International Standard

ISO 28037

Determination and use of straight-line calibration functions

Détermination et utilisation des fonctions d'étalonnage linéaire

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ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Email: copyright@iso.org
Website: www.iso.org

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

The main changes are as follows:

— improved structuring has been implemented throughout and more user-friendly information incorporated;

— some definitions have been removed (functional model, structural model, etc.) 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 $\left(x_i, y_j\right)$ $(i \neq j)$ has been deleted since its occurrence seems not to arise in calibration problems;

— GUM-consistent solutions are provided in the main text for all uncertainty structures considered, with a calculation procedure added as an annex;

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— solutions in the withdrawn TS, which are strictly inconsistent with the GUM, are valid for sufficiently small x-uncertainties and 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-consistent solutions have been added as an annex. Some existing examples in the TS are retained because of the preceding bullet;

— some 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).

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.

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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 $(x_i, y_i), i = 1, \ldots, m$, 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 way consistent with ISO/IEC Guide 98-3 and other guides in the ISO/IEC Guide 98 series. 'GUM-consistency' 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 generally constitute an implicit multivariate model: see ISO Guide 98-3:2008, Suppl.2., 6.3. 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 Reference [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:

a) Obtaining measured data and associated uncertainty and covariance information.

b) Providing estimates of the straight-line parameters accounting for the information in Step a).

c) 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?).

d) Obtaining the standard uncertainties and covariance associated with the estimates of the straight-line parameters.

e) 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.

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Figure 1 shows a related dependency chart.

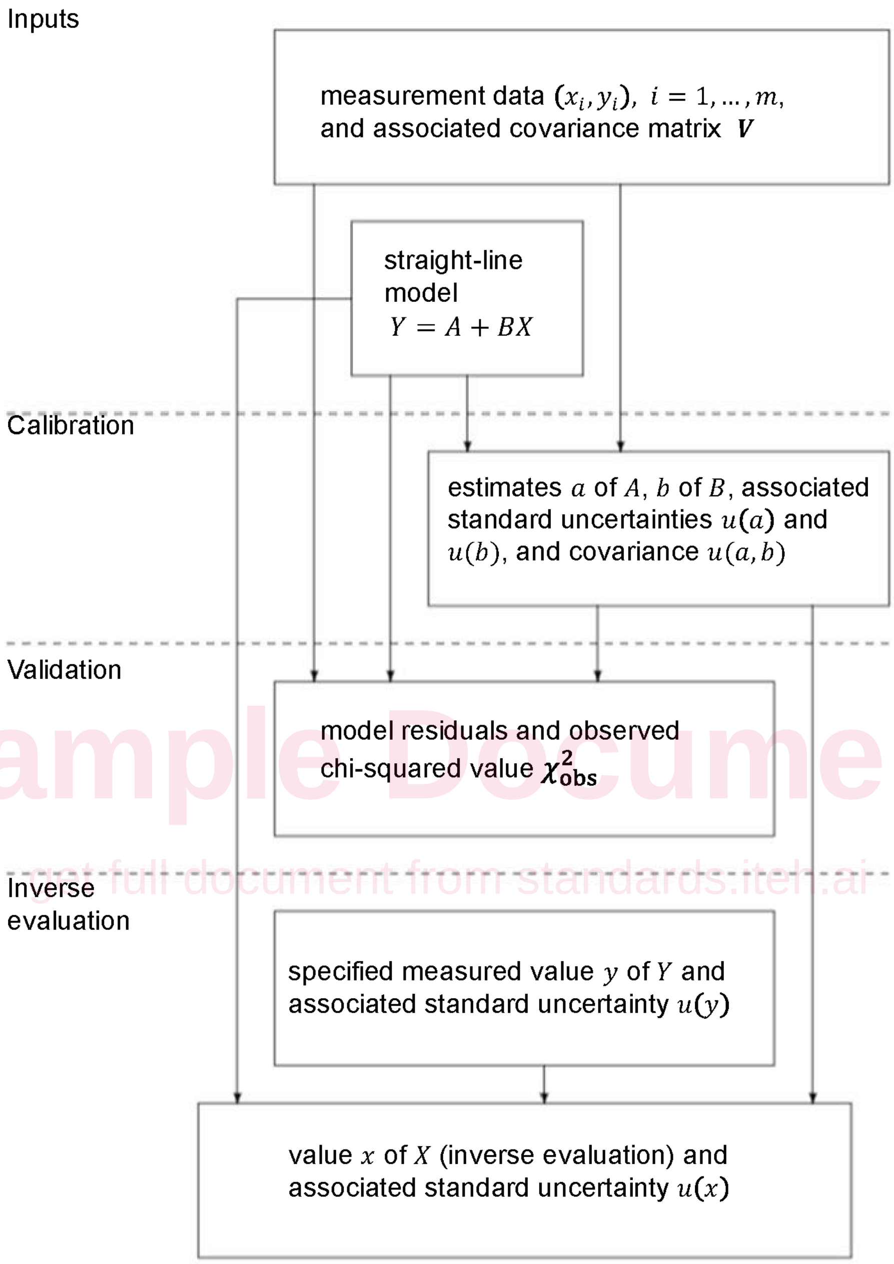

Figure 1 — Dependency chart for determining and using straight-line calibration functions

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

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are provided. Moreover, the systematic errors in the data may be appreciable. 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-consistent

The provisions of this document are supported by Annexes A to H:

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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), $i = 1, \ldots m$. 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 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.

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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.

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The document also describes the use of the estimates of the calibration-function parameters 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 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 (see Annex D).

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 3534-1, *Statistics — Vocabulary and symbols — Part 1: Probability and general statistical terms*

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

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

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3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 3534-1, ISO/IEC Guide 98-3 and ISO/IEC Guide 99 and the following apply.

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/

NOTE ISO/IEC Guide 99 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'.

3.1
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 $\boldsymbol{R_x}$ of dimension $N \times N$ associated with the estimate $\boldsymbol{x}$ of a vector quantity $\boldsymbol{X}$ has the representation

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$$\boldsymbol{R_x} = \begin{bmatrix} r(x_1,x_1) & \cdots & r(x_1,x_N) \\ \vdots & \ddots & \vdots \\ r(x_N,x_1) & \cdots & r(x_N,x_N) \end{bmatrix},$$

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

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

Note 3 to entry: $\boldsymbol{R_x}$ is related to the covariance matrix $\boldsymbol{V_x}$ by

$$\boldsymbol{R_x} = \boldsymbol{D_x} \boldsymbol{V_x} \boldsymbol{D_x},$$

where $\boldsymbol{D_x}$ is a diagonal matrix of dimension $N \times N$ with diagonal elements $u^{-1}(x_1),\ldots,u^{-1}(x_N)$ and $u(x_i)$ is the standard uncertainty associated with x_i. Element (i,j) of $\boldsymbol{R_x}$, with $u(x_i,y_i)$ the covariance associated with x_i and x_j, is

$$r(x_i,x_j) = \frac{u(x_i,x_j)}{\left[u(x_i)u(x_j)\right]},$$

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

3.2
normal distribution
probability distribution of a continuous random variable X having the probability density function

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

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.

3.3
***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

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

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is the gamma function

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

3.4
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 $0 \le \xi < \infty$, 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, *termed* the degrees of freedom.

3.5
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 $n \times 1$

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3.6
positive semi-definite matrix

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

3.7
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 = 0,562 5 and their ratio is 9:16.

4 Conventions and notation

4.1 General

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.

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

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

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

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

a, b, and the x_i^* and y_i^* satisfy $y_i^* = a + bx_i^*$, $i = 1, ..., m$.

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

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}, \quad \boldsymbol{x}^{\bullet} = \begin{bmatrix} x_1 & \ldots & x_m \end{bmatrix},$$

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

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & \ldots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \ldots & a_{mn} \end{bmatrix}, \quad \boldsymbol{A}^{\bullet} = \begin{bmatrix} a_{11} & \ldots & a_{m1} \\ \vdots & \ddots & \vdots \\ a_{1n} & \ldots & a_{mn} \end{bmatrix}.$$

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

The zero matrix or vector is denoted by **0** and the unit vector by **1**.

In matrices, a zero element is often indicated by a blank. A zero submatrix is often indicated by **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.

4.2 Symbols

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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 $(a,b)^{\bullet}$ 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
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 in terms of A and B
u_{R}	standard deviation of random variable with distribution encoding knowledge of a random effect
u_{S}	as for u_{R} but for distribution encoding knowledge of a systematic effect
$u(z)$	standard uncertainty associated with z denoting a, b, x_i, y_i, etc.
$u(a,b)$	covariance associated with a and b
$\boldsymbol{V}$	covariance matrix of dimension $2m \times 2m$ associated with the data $(x_i, y_i), i = 1, \ldots, m$
$\boldsymbol{V_a}$	covariance matrix of dimension 2×2 associated with $\boldsymbol{a}$

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