



BSI Standards Publication

Accuracy (trueness and precision) of measurement methods and results

Part 5: Alternative methods for the determination of the precision of a standard measurement method

National foreword

This British Standard is the UK implementation of ISO 5725-5:2025. It supersedes BS ISO 5725-5:1998, which is withdrawn.

The UK participation in its preparation was entrusted to Technical Committee SS/6, Statistical procedures for measurement methods and results.

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

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© The British Standards Institution 2025
Published by BSI Standards Limited 2025

ISBN 978 0 539 27966 5

ICS 03.120.30; 17.020

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This British Standard was published under the authority of the Standards Policy and Strategy Committee on 31 October 2025.

Amendments/corrigenda issued since publication

Date	Text affected
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International
Standard

ISO 5725-5

**Accuracy (trueness and precision)
of measurement methods and
results —**

**Part 5:
Alternative methods for the
determination of the precision of a
standard measurement method**

*Exactitude (justesse et fidélité) des résultats et méthodes de
mesure —*

*Partie 5: Méthodes alternatives pour la détermination de la
fidélité d'une méthode de mesure normalisée*

**Second edition
2025-10**

Reference number
ISO 5725-5:2025(en)

Full document details: BS ISO 5725-5:2025

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Published in Switzerland

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Foreword

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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 document 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).

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

This second edition cancels and replaces the first edition (ISO 5725-5:1998), which has been technically revised. It also incorporates the Technical Corrigendum ISO 5725-5:1998/Cor.1:2005.

The main changes are as follows:

- alternative experimental designs (split-level and design for heterogeneous material) have been transferred to ISO 5725-3;
- an additional robust approach, the Q method, which has improved breakdown properties, has been added.

A list of all parts in the ISO 5725 series can be found on the ISO website.

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.

Introduction

This document uses two terms, trueness and precision, to describe the accuracy of a measurement method. Trueness refers to the closeness of agreement between the average value of a large number of test results and the true or accepted reference value. Precision refers to the closeness of agreement between test results.

General consideration of these quantities is given in ISO 5725-1 and so is not repeated here. This document should be read in conjunction with ISO 5725-1 because the underlying definitions and general principles are given there.

ISO 5725-2 is concerned with estimating, by means of interlaboratory experiments, standard measures of precision, namely the repeatability standard deviation and the reproducibility standard deviation. It gives a basic method for doing this, including methods of calculation. This document describes alternative calculation methods to this basic method:

- The basic method requires the preparation of a number of identical samples of the material for use in the experiment. With heterogeneous materials this may not be possible, so that the use of the basic method then gives estimates of the reproducibility standard deviation that are inflated by the variation between the samples. The design for a heterogeneous material given in this document yields information about the variability between samples which is not obtainable from the basic method; it may be used to calculate an estimate of reproducibility from which the between-sample variation has been removed.
- The basic method requires tests for outliers to be used to identify data that should be excluded from the calculation of the repeatability and reproducibility standard deviations. Excluding outliers can sometimes have a large effect on the estimates of repeatability and reproducibility standard deviations, but in practice, when applying the outlier tests, the statistical expert may have to use judgement to decide which data to exclude. This document describes robust methods of data analysis that may be used to calculate repeatability and reproducibility standard deviations from data containing outliers without using tests for outliers to exclude data, so that the results are no longer affected by the statistical expert's judgement.

Accuracy (trueness and precision) of measurement methods and results —

Part 5:

Alternative methods for the determination of the precision of a standard measurement method

1 Scope

This document describes the use of robust methods for analysing the results of precision experiments without using outlier tests to exclude data from the calculations, and in particular, the detailed use of several such methods. The robust methods described in this document allow the data to be analysed in such a way that it is not required to make decisions about outliers that affect the results of the calculations.

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 3534-1, *Statistics — Vocabulary and symbols — Part 1: General statistical terms and terms used in probability*

ISO 5725-1, *Accuracy (trueness and precision) of measurement methods and results — Part 1: General principles and definitions*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 3534-1 and in ISO 5725-1 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/>

4 Symbols and abbreviations

- | | |
|-----------------|--|
| b_p | Correction factor used for reproducibility standard deviation in the Q method |
| c_p | Correction factor used for repeatability standard deviation in the Q method |
| D | Within-cell difference between measurement results (used with subscripts as required). |
| $\bar{D}$ | Average of within-cell differences |
| $d_1 \dots d_6$ | Interpolation nodes for each value y_i (Hampel estimator, non-iterative) |
| $E\{\}$ | Expectation of a statistical variable |

$G_1(x)$	Interpolation function (Q method, robust reproducibility standard deviation)
$G_1^{-1}()$	Function returning a given quantile of $G_1(x)$ (Q method, robust reproducibility standard deviation)
$G_1(x_i)$	Function of individual discontinuity points (Q method, robust reproducibility standard deviation)
$G_2(x)$	Interpolation function (Q method, robust repeatability standard deviation)
$G_2^{-1}()$	Function returning a given quantile of $G_2(x)$ (Q method, robust repeatability standard deviation)
$G_2(x_i)$	Function of individual discontinuity points (Q method, robust repeatability standard deviation)
$H_1(x)$	Cumulative distribution function of absolute between-laboratory differences (Q method)
$H_2(x)$	Cumulative distribution function of within-laboratory differences (Q method)
$I\{\}$	Indicator function returning 1 when a condition (in $\{\}$) is met and 0 otherwise
i	Identifier for a particular laboratory
j	Identifier for a particular replicate observation
n	Number of test results obtained in one laboratory at one level (i.e. per cell)
P	Probability
P_ξ	Probability used in calculation of adjustment factor for Algorithm S
p	Number of laboratories participating in the interlaboratory experiment
p_m	Check value for solutions in non-iterative Hampel estimator
p'	Number of laboratories participating in an interlaboratory experiment (heterogeneous material)
SS	Sum of squares
SS_H	Robust estimate of between-sample sum of squares (heterogeneous material)
SS_r	Robust estimate of repeatability sum of squares (heterogeneous material)
s	Estimate of a standard deviation
s'	standard deviation of a subset of data items between limits calculated in Algorithm A
s^*	Robust estimate of standard deviation
s_D	Estimate of standard deviation of cell differences in a split-level design
s_d	Robust estimate of standard deviation of cell averages
s_H	Robust estimate of between-sample standard deviation for a heterogeneous material
$s_{I(1)}$	Robust estimate of intermediate standard deviation
s_L	Estimate of between-laboratory standard deviation
s_R	Estimate of reproducibility standard deviation
s_r	Estimate of repeatability standard deviation
s_y	Estimate of standard deviation of cell averages for a level in a split-level design

t	Test sample number in an experiment for a heterogeneous material
u_L	Number of data items below a calculated threshold in Algorithm A
u_U	Number of data items above a calculated threshold in Algorithm A
w_i	i^{th} item of data in Algorithm S
x_i	i^{th} data point in a set of data
x_i^*	Updated value for i^{th} data point in iterative robust estimation
x^*	Robust estimate of mean value
x'	Average of a subset of data items between limits calculated in Algorithm A
y_i	i^{th} measurement result in a set of measurement results
$\bar{y}$	Average of a set of measurement results
y_{ij}	j^{th} measurement for laboratory i in a set of results grouped by laboratory
y_{itk}	k^{th} measurement on sample t in laboratory i at a particular level of a design for a heterogeneous material (adapted from ISO 5725-3)
ξ	Adjustment factor used in robust analysis (Algorithm S)
ν	Number of degrees of freedom
σ	True value of a standard deviation
$\Phi^{-1}(q)$	q^{th} quantile of the standard normal distribution
φ	Limit used in robust analysis (Algorithm A)
η	Limit factor used in robust analysis (Algorithm S)
ψ	Limit used in robust analysis (Algorithm S)
$\psi(q)$	Influence function (Hampel estimator)

5 Robust methods for data analysis: Algorithms A and S

5.1 Applications of robust methods of data analysis

5.1.1 In ISO 5725-2, it is recommended that two tests for outliers (Cochran's test and Grubbs' test) should be applied to the data obtained in a precision experiment, and any data that give rise to a test statistic in one or other of these tests that exceeds the critical value of the test at the 1 % significance level should be discarded (unless the statistical expert has good reason to retain the data). In practice, this procedure is often not easy to apply. Consider the results of the outlier tests in Example C.2. These are given in Table C.4. Laboratory 5 gives only one cell average (at Level 10) that is sufficiently extreme to be classed as an outlier by Grubbs' test, but gives three other stragglers, and a strong indication in Figure C.2 that something is amiss in this laboratory. The statistical expert, in this situation, must decide between:

- retaining all the data for Laboratory 5;
- discarding only the data from Level 10 for Laboratory 5;
- discarding all the data for Laboratory 5.

The decision will have a substantial influence on the calculated values for the repeatability and reproducibility standard deviations. It is a common experience when analysing data from precision experiments to find data that are on the borderline between stragglers and outliers, so that judgements may have to be made that affect the results of the calculation. This can be unsatisfactory. The robust methods described in this clause allow the data to be analysed in such a way that it is not required to make decisions that affect the results of the calculations. Thus, if there is reason to expect that the results of a precision experiment will contain outliers, robust methods may be preferred.

NOTE In this document, the statistical expert is the person designated to undertake analysis of the data and to provide a report of the data analysis to the panel, as described in ISO 5725-2.

5.1.2 The basic model discussed in ISO 5725-2 contains the assumption that establishing a common value for the repeatability standard deviation for all laboratories using the measurement method is justifiable. In practice it is often found that some laboratories achieve poorer repeatability than others. Some participants in a precision experiment might achieve poor repeatability when a measurement method is subjected to an interlaboratory precision experiment for the first time, or when they have little experience of the measurement method, and these are situations when the use of robust methods will be particularly appropriate.

5.1.3 The object of using robust methods^[10], when analysing the data from a precision experiment, is to calculate values for the repeatability and reproducibility standard deviations in such a way that they are not influenced by outlying data. If the participants in the experiment can be considered to be divided into two classes, those that produce good-quality data, and those that produce poor-quality data, then the robust methods should yield values for the repeatability and reproducibility standard deviations that are valid for the good-quality-data class, and not affected by the poor-quality data (provided that the poor-quality-data class is not too large).

5.1.4 The use of robust methods of data analysis does not affect the planning, organization or execution of a precision experiment. The decision as to whether to use robust methods or methods that require outliers to be discarded should be made by the statistical expert and reported to the panel.

When robust methods are used, data should be inspected visually for anomalies and the outlier tests and consistency checks described in ISO 5725-2 should be applied to the data, and the causes of any outliers, or patterns in the h and k statistics, should be investigated. However, data should not be discarded as a result of these tests and checks unless the check identifies a clear deviation from the prescribed measurement or test method. Additional statistical methods of identifying anomalous results or unexpected patterns may be applied, including, for example, z -scores for laboratory means, or the graphical methods illustrated in ISO 5725-2.

NOTE A z -score can be calculated as $(x_i - \bar{x}^*) / s^*$ where x_i is the mean for laboratory i , and $\bar{x}^*$ and s^* are respectively the robust mean and standard deviation of the laboratory means x_i as calculated by, for example, Algorithm A (see 5.2) or the Q/Hampel method (see 7.2 for s^* and 7.4 for $\bar{x}^*$).

5.1.5 The denominators in the h and k statistics are standard deviations that, according to the methods of calculating these statistics described in ISO 5725-2, are calculated from the data as reported. If outliers are present in the data then these will inflate the denominators and produce a distorted effect in the graphs of the statistics. For example, if, at one level of an experiment, one laboratory gives a cell average that is an outlier, and much more extreme than any other outlier at that level, then it will show up in a graph of h statistics as giving an exceptionally large h for that level. However, the h statistics for all the other laboratories for that level will be small, even if some of these other laboratories give outliers. The use of the overall average in the calculation of the h statistics can give rise to a similar effect. The use of robust estimates of the standard deviations as the denominators in the h and k statistics, and of robust estimates of the overall averages in the calculation of the h statistics, avoids this distortion. It is therefore recommended that they are used for this purpose.

5.1.6 The data from a precision experiment allow two types of statistic to be calculated:

- a) cell averages, from which a standard deviation can be calculated that gives a measure of between-laboratory variation;
- b) standard deviations or ranges (or differences in a split-level design) within cells that are combined to give a measure of within-laboratory variation.

The robust methods described here do not replace these cell averages, standard deviations or ranges or differences, but provide alternative ways of combining them to obtain the statistics that are used to calculate the repeatability and reproducibility standard deviations.

5.1.7 For example, with the data from one level of the uniform-level design considered in ISO 5725-2, the first stage of the analysis is to calculate the average and standard deviation of the measurement results in each cell. The cell averages are then used to calculate a standard deviation that is a measure of between-laboratory variation. When the robust methods of this clause are used, this calculation is performed using 'Algorithm A' and cell averages are not excluded from the calculation as a result of applying Grubbs' test. Also in this design, the cell standard deviations are pooled to give an estimate of the repeatability standard deviation. With robust analysis, this is performed using 'Algorithm S' and cell standard deviations are not excluded as a result of applying Cochran's test. With either approach (that described in ISO 5725-2 or that described here), the two measures are then used to calculate estimates of the repeatability and reproducibility standard deviations in the same way.

5.1.8 The robust methods that are included in this document were chosen because they can be applied to all the experimental designs given in ISO 5725-2, ISO 5725-3 and ISO 5725-4, and because the calculations they require are relatively simple. It should be noted, however, that they provide a means of combining, in a robust manner, cell averages, cell standard deviations and cell ranges. They do not combine individual test results in a robust manner, i.e. they start with the arithmetic cell averages and the cell standard deviations. There are robust methods that combine test results within cells in a robust manner, and they would be more complicated to apply in practice.

5.2 Robust analysis: Algorithm A

5.2.1 This algorithm yields robust values of the average and standard deviation of the data to which it is applied, and is applied to:

- a) cell averages, in any design;
- b) cell differences, in the split-level design.

5.2.2 Denote the p items of data by:

$$x_1, x_2, \dots, x_i, \dots, x_p$$

Denote the robust average and robust standard deviation of these data by x^* and s^* .

5.2.3 Calculate initial values for x^* and s^* as given by [Formulae \(1\)](#) and [\(2\)](#):

$$x^* = \text{median of } x_i, \quad (i=1, 2, \dots, p) \tag{1}$$

$$s^* = 1,483 \times \text{median of } |x_i - x^*|, \quad (i=1, 2, \dots, p) \tag{2}$$

NOTE The factor of 1,483 is the inverse of the upper quartile for the standard normal distribution ($1/0,6745 = 1,483$) and is the ratio of the standard deviation to the median absolute deviation for a normal distribution.

5.2.4 Update the values of x^* and s^* as in [Formula \(3\)](#).

Calculate:

$$\varphi = 1,5 s^* \quad (3)$$

For each x_i value ($i = 1, 2, \dots, p$), calculate updated values x_i^* following [Formula \(4\)](#):

$$x_i^* = \begin{cases} x^* - \varphi & \text{if } x_i < x^* - \varphi \\ x^* + \varphi & \text{if } x_i > x^* + \varphi \\ x_i & \text{otherwise} \end{cases} \quad (4)$$

Calculate the new values of x^* and s^* from [Formulae \(5\)](#) and [\(6\)](#):

$$x^* = \sum_{i=1}^p x_i^* / p \quad (5)$$

$$s^* = 1,134 \sqrt{\sum_{i=1}^p (x_i^* - x^*)^2 / (p-1)} \quad (6)$$

NOTE The factor 1,134 is a correction factor calculated from the standard deviation for a standard normal distribution with values outside $\pm 1,5$ treated as in [Formula \(4\)](#).

5.2.5 The robust estimates x^* and s^* may be derived by an iterative calculation, i.e. by repeating the calculations in [5.2.4](#) several times, until the change in the estimates of x^* and s^* from one calculation to the next is small (for example, a change of less than 10^{-4} of the previous estimate of either x^* and s^*). This is a simple method to program on a computer.

NOTE It can be useful to check that the results of iterative methods do not change materially with a smaller convergence criterion.

5.2.6 An alternative method that does not involve iteration and so may be easier to apply if the calculations are being done by hand, is derived by observing that [Formulae \(5\)](#) and [\(6\)](#) in [5.2.4](#) may be written as in [Formulae \(7\)](#) and [\(8\)](#):

$$x^* = x' + 1,5(u_U - u_L) s^* / (p - u_L - u_U) \quad (7)$$

$$(s^*)^2 = (p - u_L - u_U - 1)(s')^2 / \left[(p-1) / 1,134^2 - 1,5^2 (pu_L + pu_U - 4u_L u_U) / (p - u_L - u_U) \right] \quad (8)$$

where

u_L is the number of data items x_i for which $x_i < x^* - \varphi$;

u_U is the number of data items x_i for which $x_i > x^* + \varphi$;

x' and s' are the average and standard deviation of the $(p - u_L - u_U)$ data items x_i for which $|x_i - x^*| \leq \varphi$

These may be used to calculate x^* and s^* directly if u_L and u_U are known. One approach is to try the various possibilities in a systematic order (i.e. try $u_L = 0$, $u_U = 0$; then $u_L = 0$, $u_U = 1$; then $u_L = 1$, $u_U = 0$; then $u_L = 1$, $u_U = 1$; and so on) until a valid solution is found in which the actual numbers of items of data more than $1,5 s^*$ from x^* equal the values of u_L and u_U used to calculate x^* and s^* . In practice, the statistical expert will be able to use graphical methods to identify the values that are likely to differ from x^* by more than $1,5 s^*$, and so find the solution by evaluating a small number of cases.

NOTE The derivation for [Formulae \(7\)](#) and [\(8\)](#) is included in [Annex B](#).

5.2.7 A further possibility is to use the iterative method to find an approximate solution, then solve [Formulae \(7\)](#) and [\(8\)](#) to find the exact solution. This approach is illustrated in examples 1 and 3 in [Annex C](#).

5.3 Robust analysis: Algorithm S

5.3.1 This algorithm is applied to within-laboratory standard deviations (or within-laboratory ranges) in any balanced design. It yields a robust pooled value of the standard deviations or ranges to which it is applied.

5.3.2 Denote the p items of data by:

$$w_1, w_2, \dots, w_i, w_p$$

(These may be ranges or standard deviations).

Denote the robust pooled value by w^* , and the degrees of freedom associated with each w_i by v . (When w_i is a range, $v = 1$. When w_i is the standard deviation of n results, $v = n - 1$.) Obtain the values of ξ and η required by the algorithm from [Table 1](#).

5.3.3 Calculate an initial value for w^* as in [Formula \(9\)](#):

$$w^* = \text{median of } w_i \ (i = 1, 2, \dots, p) \quad (9)$$

5.3.4 Update the value of w^* as in [Formula \(10\)](#).

a) Calculate:

$$\psi = \eta \times w^* \quad (10)$$

b) For each $w_i \ (i = 1, 2, \dots, p)$, calculate updated values w_i^* following [Formula \(11\)](#):

$$w_i^* = \begin{cases} \psi & \text{if } w_i > \psi \\ w_i & \text{otherwise} \end{cases} \quad (11)$$

c) Calculate the new value of w^* from [Formula \(12\)](#):

$$w^* = \xi \sqrt{\sum_{i=1}^p (w_i^*)^2 / p} \quad (12)$$

5.3.5 The robust estimate w^* may be derived by an iterative calculation by repeating the calculations in [5.3.4](#) several times, until the change in the estimate of w^* from one calculation to the next is small (for example, 10^{-4} of the previous value). This is a simple method to program on a computer.

5.3.6 An alternative method, that does not involve iteration, and so may be easier to apply if the calculations are being done by hand, is similar to that described in [5.2.6](#). [Formula \(12\)](#) in [5.3.4](#) may be written as in [Formula \(13\)](#):

$$(w^*)^2 = \left[\frac{\xi^2}{p} \right] \times \left[\sum' (w_i^*)^2 + u_U \times (\eta w^*)^2 \right] \quad (13)$$

where

$\sum'$ is the summation over the w_i for which $w_i \leq \psi$
 u_U is the number of w_i for which $w_i > \psi$