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Determination and use of polynomial calibration functions

Détermination et utilisation des fonctions d'étalonnage polynômial

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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;

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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.

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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.

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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

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