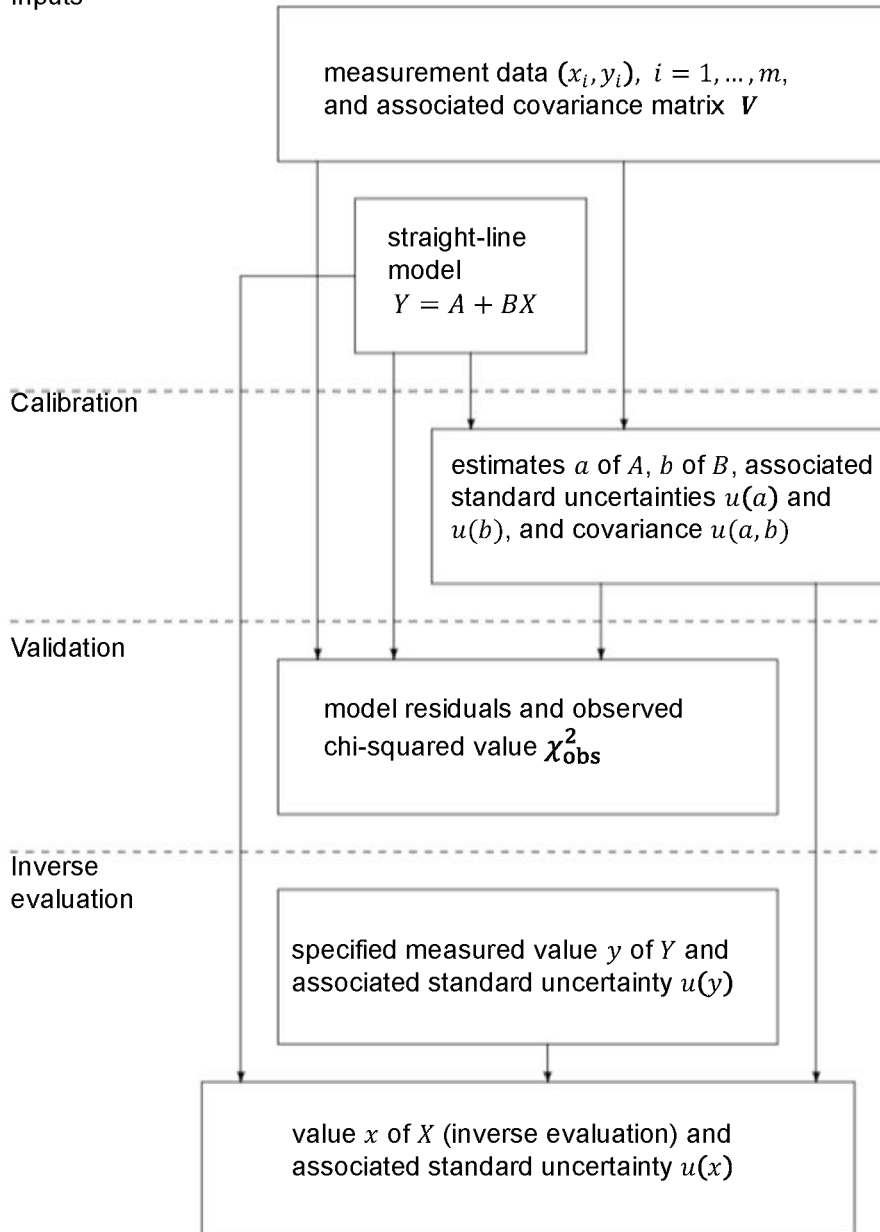


Figure 1 — Dependency chart for determining and using straight-line calibration functions

The main aim of this document is the consideration of Steps 2 to 5. Therefore, as part of Step 1, before using this document, 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. Some guidance is given in [Annex C](#). Account is taken of the principles of the GUM in evaluating these uncertainties based on a measurement model that is specific to the input uncertainty structure.

ISO 11095:1996^[20] is concerned with linear calibration using reference materials. It differs from this document in the ways given in [Table 1](#). For example, the present document addresses data x -values that may not be known exactly but their associated uncertainties and, when appropriate, covariances are provided. Moreover, the systematic errors in the data may be appreciable. In the present document. Ways to account for such effects are given.

Table 1 — Differences between ISO 11095:1996 and this document

Feature	ISO 11095:1996	This document
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	Not totally	Yes
Types of uncertainty structure treated	Two	Four, including the most general case
Only uncertainty associated with random errors	Yes	More general uncertainty information
Consistency test	ANOVA	Chi-squared
Uncertainty associated with inverse evaluation	Ad hoc	GUM-compliant

The provisions of this international standard are supported by several informative annexes:

[Annex A](#): Matrix operations and definitions used in this document.

[Annex B](#): Orthogonal factorization approach to solving the generalized Gauss-Markov problem.

[Annex C](#): Provision of uncertainties and covariances associated with the measured data.

[Annex D](#): Uncertainties known only up to a scale factor.

[Annex E](#): Examples illustrating straight-line regression for all uncertainty structures.

[Annex F](#): GUM-compliant straight-line parameter uncertainties in the errors-in-variables' case.

[Annex G](#): Non-GUM-compliant calculation procedures.

[Annex H](#): Software implementations.

[Annex I](#): Glossary of principal symbols.

Determination and use of straight-line calibration functions

1 Scope

This document 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 estimated based on measured data points (x_i, y_i) , $i = 1, \dots, m$. 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 document is on using the method most appropriate for the type of measured data, that is, respecting the associated uncertainties. The most general type of covariance matrix associated with the measured 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 document also describes the use of the estimates of the calibration-function parameter 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 document does not give a general treatment of outliers in measured data, although the validation tests given can be used to indicate discrepant data. ISO 16269-4:2010 Statistical interpretation of data – Part 4: Detection and treatment of outliers can be consulted for guidance.

NOTE 2 The document describes a method to evaluate the uncertainties associated with the measured data when those uncertainties are known only up to a scale factor ([Annex D](#)).

Software to support this standard is available. See [Annex H](#).

2 Normative references

The following documents are referred to in the text in such a way that some or all their content constitutes requirements 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 98-3:2008, *Uncertainty of measurement — Part 3: Guide to the expression of uncertainty in measurement (GUM:1995)*

ISO/IEC Guide 99:2012, *International vocabulary of metrology — Basic and general concepts and associated terms (VIM)*

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 99:2012 and the following apply.

NOTE ISO/IEC Guide 99:2012 uses the term ‘measured quantity value’. Here, the term ‘measured value’, which will be used in future versions of ISO/IEC Guide 99, is adopted when there is no ambiguity. Similarly, ‘standard uncertainty’ is used instead of ‘standard measurement uncertainty’ and ‘covariance matrix’ instead of ‘measurement covariance matrix’.

A glossary of principal symbols is given in [Annex I](#).

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

- ISO Online browsing platform: available at <https://www.iso.org/obp>
- IEC Electropedia: available at <https://www.electropedia.org/>

3.1

measured quantity value

quantity value representing a measurement result

[SOURCE: ISO/IEC Guide 99:2012 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

[SOURCE: ISO/IEC Guide 99:2012 2.26]

3.3

standard measurement uncertainty

measurement uncertainty expressed as a standard deviation

[SOURCE: ISO/IEC Guide 99:2012 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

[SOURCE: ISO/IEC Guide 98-3:2008/Suppl. 1:2008, definition 3.10]

3.5

measurement 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 estimate of the quantity, and, in its off-diagonal positions, the covariances associated with pairs of components of the estimate of the quantity

Note 1 to entry: A covariance matrix V_x of dimension $N \times N$ associated with the vector estimate x of a vector quantity X has the representation.

$$V_x = \begin{bmatrix} u(x_1, x_1) & \cdots & u(x_1, x_N) \\ \vdots & \ddots & \vdots \\ u(x_N, x_1) & \cdots & u(x_N, x_N) \end{bmatrix},$$

[SOURCE: ISO/IEC Guide 98-3:2008/Suppl. 2:2011, definition 3.20]

3.6

correlation matrix

symmetric positive-definite matrix of dimension $N \times N$ associated with an estimate of a vector quantity of dimension $N \times 1$, containing the correlations associated with pairs of components of the estimate

Note 1 to entry: A correlation matrix $\mathbf{R}_x$ of dimension $N \times N$ associated with the estimate $\mathbf{x}$ of a vector quantity $\mathbf{X}$ has the representation

$$\mathbf{R}_x = \begin{bmatrix} r(x_1, x_1) & \cdots & r(x_1, x_N) \\ \vdots & \ddots & \vdots \\ r(x_N, x_1) & \cdots & r(x_N, x_N) \end{bmatrix},$$

where $r(x_i, x_i) = 1$ and $r(x_i, x_j)$ is the correlation associated with x_i and x_j . When elements X_i and X_j of $\mathbf{X}$ are uncorrelated, $r(x_i, x_j) = 0$.

Note 2 to entry: Correlations are also known as correlation coefficients.

Note 3 to entry: $\mathbf{R}_x$ is related to the covariance matrix $\mathbf{V}_x$ (see [definition 3.5](#)) by

$$\mathbf{R}_x = \mathbf{D}_x \mathbf{V}_x \mathbf{D}_x,$$

where $\mathbf{D}_x$ is a diagonal matrix of dimension $N \times N$ with diagonal elements $u^{-1}(x_1), \dots, u^{-1}(x_N)$. Element (i, j) of $\mathbf{R}_x$ is

$$r(x_i, x_j) = u(x_i, x_j) / [u(x_i)u(x_j)].$$

[SOURCE: ISO/IEC Guide 98-3:2008/Suppl. 2:2011, 3.21, slightly modified, Notes 4 and 5 deleted.]

3.7

measurement model

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

[SOURCE: ISO/IEC Guide 99:2012 2.48]

3.8

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 to entry: 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 to entry: Calibration does not relate to the adjustment of a measuring system, often mistakenly called 'self-calibration', nor with verification of calibration.

Note 3 to entry: Often the first step alone in the above definition is perceived as being calibration.

[SOURCE: ISO/IEC Guide 99:2012 2.39]

3.9

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 to entry: The probability on the whole set of values of the random variable equals 1.

Note 2 to entry: 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 to entry: A probability distribution can take the form of a distribution function or a probability density function.

Note 4 to entry: Definition and note 1 are adapted from ISO 3534-1:1993, definition 1.3 and ISO/IEC Guide 98 3:2008, definition C.2.3; notes 2 and 3 are adapted from ISO/IEC Guide 98 3:2008/Suppl. 1:2008, definition 3.1^[16].

3.10

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 to entry: μ is the expectation and σ is the standard deviation of X .

Note 2 to entry: The normal distribution is also known as the Gaussian distribution.

Note 3 to entry: 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.

3.11

t-distribution

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

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

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

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

is the gamma function

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

3.12

chi-squared distribution

probability distribution of a continuous random variable X having the χ^2 probability density function

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

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

Note 1 to entry: 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.

3.13

positive definite matrix

matrix M of dimension $n \times n$ having the property $z^T M z > 0$ for all non-zero vectors z of dimension $n \times 1$

3.14**positive semi-definite matrix**

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

3.15**quotient**

value of N_1 / N_2 resulting from the division of the real number N_1 by the real number N_2

Note 1 to entry: 'Ratio' is not a synonym for 'quotient', the former being a statement of the relative proportions of two numbers in the form $N_1 : N_2$. To illustrate, for $N_1 = 9$ and $N_2 = 16$, their quotient is $9/16 = 0,5625$ and their ratio is 9:16.

4 Conventions and notation

The following conventions and notation are adopted in this document.

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.

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 random variables in expressions involving the calibration function parameters.

The quantities X_i and Y_i are used as random variables to denote the coordinates of the i th data point, $i = 1, \dots, m$.

The constants x_i and y_i are the measured values of the coordinates of the i th data point X_i and Y_i .

The constants x_i^* and y_i^* are estimates of the coordinates of the i th data point X_i and Y_i .

The constants a and b are estimates of A and B that specify the straight-line calibration function for a particular measuring system.

The constants a , b , x_i^* and y_i^* satisfy $y_i^* = a + bx_i^*$, $i = 1, \dots, m$.

The constants a and b specify the estimated (fitted) straight-line calibration function $Y = a + bX$ for a particular measuring system.

A vector of dimension $m \times 1$ and its transpose are generically denoted by

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}, \quad \mathbf{x}^\top = [x_1 \quad \dots \quad x_m],$$

where $^\top$ denotes transpose, and a matrix of dimension $m \times n$ by

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

The dimension of a vector or matrix is often specified to avoid possible confusion.

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

In matrices, a zero element is often indicated by a blank. A zero submatrix is often indicated by $\mathbf{0}$.

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

Numbers displayed in tables to a given number of decimal places are correctly rounded representations of numbers stored to higher numerical precision, as would be the case in a spreadsheet, for example. Therefore,

minor inconsistencies may be perceived, for instance, between displayed column sums and the column sums of the displayed numbers.

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

The mathematical symbols used in [Annex A](#) and [Annex B](#) have generally a different interpretation from those in the bulk of this document,

In the examples, while data values are provided to a given numerical precision, the results of calculations are sometimes 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

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 measured data. In the context of calibration, the measured 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 x_i of X_i given in standard units, of a property of the artefacts, and the corresponding 'responses' or indications y_i of 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'.

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

5.2 Inputs to determining the calibration function

5.2.1 Measured data

The information required to determine the straight-line calibration function is the measured data and their associated standard uncertainties and covariances. In this document, the measured data are denoted by (x_i, y_i) , $i = 1, \dots, m$, that is, m pairs of measured values of X and Y . It is assumed that m is at least two and at least two of the x_i are distinct.

NOTE 1 The uncertainties associated with the estimates a and b generally decrease as m increases. Therefore, calibration aims to use as many measured data points as is economically viable.

NOTE 2 It is beyond the scope of this document to consider strategies for selecting the measured points. For this purpose, references on the theory of optimal experimental design such as [\[29\]](#) can be consulted. Often, however, the choice of measured points is dictated by the calibration experiment.

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 $u(x_i, x_j)$. Similarly, the covariances associated with y_i and y_j , and with x_i and y_j , are denoted by $u(y_i, y_j)$ and $u(x_i, y_j)$, respectively. [Annex C](#) 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) V of dimension $2m \times 2m$ holding the variances (squared standard uncertainties) $u^2(x_i)$ and $u^2(y_i)$ and the covariances:

$$V = \begin{bmatrix} u^2(x_1) & \dots & u(x_1, x_m) & u(x_1, y_1) & \dots & u(x_1, y_m) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ u(x_m, x_1) & \dots & u^2(x_m) & u(x_m, y_1) & \dots & u(x_m, y_m) \\ u(y_1, x_1) & \dots & u(y_1, x_m) & u^2(y_1) & \dots & u(y_1, y_m) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ u(y_m, x_1) & \dots & u(y_m, x_m) & u(y_m, y_1) & \dots & u^2(y_m) \end{bmatrix}.$$

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

NOTE 1 This document is concerned with problems in which the $u(x_i)$ and the $u(y_i)$ can take any appropriate values.

NOTE 2 The data x_i and y_i and the associated uncertainties and covariances are assumed to be the only input information available.

5.3 Determining the calibration function

5.3.1 Line parameters

The inputs to determining the calibration function are the measured data and their associated uncertainties and possibly covariances. The inputs can be used to provide a measure of the departure of the i th data point (x_i, y_i) from the line $Y = A + BX$. The estimates a and b of A and B are determined by minimizing a weighted sum of squares of these departures, or a more general measure when any covariances are non-zero. The way this computation is carried out depends on the 'uncertainty structure' associated with the measured 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 Input uncertainty information

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 document:

- 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) 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 8](#)).
- d) Uncertainties are associated with the measured value x_i and y_i and covariances associated with all pairs of values of the x_i and the x_j and with the y_k and the y_ℓ (the most general case considered, [Clause 9](#)).

The case of non-zero cross-covariances $u(x_i, y_j)$ ($i \neq j$) is not considered since its occurrence is extremely rare in calibration problems. The covariance matrix in 5.2.2 accordingly reduces to

$$V = \begin{bmatrix} V_x & \\ & V_y \end{bmatrix},$$

where V_x is the covariance matrix associated with the x_i and V_y that associated with the y_i .

NOTE In all cases, it is assumed that no further information is available.

Given for each case are:

- (i) the prescribed measured data and uncertainty structure,
- (ii) the corresponding statistical model,
- (iii) the least-squares' problem addressed,
- (iv) the calculation steps,
- (v) properties of the statistical model,
- (vi) validation of the model,
- (vii) organization of the calculations for the computer, where appropriate,
- (viii) a numerical algorithm, where appropriate, and
- (ix) one or more worked examples.

5.3.3 Output uncertainty information

In the Technical Specification ISO/TS 28037 that preceded this standard, provision of uncertainties and covariance associated with the estimated line parameters a and b was not entirely compliant with the provisions of ISO/IEC Guide 98-3:2008 (GUM), which applies predominantly to linear measurement models. For cases a) and c) in 5.3.2, they were compliant since a and b depending linearly on the input values x_i and y_i . For cases b) and d) in 5.3.2, provision of uncertainties and covariance associated with a and b were not GUM-compliant in ISO/TS 28037 since the dependence is nonlinear. GUM-compliant uncertainties are provided in this document for these cases. For compatibility with ISO/TS 28037 and users who wish to continue with its provisions, the non-compliant treatments are also given in this document. That treatment is adequate for sufficiently small input uncertainties^[22].

5.4 Numerical treatment

In clause 9, an approach to the most general case d) in 5.3.2 is given. It can be used to treat all the other cases and uses sophisticated numerical methods. The cases a) and c) in 5.3.2 can, however, be treated using elementary operations, which can be implemented in a spreadsheet, for example. The cases b) and d) 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 Line parameter uncertainties

Following the GUM, the intercept A and slope B in straight-line regression can be estimated and their uncertainties evaluated once a relevant measurement model has been specified. Equations that specify such a measurement model are obtained by equating to zero the first order partial derivatives of a (generalized) least-squares' objective function that depends on the nature of the uncertainties associated with the measured data [see cases a) to d) in 5.3.2]. For cases a) and c) in 5.3.2, the line parameters A and B can be

expressed explicitly and linearly in terms of the input data with the result that the law of propagation of uncertainty in the GUM can be applied directly and exactly to evaluate the standard uncertainties $u(a)$ and $u(b)$ and the covariance $u(a,b)$.

For cases b) and d) in 5.3.2, A and B cannot be expressed explicitly and linearly in terms of the input data. To provide estimates a and b of A and B not only requires iterative solution but it is more complicated to evaluate $u(a)$, $u(b)$ and $u(a,b)$. The forerunner ISO/TS 28037:2010 to this International Standard provided an approximate evaluation of $u(a)$, $u(b)$ and $u(a,b)$ in those cases. That evaluation is not GUM-compliant although adequate when the input uncertainties are sufficiently small. A general relationship between the magnitudes of the input uncertainties and the extent of the approximation is not available (but see [22] for useful information). However, this document provides a solution that is GUM-compliant. In that solution, the sensitivity coefficients, that is, the first-order partial derivatives of a and b with respect to the inputs are evaluated at the x - and y -data as required by the law of propagation of uncertainty.

The body of this document contains exact propagation according to the GUM, whereas the approximate propagation (as in ISO/TS 28037:2010) is given in informative annexes for compatibility with the TS, which is now withdrawn.

NOTE 1 These approximate uncertainty evaluations are retained for users who consider them fit for purpose and so avoid the increased complexity of the GUM-compliant evaluations.

NOTE 2 An alternative treatment, also avoiding the complexity of the calculation, is the use of a Monte Carlo approach based on the propagation of distributions (not treated in this document). See ISO/IEC Guides 98-3:2008/Suppl. 1:2008 and 98-3:2008/Suppl. 2:2011].

5.5.2 Primary outputs

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

$$\mathbf{a} = \begin{bmatrix} a \\ b \end{bmatrix}, \quad \mathbf{V}_a = \begin{bmatrix} u^2(a) & u(a,b) \\ u(b,a) & u^2(b) \end{bmatrix}.$$

5.6 Validation of the model

5.6.1 Departure of data points from fitted calibration function

In determining 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 measured data give a credible measure of the departure of the measured data from a straight line. Once a and b have been determined, the actual departure of the data points from the fitted 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_{obs}^2 of m weighted residuals, the i th weighted residual being a measure of the departure of the i th data point from the line, or, when the covariance associated with the i th data point (x_i, y_i) is non-zero, a more general form. If χ_{obs}^2 is much larger than expected, on statistical grounds there is reason to question the validity of the model assumptions.

NOTE The R-squared statistic, also a measure of the goodness of fit of a model, could be used instead of chi-squared. However, it does not account for uncertainties in the data, the main rationale for this document.

5.6.2 Testing under normality

Statistically, the measured 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_{obs}^2 , regarded as a draw from this aggregate distribution, exceeded any specified 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_v^2 with $\nu = m - 2$ degrees of freedom. Accordingly, the probability that χ_{obs}^2 exceeds any specified quantile of χ_v^2 can be determined (see [6.3](#), [7.3](#), [8.3](#) and [9.3](#)). The 95 % quantile is used.

NOTE 1 If χ_{obs}^2 exceeds the 95 % quantile of χ_v^2 , 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 can 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 contemplated. See ISO/TS 28038:2018^[21] for the determination and use of polynomial calibration functions.

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

5.6.3 Relevance of prior uncertainty information

To obtain as much value as possible from a calibration, it is highly desirable that input uncertainties are derived prior to estimating 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 D](#).

5.6.4 Failure of model validation

If, in any particular case, the validation of the model fails, that is, χ_{obs}^2 exceeds the 95 % quantile of χ_v^2 , the calculated standard uncertainties $u(a)$ and $u(b)$ and covariance $u(a,b)$ (see [Clause 5.5.2](#)) should be regarded as unreliable, as should the uncertainty associated with use of the calibration function (see [Clause 5.7](#)).

5.7 Use of the calibration function

5.7.1 Inverse evaluation

The calibration function is typically used for inverse evaluation given an estimate of Y and its associated standard uncertainty, the corresponding value of X is estimated and its associated standard uncertainty 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 [10.2](#).

5.7.2 Forward evaluation

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 [10.3](#).

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

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

5.8.1 Ordinary least-squares objective function

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

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

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

5.8.2 Steps in the calculation

The estimates a and b can be calculated in the following steps:

1. $x_0 = \frac{1}{m} \sum_{i=1}^m x_i$;
2. $y_0 = \frac{1}{m} \sum_{i=1}^m y_i$;
3. $\tilde{x}_i = x_i - x_0$, $i = 1, \dots, m$;
4. $\tilde{y}_i = y_i - y_0$, $i = 1, \dots, m$;
5. $b = \frac{\sum_{i=1}^m \tilde{x}_i \tilde{y}_i}{\sum_{i=1}^m \tilde{x}_i^2}$;
6. $a = y_0 - bx_0$.

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

NOTE Mathematically, estimates a and b of the parameters of the straight line 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 and generally more reliably. Translating the data also has a beneficial effect in terms of numerical accuracy of the computed solution ([4], page 33).

5.8.3 Extension to other forms of input uncertainty information

The methods described in [Clauses 6](#) to [9](#) constitute extensions of the calculations in this clause that use the prescribed uncertainty information.

6 Uncertainties associated with the response data only and no covariance

6.1 Model

6.1.1 Input information

This clause considers the case a) in [5.3.2](#), namely, when the following values are provided for $i = 1, \dots, m$, there is no uncertainty associated with the x -values and no covariance associated with the data:

- a) measured data (x_i, y_i) , and
- b) standard uncertainty $u(y_i)$ associated with y_i .

[Annex C](#) provides guidance on obtaining these uncertainties. All other uncertainties and covariances associated with the data are regarded as negligible.

6.1.2 Statistical model

Case a) in [5.3.2](#) corresponds to that described by the statistical model

$$y_i = A + Bx_i + e_i, \quad i = 1, \dots, m,$$

where the e_i are realizations of independent random variables with expectations zero and variances $u^2(y_i)$ ([11] page 1), and A and B are the calibration function parameters for the measuring system for which a calibration is required and which provides the measured data. This model has no uncertainty associated with the x_i .

6.1.3 Objective function

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

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

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 this expression with respect to A and B .

6.2 Calibration parameter estimates and associated standard uncertainties and covariance

6.2.1 Steps in the calculation

Estimates a and b are calculated in Steps 1 to 5; the standard uncertainties $u(a)$ and $u(b)$ and covariance $u(a, b)$ are evaluated in Step 6. Set

1. Set $w_i = \frac{1}{u(y_i)}$, $i = 1, \dots, m$, and $F^2 = \sum_{i=1}^m w_i^2$;
2. Set $g_0 = \frac{1}{F^2} \sum_{i=1}^m w_i^2 x_i$ and $h_0 = \frac{1}{F^2} \sum_{i=1}^m w_i^2 y_i$;
3. Set $g_i = w_i (x_i - g_0)$, $i = 1, \dots, m$, and $h_i = w_i (y_i - h_0)$, $i = 1, \dots, m$;
4. Set $G^2 = \sum_{i=1}^m g_i^2$;
5. Set $b = \frac{1}{G^2} \sum_{i=1}^m g_i h_i$ and $a = h_0 - b g_0$;
6. Set $u^2(a) = \frac{1}{F^2} + \frac{g_0^2}{G^2}$, $u^2(b) = \frac{1}{G^2}$ and $u(a, b) = -\frac{g_0}{G^2}$.

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

$$i) \quad \text{Set } w_i = \frac{1}{u(y_i)}, \quad i = 1, \dots, m, \quad x_0 = \frac{\sum_{i=1}^m w_i^2 x_i}{\sum_{i=1}^m w_i^2} \text{ and } y_0 = \frac{\sum_{i=1}^m w_i^2 y_i}{\sum_{i=1}^m w_i^2};$$

$$ii) \quad \text{Set } \check{x}_i = x_i - x_0, \quad i = 1, \dots, m, \text{ and } \check{y}_i = y_i - y_0, \quad i = 1, \dots, m;$$

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

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

$$w_i a + w_i x_i b = w_i y_i, \quad i = 1, \dots, m.$$

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 line fit in [5.8.2](#).

NOTE 4 The first part of Step 2 may alternatively be re-expressed as $g_0 = \sum_{i=1}^m (w_i^2 / F^2) x_i$. Since floating-point error analyses indicate the numerical stability of both formulae is comparable, either can be used. A similar remark can be made concerning h_0 in Step 2 and other formulae elsewhere in this document. Regarding the possibility of overflow or underflow in such calculations, it is the user's responsibility to ensure sensible scaling of the data. Calibration data is nearly always such that the risk of overflow or underflow is extremely small.

NOTE $u^2(a)$, $u^2(b)$ and $u(a, b)$ 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 Solution properties

The estimates a and b determined in [6.2.1](#) have the following properties^[23] for data y_i according to the model in [6.1.2](#):

- 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 to estimate A and B that specify the straight-line calibration function for a particular measuring system.
- iii) The covariance matrix for the random variables in ii) is specified by $u^2(a)$, $u^2(b)$ and $u(a, b)$.

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 constants a and b specify the estimated (fitted) straight-line calibration function $Y = a + bX$ for a particular measuring system.

The estimation method of [6.2.1](#) has the following optimal property for data y_i according to the model in [6.1.2](#):

- iv) The estimates $\check{a}$ and $\check{b}$ 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 $u(c\check{a} + d\check{b})$ associated with a linear combination of the estimates $\check{a}$ and $\check{b}$ 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 in [6.1.2](#). 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, 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 $u(a,b)$.
- 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 measured data y_i .
- vii) Because of properties i) and v), and the x_i being exact, the probability distribution for A and B is bivariate normal centred on a and b with covariance matrix specified by $u^2(a)$, $u^2(b)$ and $u(a,b)$.

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 $r_i = w_i (y_i - a - bx_i)$, $i = 1, \dots, m$;
8. Form the observed chi-squared value $\chi_{\text{obs}}^2 = \sum_{i=1}^m r_i^2$ and degrees of freedom $\nu = m - 2$;
9. Check whether χ_{obs}^2 exceeds the 95 % quantile of χ_{ν}^2 , and if it does reject the straight-line model.

NOTE The chi-squared test is a test of the hypothesis that the measured data (a) can be modelled by a straight line and (b) errors in the data are regarded as drawn from a multivariate normal distribution consistent with the specified uncertainty structure. A significant chi-squared value indicates that (a) or (b) or both do not apply.

6.4 Organization of the calculation

The calculations in 6.2.1 and 6.3 can be organized into one or two tableaux for implementation in a spreadsheet as in Table 2 and Table 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	$u(y_1)$
$\vdots$	$\vdots$	$\vdots$
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
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
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
$F^2 = \sum w_i^2$		$\sum w_i^2 x_i$	$\sum w_i^2 y_i$	$G^2 = \sum g_i^2$		$\sum g_i h_i$	b	$\chi_{\text{obs}}^2 = \sum r_i^2$

6.5 Illustrative examples

Examples of application of the provisions of this annex are given in E.2.

7 Uncertainties associated with the stimulus and the response data and no covariance

7.1 Model

7.1.1 Input information

This clause considers case b) in [5.3.2](#), namely, when the following are provided for $i=1, \dots, m$ and there is no or negligible covariance:

- a) measured 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 C](#) provides guidance on obtaining these input uncertainties.

7.1.2 Statistical model

Case b) in [5.3.2](#) corresponds to that described by the statistical model

$$x_i = X_i + d_i, \quad y_i = Y_i + e_i, \quad Y_i = A + BX_i, \quad i = 1, \dots, m, \quad (1)$$

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. In the model, (x_i, y_i) represent the measured coordinates of the (unobserved) point (X_i, Y_i) lying on the line $Y = A + BX$.

7.1.3 Objective function

7.1.3.1 General

As the x_i (in addition to the y_i) 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)^[4] or generalized distance regression (GDR).^[3] In the statistical literature it is referred to as an errors-in-variables model^{[10], [12]} page 50^[26], page 189. The estimates a and b are those that minimize the sum of squares

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

with respect to A, B and X_i , $i = 1, \dots, m$, for weights $v_i = 1/u(x_i)$ and $w_i = 1/u(y_i)$. Here, a and b , along with the x_i^* , specify the line $y_i^* = a + bx_i^*$ with the point (x_i^*, y_i^*) estimating (X_i, Y_i) in model (1).

7.1.3.2 Reduced objective function

In terms of A and B , the values x_i^* that minimize the sum of squares) with respect to X_i are

$$x_i^* = x_i^*(A, B) = \left[x_i u^2(y_i) + (y_i - A) B u^2(x_i) \right] T_i, \quad T_i = \frac{1}{u^2(y_i) + B^2 u^2(x_i)}. \quad (3)$$