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# Determination and use of polynomial calibration functions

*Détermination et utilisation des fonctions d'étalonnage polynômial*



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# Contents

# Foreword

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

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# Introduction

**0.1** Calibration is central to measurement science and involves fitting to measured data a function that describes the relationship of a response (dependent) variable $y$ to a stimulus (independent) variable $x$. It also involves the use of that calibration function. This document considers calibration functions in the form of polynomial models that depend on a set of parameters (coefficients). The purpose of a calibration procedure is the following.

a) To estimate the parameters of the calibration function given suitable calibration data provided by a measuring system and evaluate the covariance matrix associated with these parameter estimates. Any uncertainties provided with the data are taken into consideration.

b) To use an accepted calibration function for inverse evaluation, that is, to determine the stimulus value corresponding to a further measured response value, and also to obtain the stimulus value standard uncertainty given the response value standard uncertainty. A calibration function is sometimes used for direct evaluation, that is, to determine the response value corresponding to a further stimulus value, and also to obtain the response value standard uncertainty given the stimulus value standard uncertainty.

This document describes how these calculations can be undertaken using recognized algorithms. It provides examples from a number of disciplines: absorbed dose determination (NPL), flow meter characterization (INRIM), natural gas analysis (VSL), resistance thermometry (DFM) and isotope-based quantitation (NRC).



**0.2** The nature of the calibration data uncertainty information influences the manner in which the calibration function parameters are estimated and how their associated covariance matrix is provided. This uncertainty information may include quantified measurement covariance effects relating to dependencies among the quantities involved.



**0.3** Since in any particular instance the degree of the polynomial calibration function is not generally known, this document recommends the determination of polynomial functions of all degrees up to a stipulated maximum (limited by the quantity of data available), followed by the selection of one of these degrees according to suitable criteria. One criterion relates to the requirement that the calibration function is monotonic (strictly increasing or decreasing) over its domain. A second criterion relates to striking a balance between the polynomial calibration function providing a satisfactory explanation of the data and the number of parameters required to describe that polynomial. A further criterion relates to visual acceptance of the polynomial function.

**0.4** The determination and use of a polynomial calibration function thus consist of the following steps:

1 obtaining calibration data and available uncertainty information including covariance information when available;

2 determining polynomial functions of all degrees up to a prescribed maximum in a manner that respects the uncertainty information;

3 selecting an appropriate function from this set of polynomial functions according to the criteria in Subclause 0.3;

4 providing estimates of the parameters of the chosen polynomial function and obtaining the covariance matrix associated with those estimates;

5 using the calibration function for inverse evaluation and associated uncertainty evaluation;

6 using the calibration function for direct evaluation and associated uncertainty evaluation.

**0.5** This document treats steps 2 to 6 listed in Subclause 0.4 employing the principles of ISO/IEC Guide 98-3:2008 (GUM). Therefore, as part of step 1, before using this document, the user should provide available standard uncertainties and covariances associated with the measured $x$- and $y$-values. Account should be taken of the provisions of the GUM in obtaining these uncertainties on the basis of a measurement model that is specific to the area of concern.

# Determination and use of polynomial calibration functions

## 1 Scope

**1.1** This document is concerned with polynomial calibration functions that describe the relationship between a stimulus variable and a response variable. These functions contain parameters estimated from calibration data consisting of a set of pairs of stimulus value and response value. Various cases are considered relating to the nature of any uncertainties associated with the data.

**1.2** Estimates of the polynomial function parameters are determined using least-squares methods, taking account of the specified uncertainty information. It is assumed that the calibration data are fit for purpose and thus the treatment of outliers is not considered. It is also assumed that the calibration data errors are regarded as drawn from normal distributions. An emphasis of this document is on choosing the least-squares method appropriate for the nature of the data uncertainties in any particular case. Since these methods are well documented in the technical literature and software that implements them is freely available, they are not described in this document.



**1.3** Commonly occurring types of covariance matrix associated with the calibration data are considered covering (a) response data uncertainties, (b) response data uncertainties and covariances, (c) stimulus and response data uncertainties, and (d) stimulus data uncertainties and covariances, and response data uncertainties and covariances. The case where the data uncertainties are unknown is also treated.



**1.4** Methods for selecting the degree of the polynomial calibration function according to prescribed criteria are given. The covariance matrix associated with the estimates of the parameters in the selected polynomial function is available as a by-product of the least-squares methods used.

**1.5** For the chosen polynomial function this document describes the use of the parameter estimates and their associated covariance matrix for inverse and direct evaluation. It also describes how the provisions of ISO/IEC Guide 98-3:2008 (GUM) can be used to provide the associated standard uncertainties.

**1.6** Consideration is given to accounting for certain constraints (such as the polynomial passing through the origin) that may need to be imposed and also to the use of transformations of the variables that may render the behaviour of the calibration function more polynomial-like. Interchanging the roles of the variables is also considered.

**1.7** Examples from several areas of measurement science illustrate the use of this document.

## 2 Normative references

The following documents are referred to in the text in such a way that some or all of 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 99:2007 (corr. 2010), *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.

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

— IEC Electropedia: available at http://www.electropedia.org/

— ISO Online browsing platform: available at https://www.iso.org/obp

**3.1**
**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 99:2007 (corr. 2010), 2.26, modified - Notes 1 to 4 have been deleted.]



**3.2**
**standard measurement uncertainty**
**standard uncertainty**
*measurement uncertainty* (3.1) expressed as a standard deviation

[SOURCE: ISO/IEC Guide 99:2007 (corr. 2010), 2.30.]

**3.3**
**measurement covariance matrix**
**covariance matrix**
symmetric positive-definite matrix of dimension $N \times N$ associated with an estimate of a vector quantity of dimension $N \times 1$, containing on its diagonal the squared standard uncertainties associated with the 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 measurement covariance matrix $\boldsymbol{V}_{\boldsymbol{x}}$ of dimension $N \times N$ associated with the estimate $\boldsymbol{x}$ of a vector quantity $\boldsymbol{X}$ has the representation

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

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

Note 2 to entry: A covariance matrix is also known as a variance-covariance matrix.

[SOURCE: ISO/IEC Guide 98-3:2008/Suppl. 1:2008, 3.11 (definition of uncertainty matrix), modified - definition slightly modified, Note 2 deleted, Note 3 becomes Note 2 to entry, slightly modified.]

**3.4**
**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 $\boldsymbol{R}_{\boldsymbol{x}}$ of dimension $N \times N$ associated with the estimate $\boldsymbol{x}$ of a vector quantity $\boldsymbol{X}$ has the representation



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



where $r(x_i,x_i) = 1$ and $r(x_i,x_j)$ is the correlation associated with $x_i$ 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: $\boldsymbol{R}_{\boldsymbol{x}}$ is related to $\boldsymbol{V}_{\boldsymbol{x}}$ (see definition 3.3) by

$$\boldsymbol{V}_{\boldsymbol{x}} = \boldsymbol{D}_{\boldsymbol{x}} \boldsymbol{R}_{\boldsymbol{x}} \boldsymbol{D}_{\boldsymbol{x}},$$

where $\boldsymbol{D}_{\boldsymbol{x}}$ is a diagonal matrix of dimension $N \times N$ with diagonal elements $u(x_1),\ldots,u(x_N)$. Element $(i,j)$ of $\boldsymbol{V}_{\boldsymbol{x}}$ is given by

$$u(x_i,x_j) = r(x_i,x_j)u(x_i)u(x_j).$$

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

**3.5**
**measurement model**
mathematical relation among all quantities known to be involved in a measurement

[SOURCE: ISO/IEC Guide 99:2007 (corr. 2010), 2.48, modified - Notes 1 and 2 deleted.]

**3.6**
**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* (3.1).

Note 2 to entry: Calibration should not be confused with 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 99:2007 (corr. 2010), 2.39.]

**3.7**
**stimulus interval**
interval in the stimulus variable over which a calibration function is defined



**3.8**
**stimulus**
quantity that effects a *response* (3.9) in a measuring system

**3.9**
**response**
quantity resulting from stimulating a measuring system

**3.10**
**inverse evaluation**
use of a calibration function to provide the stimulus value corresponding to a response value

**3.11**
**direct evaluation**
use of a calibration function to provide the response value corresponding to a stimulus value

## 4 Conventions and notation

For the purposes of this document the following conventions and notations are adopted.

**4.1** The quantity whose values are provided by measurement standards is termed the independent variable $x$ (also called 'stimulus') and the quantity described by measuring system indication values is termed the dependent variable $y$ (also called 'response').

**4.2** $x_i$ and $y_i$ denote the measured values of the Cartesian co-ordinates of the $i$th point $(x_i, y_i)$, $i = 1, \ldots, m$, in a calibration data set of $m$ points. Vector and matrix notation is frequently used. The values of $x_i$ and $y_i$ are often expressed as vectors, with '$\mathsf{T}$' denoting 'transpose':

$$\boldsymbol{x} = \left[x_1, \ldots, x_m\right]^{\mathsf{T}}, \quad \boldsymbol{y} = \left[y_1, \ldots, y_m\right]^{\mathsf{T}}.$$

A matrix or vector of zeros is denoted by $\mathbf{0}$.

**4.3** True values (that would be achieved with perfect measurement) of the co-ordinates of the $i$th point are denoted by $\xi_i$ and $\eta_i$. Measured values of points expressed in Cartesian co-ordinates and corresponding true values are related by:

$$x_i = \xi_i + d_i, \quad y_i = \eta_i + e_i,$$

where $d_i$ and $e_i$ denote the errors in $x_i$ and $y_i$, respectively. Errors are unknowable, but can often be estimated.

**4.4** 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 covariance associated with $y_i$ and $y_j$ is denoted by $u(y_i, y_j)$.



NOTE This document does not consider cross-variances $u(x_i, y_j)$ since no practical calibration application has been identified in which cross-variances are prescribed.



**4.5** The uncertainty information for the specification of a polynomial calibration problem is represented by matrices $\boldsymbol{V}_{\boldsymbol{x}}$ and $\boldsymbol{V}_{\boldsymbol{y}}$ each of dimension $m \times m$ holding the variances (squared standard uncertainties) $u^2(x_i) \equiv u(x_i, x_i)$ and $u^2(y_i) \equiv u(y_i, y_i)$, and the covariances $u(x_i, x_j)$ and $u(y_i, y_j)$. Formula (1) denotes the covariance matrix associated with $\boldsymbol{x}$ and Formula (2) denotes the covariance matrix associated with $\boldsymbol{y}$:

$$\boldsymbol{V}_x = \begin{bmatrix} u(x_1, x_1) & \cdots & u(x_1, x_m) \\ \vdots & \ddots & \vdots \\ u(x_m, x_1) & \cdots & u(x_m, x_m) \end{bmatrix}, \tag{1}$$

$$\boldsymbol{V}_y = \begin{bmatrix} u(y_1, y_1) & \cdots & u(y_1, y_m) \\ \vdots & \ddots & \vdots \\ u(y_m, y_1) & \cdots & u(y_m, y_m) \end{bmatrix}. \tag{2}$$

For a particular calibration problem, either of $\boldsymbol{V_x}$ and $\boldsymbol{V_y}$ may be equal to $\boldsymbol{0}$.

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

**4.6** If the covariances $u(x_i, x_j)$ $(i \neq j)$ are all zero, $\boldsymbol{V_x}$ is a diagonal matrix:

$$V_x = \begin{bmatrix} u^2(x_1) & & \\ & \ddots & \\ & & u^2(x_m) \end{bmatrix} = \mathrm{diag}\left[u^2(x_1), \ldots, u^2(x_m)\right] \quad (3)$$

and similarly for the $u(y_i, y_j)$.

**4.7** The elements below the main diagonal of a symmetric matrix are generally not displayed. Thus, for instance, the representation of the matrix

$$\begin{bmatrix} 1,2 & -0,7 & 0,8 \\ -0,7 & 2,5 & 0,5 \\ 0,8 & 0,5 & 1,7 \end{bmatrix} \text{ is } \begin{bmatrix} 1,2 & -0,7 & 0,8 \\ & 2,5 & 0,5 \\ \text{sym.} & & 1,7 \end{bmatrix}.$$



**4.8** A polynomial calibration function relating $y$ and $x$ is denoted by $p_n(x)$, where $n$ is the degree of the polynomial. It is denoted by $p_n(x, \boldsymbol{a})$ when it is necessary to indicate that it depends on $n+1$ parameters $\boldsymbol{a} = [a_0, \ldots, a_n]^\mathrm{T}$.



**4.9** An estimate of a quantity $q$ is denoted by $\hat{q}$. Model values corresponding to the data point $(x_i, y_i)$, namely, satisfying $\hat{y}_i = p_n(\hat{x}_i, \hat{\boldsymbol{a}})$ are denoted by $\hat{x}_i$ and $\hat{y}_i$.

**4.10** The function that is minimized to estimate the polynomial function parameters $\boldsymbol{a}$ is termed the objective function.

**4.11** While data values in examples are provided to a given number of decimal digits, results of calculations are sometimes provided to a greater number, for comparison purposes, for example.

## 5 Other Standards using polynomial calibration functions

Other Standards concerned with polynomial calibration are as follows.

a) ISO 6143:2006[23] is concerned with comparison methods for determining and checking the composition of calibration gas mixtures. It contains clauses on the determination (and use) of ‘analysis functions’ given calibration data. The analysis functions considered are polynomials of degrees 1, 2 and 3 representing the stimulus as a function of response. Uncertainties are permitted in the stimulus data values and the response data values. Covariances are permitted in the stimulus data, but not in the response data.

b) ISO 7066-2:1988[24] covers basic methods for determining and using polynomial calibration functions in the context of the measurement of fluid flow: assessment of uncertainty in the calibration and use of flow measurement devices. It handles, in the language of this document, standard uncertainties associated with the data y-values, and inverse evaluation.

c) ISO 11095:1996[20] specifically addresses reference materials, outlining general principles needed to calibrate a measuring system and to maintain that system in a state of statistical control. It provides a basic method for estimating a straight-line calibration function when stimulus values are known exactly.

d) ISO 11843-2:2000[21] concerned with capability of detection, uses straight-line calibration functions when the standard uncertainties in the response values are constant or depend linearly on stimulus. ISO 11843-5:2008[22] extends the provisions of ISO 11843:2000 to the non-linear case.

e) ISO/TS 28037:2010[25] covers the same uncertainty structures as in the current document, and is concerned with straight-line calibration. The current document can be regarded as an extension of ISO/TS 28037 to polynomial functions of general degree.

## 6 Calibration data and associated uncertainties



**6.1** Calibration consists of two stages (definition 3.6). The first stage establishes a relation between (stimulus) values provided by measurement standards and corresponding instrument response values. The second stage uses this relation to obtain stimulus values from further instrument response values (inverse evaluation). The relation also allows a response value to be obtained given a further stimulus value (direct evaluation). In this document the relation takes the form of a polynomial calibration function, which is described by a set of parameters, estimates of which are deduced from the calibration data and the associated uncertainties.

NOTE This document is not concerned with determining a mathematical form from which a stimulus value can be determined explicitly given a response value. Such a form is known in some fields of application as an analysis function.

**6.2** The calibration of a measuring system should take into account prescribed calibration data uncertainties and any prescribed covariances.

**6.3** An acceptable calibration function will satisfy a statistical test for compatibility with the calibration data and the accompanying uncertainties. In many circumstances it will also have to be monotonic (strictly increasing or decreasing).

**6.4** Standard uncertainties and covariances accompany the parameter estimates, and the information concerning the calibration function is used to provide a stimulus value (or response value) and the associated standard uncertainty corresponding to a given response value (or stimulus value, respectively).

**6.5** Any particular set of calibration data $\left(x_i, y_i\right)$, $i = 1, \ldots, m$, will have an uncertainty structure specific to that data. At one extreme, nothing is known about the uncertainties and covariances and, to proceed, assumptions are necessary. At the other extreme, all standard uncertainties $u\left(x_i\right)$ and $u\left(y_i\right)$

and all covariances $u\left(x_i, x_j\right)$ and $u\left(y_i, y_j\right)$ are prescribed. In practice, the provided information often lies between these extremes.

NOTE In this document any uncertainty or covariance that is not prescribed is taken as zero.

**6.6** The following five cases can be distinguished, the first four in approximately increasing order of complexity of uncertainty structure. The fifth is different in character in the sense that the uncertainty information is unknown.

a) *Response data uncertainties*. Standard uncertainties $u(y_i)$, $i = 1,...,m$, prescribed.

b) *Response data uncertainties and covariances*. As 6.6 a) with covariances $u(y_i, y_j)$, $i = 1,...,m$, $j = 1,...,m$ ($i \neq j$), also prescribed.

c) *Stimulus and response data uncertainties*. As 6.6 a) with standard uncertainties $u(x_i)$, $i = 1,...,m$, also prescribed.

d) *Stimulus and response data uncertainties and covariances*. As 6.6 c) with covariances $u(x_i, x_j)$ and $u(y_i, y_j)$, $i = 1,...,m$, $j = 1,...,m$ ($i \neq j$), also prescribed.

e) *Unknown data uncertainties*.

In cases 6.6 a) to 6.6 d), the prescribed uncertainties and covariances are summarized as covariance matrices $\boldsymbol{V_x}$ and $\boldsymbol{V_y}$ as appropriate according to Subclause 4.5.



NOTE Cases 6.6 a) to 6.6 c) can be treated as special cases of 6.6 d), but computationally less efficiently.

**6.7** The key distinction between calibration data with prescribed uncertainties and calibration data with unknown uncertainties made in this document is the following.

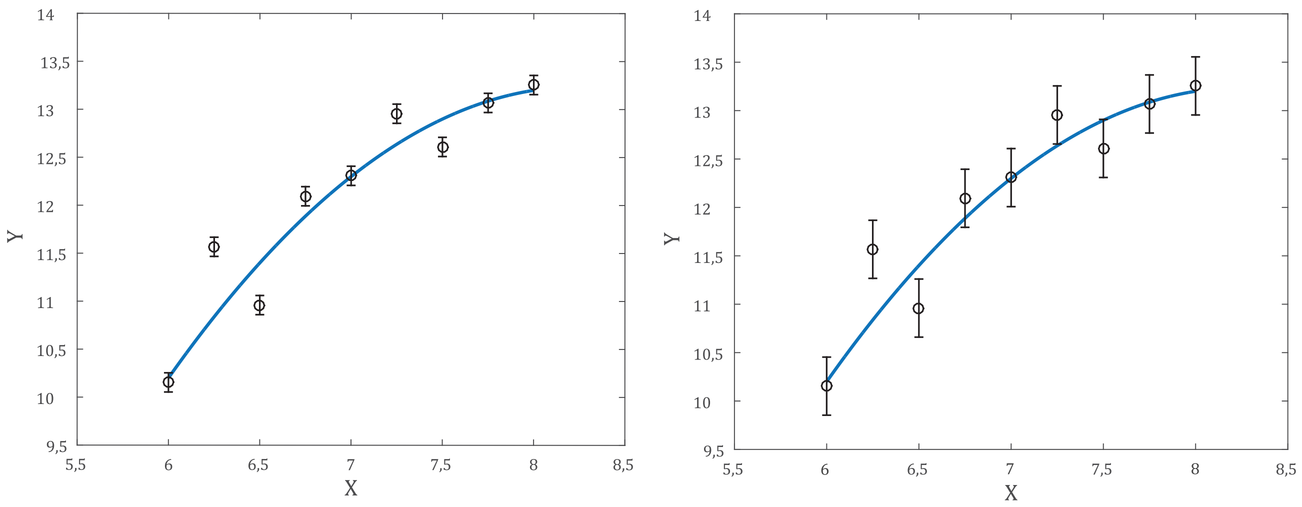


a) For calibration data with prescribed uncertainties and covariances [cases 6.6 a) to 6.6 d)] a metric, such as the chi-squared statistic (Subclause 7.7.1), that uses the uncertainties and covariances may be employed to decide whether a candidate calibration function, in this document a polynomial of a particular degree, is statistically valid. This approach assumes the plausibility of the specified uncertainty information.

b) For calibration data with unknown uncertainties [case 6.6 e)] a chi-squared statistic can still be calculated for candidate polynomial models. The assumptions are made that the data errors in the response variable are homogeneous and the data errors in the stimulus variable are negligible. The value of the chi-squared statistic can be used to estimate the response variable standard uncertainty and the provisions of 6.7 a) then applied.

**6.8** A polynomial is selected from a set of candidate polynomials of various degrees according to a suitable criterion such as AIC (Subclause 7.7.3). For some data sets with prescribed uncertainties there might be no suitable polynomial (or any other smooth) representation consistent with this information. For the data in Figure 1 a), the only uncertainties are associated with the *y*-values, the vertical bars represent ± 1 standard uncertainty, and the covariances are zero. The smallness of the standard uncertainties prevent a monotonic function that is consistent with the data from being obtained. For the data in Figure 1 b), identical to those in Figure 1 a) except that the standard uncertainties are some three times as large, a monotonic polynomial of low degree is suitable. An acceptable calibration function should be both monotonic (Subclause 7.6) and statistically adequate[30].




**a) Statistical inadequacy** **b) Statistical adequacy**

**Key**

X stimulus (a.u.)

Y response (a.u.)

NOTE Error bars denote ±1 standard uncertainty. 'a.u.' denotes arbitrary units.

**Figure 1 — Statistical inadequacy and adequacy**



NOTE Figure 1 a) appears to relate to mis-specification of the standard uncertainties associated with the calibration data; their possible rectification is beyond the scope of this document.

**6.9** Estimates of the calibration function parameters depend on the calibration data and, apart from case 6.6 e), the prescribed data uncertainties and covariances. The law of propagation of uncertainty (LPU) in the ISO/IEC Guide 98-3:2008 (GUM) can be applied to propagate calibration data uncertainties and covariances through the computation of the calibration function parameters to obtain parameter uncertainties and covariances. When there is no uncertainty associated with the stimulus values (Subclauses 9.2, 9.3 and 9.6), the propagation is exact, since the parameters of a polynomial calibration function depend linearly on the data response values and LPU applies with no approximation error in such cases (see Subclause 7.2.1). For other cases (Subclauses 9.4 and 9.5), the propagation is approximate, based on a linearization about the parameter estimates. The approximation incurred by the linearization will often be fit for purpose for practical calibration problems.

NOTE If linearization is unfit for purpose, such as when the stimulus value uncertainties are large, the propagation of distributions may be used to obtain parameter estimates, uncertainties and covariances. This approach (ISO/IEC Guide 98-3:2008/Suppl. 2:2011), which uses a Monte Carlo method, is beyond the scope of this document.

**6.10** Uncertainty information concerning the calibration function parameters takes the form of a covariance matrix for (estimates of) those parameters. That information can equally be represented as the standard uncertainties associated with those parameters together with their correlation matrix (definition 3.4), which may be a more useful form. Either form can be used in the evaluation of the standard uncertainty associated with inverse or direct evaluation.

**6.11** When the calibration function is used for inverse evaluation (Subclause 12.2), the application of LPU is approximate, even for polynomials of degree one, because when used inversely the polynomial is