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МЕЖДУНАРОДНАЯ ОРГАНИЗАЦИЯ ПО СТАНДАРТИЗАЦИИ

Assessment of uncertainty in the calibration and use of flow measurement devices —

Part 2: Non-linear calibration relationships

Évaluation de l'incertitude dans l'étalonnage et l'utilisation des appareils de mesure du débit —

Partie 2: Relations d'étalonnage non linéaires

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Foreword

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Draft International Standards adopted by the technical committees are circulated to the member bodies for approval before their acceptance as International Standards by the ISO Council. They are approved in accordance with ISO procedures requiring at least 75 % approval by the member bodies voting.

International Standard ISO 7066-2 was prepared by Technical Committee ISO/TC 30, *Measurement of fluid flow in closed conduits*.

Users should note that all International Standards undergo revision from time to time and that any reference made herein to any other International Standard implies its latest edition, unless otherwise stated.

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Assessment of uncertainty in the calibration and use of flow measurement devices —

Part 2: Non-linear calibration relationships

0 Introduction

The method of fitting a straight line to flow measurement calibration data and of assessing the uncertainty in the calibration are dealt with in ISO 7066-1. ISO 7066-2 deals with the case where a straight line is inadequate for representing the calibration data.

1 Scope and field of application

This part of ISO 7066 describes the procedures for fitting a quadratic, cubic or higher degree polynomial expression to a non-linear[1] set of calibration data, using the least-squares criterion, and of assessing the uncertainty associated with the resulting calibration curve. It considers only the use of polynomials with powers which are integers.

Because it is generally not practicable to carry out this type of curve fitting and assessment of uncertainty without using a computer, it is assumed in this part of ISO 7066 that the user has access to one. In many cases it will be possible to use standard routines available on most computers; as an alternative the FORTRAN program listed in annex C may be used.

Examples of the use of these methods are given in annex D.

Extrapolation beyond the range of the data is not permitted.

Annexes A, B, C, D and E do not form integral parts of this part of ISO 7066.

2 References

ISO 5168, *Measurement of fluid flow — Estimation of uncertainty of a flow-rate measurement.*[2]

ISO 7066-1, *Assessment of uncertainty in the calibration and use of flow measurement devices — Part 1: Linear calibration relationships.*[3]

3 Definitions

For the purposes of this part of ISO 7066, the following definitions apply.

3.1 method of least squares: Technique used to compute the coefficients of a particular form of an equation which is chosen for fitting a curve to data. The principle of least squares is the minimization of the sum of squares of deviations of the data from the curve.

3.2 polynomial (function): For a variable x, a series of terms with increasing integer powers of x.

3.3 regression analysis: The process of quantifying the dependence of one variable on one or more other variables.

NOTE — Many of the available computer programs suitable for curve fitting have the word "regression" in the title. For the purposes of this part of ISO 7066, the terms regression and least squares may be regarded as interchangeable.

3.4 standard deviation: The positive square root of the variance.

3.5 variance: A measure of dispersion based on the mean of the squares of deviations of values of a variable from its expected value.

4 Symbols and abbreviations

b_j coefficient of x_j

C_{jb} element of the inverse matrix

1) These procedures are also suitable for a linear set of calibration data.

2) At present at the stage of draft. (Revision of ISO 5168 : 1978.)

3) At present at the stage of draft.

$e_r(\ )$ random uncertainty of variable contained in parentheses[1)]

$e_s(\ )$ systematic uncertainty of variable contained in parentheses[1)]

$e(\hat{y}_c)$ total uncertainty of calibration coefficient[1)]

g_j coefficient of jth orthogonal polynomial

m degree of polynomial

n number of data values

$p_j(x)$ jth orthogonal polynomial

$s(\ )$ experimental standard deviation of variable contained in parentheses

s_r residual standard deviation of data values about the curve

t Student's t

x the independent variable

x^* arbitrary specified value of x

$\bar{x}$ arithmetic mean of the data values x_i

x_i value of x at the ith data point

x_j jth independent variable (in multiple linear regression)

x_{ji} value of x_j at the ith data point

y the dependent variable

$\bar{y}$ arithmetic mean of the data values y_i

$\hat{y}$ value of y predicted by the equation of the fitted curve

y_i value of y at the ith data point

$\hat{y}_i$ value of $\hat{y}$ at $x = x_i$

ν number of degrees of freedom

5 Curve fitting

5.1 General

Before attempting polynomial curve fitting, consideration should be given to whether a simple transformation of the x variable or the y variable or both may effectively linearize the data to enable the straight line methods described in ISO 7066-1 to be used. Some appropriate transformations are suggested in ISO 7066-1.

If it is not possible to establish a straight line, then the objective is to find the degree and coefficients of the polynomial function which best represents a set of n pairs of (x_i, y_i) data values obtained from calibration. If, for example, a quadratic expression is chosen, the curve will be of the form

$$\hat{y} = b_0 + b_1 x + b_2 x^2 \qquad \ldots (1)$$

The general polynomial expression is

$$\hat{y} = b_0 + b_1 x + \ldots + b_j x^j + \ldots + b_m x^m$$

or

$$\hat{y} = \sum_{j=0}^{m} b_j x^j \qquad \ldots (2)$$

By applying the least-squares criterion, the coefficients b_j are computed to minimize the sum of squares of deviations of the data points from the curve:

$$\sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

where $\hat{y}_i$ is the value predicted by equation (2) at $x = x_i$.

In some cases, the degree m of the polynomial will be predetermined; for example, it may be known from experience that the calibration data will be satisfactorily represented by a cubic $(m = 3)$ expression. Otherwise, the degree of fit is chosen by increasing the degree until an optimum is achieved (see 5.3).

If in increasing the degree of fit beyond a moderate degree significant improvements in the fit, as described in 5.3, continue to occur, then it is likely that the functional dependence is not suitable for representation by a polynomial; further, if the equation fitted has too many terms, the curve may display spurious oscillations. A not uncommon example is data which are virtually constant over most of the x range, but which vary strongly close to one end of the range.

In such cases, it is appropriate to divide the range into sections (see ISO 7066-1) which either are linear or can be fitted by a low-degree polynomial. Alternatively, transforming one or both variables may lead to a linear or low-degree polynomial function; transforming the independent variable to its reciprocal $1/x$ will in some cases result in adequate linearity.

The least-squares methods described in this part of ISO 7066 may not be appropriate if the effect of the random uncertainty $e_r(x)$ of the data values x_i is not negligible in comparison with that of the random uncertainty $e_r(y)$ of the y values. As in ISO 7066-1, if the magnitude of the slope[2)] of the calibration curve is always less than one-fifth of $e_r(y)/e_r(x)$, the methods may be regarded as appropriate; where this does not apply the

1) In some International Standards, the symbols U and E have been used instead of e.

2) "Slope" here means the derivative $\mathrm{d}\hat{y}/\mathrm{d}x = b_1 + 2b_2 x + \ldots$.

mathematical treatment is outside the scope of this part of ISO 7066. If therefore the normal practice in calibrating any particular meter is to plot the variables in such a way that the above condition does not hold, then either the conventional choice of abscissa and ordinate is to be reversed or this part of ISO 7066 cannot be used.

If either variable is transformed before fitting, then the uncertainties referred to above, and later (clause 6), relate to the new transformed variables. If, as a result of transforming the dependent variable, the random uncertainty $e_r(y)$ cannot be regarded as constant over the range, then a weighted least-squares method should be used. The weighted least-squares method is not described in this part of ISO 7066 but many computer library routines allow the data to be weighted.

5.2 Computational methods

Standard library routines for least-squares curve fitting are available on most computers. The method for fitting a straight line described in ISO 7066-1 is commonly known as linear or simple linear regression: the equivalent method for fitting a polynomial may be described as polynomial or curvilinear regression, which is a special type of multiple linear regression. Annex A gives further information on regression methods and how to use them.

As an alternative to the standard regression routines, the orthogonal polynomial method described in annex B may be used: this method is particularly suitable when the degree of fit is not known beforehand. Annex C lists an appropriate orthogonal polynomial computer program.

When a computer is not available and the x values are uniformly spaced, a finite-difference method (see annex E) may be used to provide a quick indication of what degree of fit may be appropriate to represent the data. The coefficients of a polynomial representing the data may also be calculated, but this will not be the least-squares polynomial. The calculation of uncertainty using this method is beyond the scope of this part of ISO 7066.

5.3 Selecting the optimum degree of fit

The optimum fit is determined by trying increasing values of the degree m, either up to a specified maximum or until no further significant improvement occurs. The residual standard deviation s_r should be computed for each degree (s_r is the square root of the residual variance) using the equation

$$s_r^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 / (n - m - 1) \qquad \ldots (3)$$

where $\hat{y}_i$ is the value predicted by the polynomial expression [equation (2)] at $x = x_i$.

NOTE — s_r^2 is equivalent to the term $s^2(y,x)$ used in ISO 7066-1.

The degree m should always be much less than the number n of data points.

If the data are well represented by a polynomial of degree m, then s_r will decrease significantly until the degree m is reached; thereafter s_r will remain approximately constant. In general, however, the degree at which the decrease in s_r ceases to be significant is not obvious, and an objective test of significance should be used as an aid to finding the optimum degree of fit.

Increasing the degree from $m-1$ to m is regarded as providing a statistically significant improvement in the fit if the new coefficient b_m differs significantly from zero, i.e. if $b_m + t_{95}\, s(b_m)$ and $b_m - t_{95}\, s(b_m)$ (the 95 % confidence limits of b_m) do not include zero.

This condition may be expressed as

$$\left| \frac{b_m}{s(b_m)} \right| > t_{95}$$

where t_{95} is the Student's t value for the 95 % confidence level with $\nu = n - m - 1$.

The value of t_{95} as a function of the number of degrees of freedom ν can be computed from the following empirical equation:

$$t_{95} = 1{,}96 + 2{,}36/\nu + 3{,}2/\nu^2 + 5{,}2/\nu^{3{,}84} \qquad \ldots (4)$$

For the orthogonal polynomial coefficient g_m (see annex B), the condition is

$$\left| \frac{g_m}{s(g_m)} \right| > t_{95}$$

Expressions for the variances of the coefficients $s^2(b_m)$ and $s^2(g_m)$ are given in annex A and annex B respectively.

It is important to test the effect of increasing the degree at least one degree beyond that which first shows no significant improvement, since it is often the case that either only the odd terms or only the even terms produce a significant improvement.

From a statistical point of view, the highest degree which produces an improvement in the fit which is significant at the 95 % confidence level may be regarded as the optimum degree. However, before this degree is selected as providing the most suitable expression to represent the data, other factors should be considered. These factors include any knowledge of the expected shape of the curve, the desirability of having a functional form which is not too complex, the range which it is necessary to represent, and the accuracy which is sought.

In assessing these factors, it is always advisable to plot graphs showing the data and the possible curves; these graphs will also highlight other possible problems. For example, if the degree is too low, then the curve will fail to represent a real trend in the data, and the predicted value $\hat{y}$ may have a bias over some of the range. If the degree is too high, the curve may be fitting the scatter of the data rather than the underlying trend.

The examples given in annex D illustrate the application of some of these principles.

6 Uncertainty

The random component of the uncertainty, at the 95 % confidence level, of a predicted value $\hat{y}$, is given by

$$e_r(\hat{y}) = t_{95}\, s(\hat{y})$$

where $s(\hat{y})$ is the square root of the variance $s^2(\hat{y})$ of $\hat{y}$. Expressions for $s^2(\hat{y})$ are given in annexes A and B; in general, $s^2(\hat{y})$ may be expressed as a polynomial function of x of degree $2m$. It is important to ensure that enough significant figures are used in the computation of $s^2(\hat{y})$ to avoid large rounding errors which result from subtraction.

It should be noted that the estimate of uncertainty provided by $e_r(\hat{y})$ will only be valid to the extent that the polynomial expression chosen is a good approximation to the true functional relationship between y and x.

The 95 % random confidence limits for the true value of y are

$$y \pm e_r(\hat{y})$$

As in ISO 7066-1, the uncertainty in the calibration coefficient is given by

$$e(\hat{y}_c) = \left[e_r^2(\hat{y}) + e_s^2(\hat{y}) \right]^{1/2}$$

where $e_s(\hat{y})$ is the systematic component of the uncertainty in $\hat{y}$.

NOTE — In the revised version of ISO 5168, in preparation, guidelines are provided for using either the linear addition or the root-sum-square combination of random and systematic errors.

If the dependent variable has been transformed, then all the above uncertainties refer to the transformed variable.

Annex A

Regression methods

(This annex does not form an integral part of the standard.)

A.1 Introduction

Regression methods for curve fitting are widely available under various names as standard routines in computer libraries. The documentation provided with these routines tends to assume a certain level of knowledge of regression analysis. The purpose of this annex is to provide a general description of the methods and terminology of regression curve fitting as a background to the documentation of the library routines.

The most widely available regression technique, apart from simple linear regression, is multiple linear regression; curve fitting can be carried out using a special type of multiple linear regression known as polynomial or curvilinear regression. If a polynomial regression routine is not available, then a multiple linear regression method can be used, although it is less convenient. "Stepwise" and "backwards elimination" or "back solution" are special types of multiple linear regression methods which may be used.

A.2 Multiple linear regression

In the following, the summation sign Σ is used to represent $\sum_{i=1}^{n}$ unless otherwise noted.

A dependent variable y is assumed to be related linearly to m independent variables $x_1, x_2, \ldots, x_m$ by

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_m x_m + U \quad \ldots (5)$$

where

β_0 to β_m are the unknown regression coefficients;

U is a measure of the random effects which cause the dependence of y on the m independent variables to depart from exact linearity.

From the n sets of observations

$$(y_i, x_{1i}, x_{2i}, \ldots, x_{mi}), \quad i = 1, 2, \ldots, n$$

the estimates of the regression coefficents are

$$b_0, b_1, \ldots, b_m$$

so that the estimate $\hat{y}$ of the true value corresponding to the ith set of observations of the independent variables is

$$\hat{y}_i = b_0 + b_1 x_{1i} + \ldots + b_m x_{mi} \quad \ldots (6)$$

The application of the least-squares procedure to minimize $\Sigma(y_i - \hat{y}_i)^2$ leads to a set of $m + 1$ simultaneous equations, commonly known as the "normal equations":

$$nb_0 + \Sigma(x_{1i})b_1 + \Sigma(x_{2i})b_2 + \ldots + \Sigma(x_{mi})b_m = \Sigma y_i$$

$$\Sigma(x_{1i})b_0 + \Sigma(x_{1i})^2 b_1 + \ldots + \Sigma(x_{1i}x_{mi})b_m = \Sigma(x_{1i}y_i) \quad \ldots (7)$$

$$\Sigma(x_{mi})b_0 + \Sigma(x_{mi}x_{1i})b_1 + \ldots + \Sigma(x_{mi})^2 b_m = \Sigma(x_{mi}y_i)$$

These can then be solved for the $m + 1$ unknowns $b_0, b_1, \ldots, b_m$.

A.3 Polynomial (curvilinear) regression

When a relationship between two variables is not linear, but may be fitted by a polynomial function

$$\hat{y} = b_0 + b_1 x + b_2 x^2 + \dots + b_m x^m$$

there is said to be a polynomial or curvilinear regression of y on x. This can be treated as a multiple linear regression with the independent variables $x_1, x_2, \dots, x_m$ replaced by $x, x^2, \dots, x^m$.

In clauses A.4 and A.5, any of the multiple linear regression expressions may be transformed to the equivalent polynomial regression expressions by replacing the jth independent variable x_j by x^j, and the corresponding data values x_{ji} by x_i^j.

A.4 Computation of coefficients and variances

Consider the multiple linear regression equation with $m = 2$

$$\hat{y} = b_0 + b_1 x_1 + b_2 x_2 \qquad \dots (8)$$

which is equivalent to

$$\hat{y} = b_0 + b_1 x + b_2 x^2 \qquad \dots (9)$$

in the polynomial regression case.

When the least-squares criterion is applied, the normal equations are

$$n b_0 + \Sigma(x_{1i}) b_1 + \Sigma(x_{2i}) b_2 = \Sigma(y_i) \qquad \dots (10)$$

$$\Sigma(x_{1i}) b_0 + \Sigma(x_{1i})^2 b_1 + \Sigma(x_{1i} x_{2i}) b_2 = \Sigma(x_{1i} y_i) \qquad \dots (11)$$

$$\Sigma(x_{2i}) b_0 + \Sigma(x_{2i} x_{1i}) b_1 + \Sigma(x_{2i})^2 b_2 = \Sigma(x_{2i} y_i) \qquad \dots (12)$$

The traditional method for solving the normal equations involves computing the inverse of the 3 × 3 matrix of coefficients of b_0, b_1 and b_2. If the elements of this inverse matrix are

$$\begin{bmatrix} C_{00} & C_{01} & C_{02} \\ C_{10} & C_{11} & C_{12} \\ C_{20} & C_{21} & C_{22} \end{bmatrix}$$

then

$$\left.\begin{aligned} b_0 &= C_{00} \Sigma y_i + C_{01} \Sigma(x_{1i} y_i) + C_{02} \Sigma(x_{2i} y_i) \\ b_1 &= C_{10} \Sigma y_i + C_{11} \Sigma(x_{1i} y_i) + C_{12} \Sigma(x_{2i} y_i) \\ b_2 &= C_{20} \Sigma y_i + C_{21} \Sigma(x_{1i} y_i) + C_{22} \Sigma(x_{2i} y_i) \end{aligned}\right\} \qquad \dots (13)$$

or, in generalized form,

$$b_j = \sum_{k=0}^{m} \left[C_{jk} \Sigma(x_{ki} y_i) \right]$$

where $x_{ki} = 1$ for $k = 0$.

Note that since the matrix from the normal equations is symmetric, the inverse matrix is also symmetric.

The variances of the coefficients are

$$s^2(b_0) = s_r^2 C_{00}$$
$$s^2(b_1) = s_r^2 C_{11}$$
$$s^2(b_2) = s_r^2 C_{22}$$

where the residual variance, s_r^2, is given as in 5.3 by

$$s_r^2 = \frac{\Sigma(y_i - \hat{y}_i)^2}{n - m - 1}$$

Because the inverse matrix is symmetric,

$$C_{01} = C_{10}$$
$$C_{02} = C_{20} \qquad \ldots (14)$$
$$C_{12} = C_{21}$$

These non-diagonal terms are used to calculate the covariances[1)] between the coefficients b_j; using COV to denote covariance,

$$\mathrm{COV}(b_0, b_1) = s_r^2 C_{01}$$
$$\mathrm{COV}(b_0, b_2) = s_r^2 C_{02} \qquad \ldots (15)$$
$$\mathrm{COV}(b_1, b_2) = s_r^2 C_{12}$$

At specified values $x_1 = x_1^*$ and $x_2 = x_2^*$, the value predicted by the regression equation is

$$\hat{y} = b_0 + b_1 x_1^* + b_2 x_2^* \qquad \ldots (16)$$

The variance of this value of $\hat{y}$ is given by

$$s^2(\hat{y}) = s_r^2 \left[C_{00} + C_{11}(x_1^*)^2 + C_{22}(x_2^*)^2 + 2C_{01}x_1^* + 2C_{02}x_2^* + 2C_{12}x_1^*x_2^* \right] \qquad \ldots (17)$$

The factor of 2 arises because $C_{jk} = C_{kj}$ for each j, k.

The general formula is

$$s^2(\hat{y}) = s_r^2 \sum_{j=0}^{m} \sum_{k=0}^{m} (C_{jk} x_j^* x_k^*) \qquad \ldots (18)$$

where x_j^*, $x_k^* = 1$ for j, $k = 0$.

For polynomial regression, $x_j^* = (x^*)^j$ and $x_k^* = (x^*)^k$, and so

$$s^2(\hat{y}) = s_r^2 \sum_{j=0}^{m} \left[\sum_{k=0}^{m} C_{jk}(x^*)^{j+k} \right]$$

Adapting this expression to the form of a polynomial of degree $2m$ gives

$$s^2(\hat{y}) = s_r^2 \sum_{j=0}^{m} \left[\left(\sum_{k=0}^{j} C_{k,j-k} \right) (x^*)^j \right] + s_r^2 \sum_{j=m+1}^{2m} \left[\left(\sum_{k=j-m}^{m} C_{k,j-k} \right) (x^*)^j \right] \qquad \ldots (19)$$

1) The covariance of two coefficients indicates the effect of a change in one on the magnitude of the other. The inverse matrix multiplied by the scalar s_r^2 is known as the variance, covariance, or variance-covariance matrix.

A.5 Centred formulation

The least-squares or regression analysis is sometimes expressed in "centred" form, in which each variable is replaced by its deviation from its mean. In this form, equation (8) is replaced by

$$\hat{y} - \bar{y} = b_1 (x_1 - \bar{x}_1) + b_2 (x_2 - \bar{x}_2) \quad \ldots (20)$$

where the bar over a symbol is used to denote the mean value of the quantity represented by the symbol for the n measurements.

A.6 Numerical techniques used in computer libraries

For the least-squares or regression computations discussed in this annex, a computer library routine may make use of one of a variety of numerical techniques. The main numerical techniques used by computers for regression and least-squares matrix manipulations are

a) Gauss or Gauss-Jordan elimination,

b) Cholesky decomposition, and

c) orthogonal decompositions (usually Householder or modified Gram-Schmidt).

The particular technique used is in general not of importance to the user. However, it should be noted that elimination methods are susceptible to the build-up of rounding error, so that the computed coefficients b_j may be significantly in error for a high-degree polynomial; for a moderate degree, up to m = 3 or 4, this should not be a problem.