PD ISO/TS 28038:2018

BSI Standards Publication

Determination and use of polynomial calibration functions

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National foreword

This Published Document is the UK implementation of ISO/TS 28038:2018.

The UK participation in its preparation was entrusted to Technical Committee SS/6, Precision of test methods.

A list of organizations represented on this committee can be obtained on request to its secretary.

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Published by BSI Standards Limited 2018

ISBN 978 0 580 98098 5

ICS 17.020

Compliance with a British Standard cannot confer immunity from legal obligations.

This Published Document was published under the authority of the Standards Policy and Strategy Committee on 31 December 2018.

Amendments/corrigenda issued since publication

Date	Text affected

PD ISO/TS 28038:2018

TECHNICAL SPECIFICATION

ISO/TS 28038

First edition
2018-12

Determination and use of polynomial calibration functions

Détermination et utilisation des fonctions d'étalonnage polynômial

Reference number
ISO/TS 28038:2018(E)

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Published in Switzerland

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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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TECHNICAL SPECIFICATION **ISO/TS 28038:2018(E)**

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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