TECHNICAL REPORT

ISO/TR 13519

First edition
2012-09-01

Guidance on the development and use of ISO statistical publications supported by software

Lignes directrices pour la rédaction et l'application de publications statistiques ISO utilisant des logiciels

Reference number
ISO/TR 13519:2012(E)

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Published in Switzerland

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

International Standards are drafted in accordance with the rules given in the ISO/IEC Directives, Part 2.

The main task of technical committees is to prepare International Standards. Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

In exceptional circumstances, when a technical committee has collected data of a different kind from that which is normally published as an International Standard ("state of the art", for example), it may decide by a simple majority vote of its participating members to publish a Technical Report. A Technical Report is entirely informative in nature and does not have to be reviewed until the data it provides are considered to be no longer valid or useful.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

ISO/TR 13519 was prepared by Technical Committee ISO/TC 69, *Applications of statistical methods*.

Introduction

This document contains guidance on software to support the development and use of ISO statistical publications.

Aspects covered within this document include

— traceability of data products (figures, tables and other numerical results),

— specification of software,

— categories of support for software, and

— software performance including the use of reference data for testing purposes.

Any references to commercial products of any kind (including but not restricted to software, data or hardware) or links to websites do not imply any approval, endorsement or recommendation by ISO, or any liability.

Guidance on the development and use of ISO statistical publications supported by software

1 Scope

This document provides guidance on the development and use of ISO publications supported by software. The software largely relates to statistical calculations considered by the subcommittees of ISO/TC 69, *Application of statistical methods*, but many other numerical calculations are covered by similar considerations.

In terms of the development of ISO publications, this document gives guidance on the traceability of data products (figures, tables and other numerical results) reproduced in normative-type documents.

In terms of assisting users of ISO publications, this document gives guidance on information that should be included in ISO publications regarding software specification, categories of support for software, and software performance including the use of reference data sets for testing purposes.

Examples are included that illustrate aspects of the guidance provided.

Reference to 'the Committee' in this document relates to the ISO body concerned with developing the relevant ISO publication.

2 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

2.1
algorithm
step-by-step procedure describing a specific calculation, given in sufficient detail that it can be implemented in software

2.2
data product
digital data, including graphical figures expressed digitally, in an ISO publication

EXAMPLE 1 A numerical table in an ISO publication.

EXAMPLE 2 A graphical figure expressed digitally as an array of pixels in an ISO publication.

2.3
domain of applicability
set of inputs for which software can be expected to operate in a valid manner

2.4
numerical accuracy
quality of a numerical value expressed in terms of the number of correct decimal digits in absolute or relative form

2.5
problem parametrization
mathematical representation of a problem involving a specific set of defining parameters

NOTE Generally, a problem has more than one parametrization.

EXAMPLE Straight line in two variables: ISO/TS 28037:2010, *Determination and use of straight-line calibration functions*.

A straight line in the variables X and Y can be parametrized as $Y = A_1 + A_2X$ and as $Y = B_1 + B_2(X - 100)$ (and in other ways). The second form is superior to the first when it is to be used as the model in straight-line regression, where X denotes Celsius temperature, taking values close to 100 °C. See ISO/TS 28037:2010[12].

2.6
reference data
data used for testing an item of software for a specific calculation

2.7
reference result
result corresponding to reference data for a specific calculation

NOTE A reference result is provided independently of test software and to a numerical accuracy that is better than that required of the result provided by the test software.

2.8
test result
result produced by test software for reference data for a specific calculation

2.9
test software
software under test

2.10
unit roundoff
distance from 1,0 to the closest floating-point number strictly less than 1,0

NOTE 1 See IEEE 754:2008[1].

NOTE 2 For the purpose of this Technical Report, floating-point numbers constitute part of the system of numerical computation used for providing statistical results.

NOTE 3 All computed values given in this Technical Report were obtained on a computer having unit roundoff of $2{,}22 \times 10^{-16}$.

3 Traceability of data products

3.1 Digital data, including figures, in an ISO document should be traceable to credible sources. Such data are termed “data product” to distinguish them from source or raw data.

3.2 Such traceability (also known as data provenance) requires knowledge of the source data and the processes by which the data product is derived from the source data. These processes are known as data transformations.

NOTE Traceability is vital in scientific work in general, and statistical applications in particular, concerning the credibility of published data.

3.3 In standards work, it is necessary to understand fully the provenance of a derived data product so that those products can be reproduced and updated as necessary.

NOTE ISO 19115:2003[5] relates to traceability considerations. It is applicable particularly to Geographic Information in the form of digital data, but its principles also apply to non-geographic data. ISO 19115:2003 is typically used for large-scale applications requiring databases. For the purposes of this Technical Report, smaller-scale considerations apply, but some concepts are usefully borrowed from this area.

3.4 For any data product, the source data used and the data transformations applied should be recorded in sufficient detail that the data product could be reproduced. Explicit reference should be given to software used for this purpose.

3.5 If the data product is a graphical figure, traceability relates to normal visual resolution. Otherwise, traceability relates to the number of decimal digits quoted in the ISO publication.

EXAMPLE ISO Technical Specification with data products provided by MATLAB and LaTeX.

Each numerical table in ISO/TS 28037:2010 was produced using a MATLAB script that generated LaTeX source, which was combined with other LaTeX source to provide a PDF version of ISO/TS 28037:2010. The table is a data product that is provided by a transformation (implemented in the MATLAB script) of a data set that corresponded to the data points — the source data — or data derived similarly from the source data. Any change at the drafting stage in the source data or transformations was hence reflected in the resulting data product. Consequently no human transcription error was incurred and the numerical tables (and accompanying text) would be reproducible through re-use of this process.

The source data and details of the transformations were recorded in ISO/TS 28037:2010.

NOTE 1 ISO Central Secretariat can provide a suitable website to hold traceability records including software.

NOTE 2 MATLAB is the trade name of a product supplied by The MathWorks Inc.

3.6 The rounding rules given in Annex B of ISO 80000-1:2009[6] apply to the expression of decimal numbers.

4 Specification of software

An ISO publication should contain a specification of software that would materially assist in using that publication. The software of concern largely relates to statistical calculations. The specification would include details of

a) the inputs to the software,

b) the outputs from the software,

c) how the outputs are obtained from the inputs,

d) how the inputs and outputs and relevant intermediate values relate to the various (sub)clauses and quantities in the ISO publication, and

e) the performance of the software, particularly in terms of the numerical accuracy required in the results produced. Also see 6.2.

EXAMPLE 1 ISO 13528:2005, *Statistical methods for use in proficiency testing by interlaboratory comparisons*

Subclause 8.6 of ISO 13528:2005[4] is concerned with producing a graph of repeatability standard deviation for each laboratory involved in a proficiency testing scheme against the corresponding average for the laboratory. It also specifies the construction of a confidence region corresponding to a particular significance level 1 – P under the assumption of normality. The generic specification in this case for such a graph is as follows:

a) Software inputs

p number of participating laboratories,

n number of replicate indication values,

x_i average indication value for laboratory i, $i = 1, \ldots, p$,

s_i within-laboratory standard deviation for laboratory i, $i = 1, \ldots, p$, and

P significance level (for example, 0,05).

b) Software outputs

x x-coordinates used in defining the boundary of the region having a significance level of 100P %, and

s corresponding y-coordinates.

c) Outputs obtained from inputs using

values of x lying in the interval $\bar{X} - (v/n)^{1/2}\bar{S}$ to $\bar{X} + (v/n)^{1/2}\bar{S}$, where $v = \chi^2_{2;1-P}$, and

values of s, corresponding to those of x, equal to $\bar{S}\exp\left(\pm(2n-2)^{-1/2}\left\{v - \left[n^{1/2}(x - \bar{X})/\bar{S}\right]^2\right\}^{1/2}\right)$,

where

$\bar{X} = x^*$, the robust average of $x_1, \ldots, x_p$, and $\bar{S} = s^*$, the robust pooled value of $s_1, \ldots, s_p$ [see d)].

d) Inputs and outputs and relevant intermediate values relate to the various (sub)clauses and quantities as follows:

Items in a) and b) and how items in b) are obtained from those in a) are described in subclause 8.6.1 of ISO 13528:2005,

x^* is calculated by Algorithm A in Annex C.1 of ISO 13528:2005,

s^* is the value of w^* calculated by Algorithm S in Annex C.2 of ISO 13528:2005, and

the expression for s is given in Formula (41) of ISO 13528:2005.

e) Performance of the software

Standard deviations are expressed to a prescribed number of significant decimal digits (usually one or two), and related averages expressed to the same number of decimal places, for inputs lying within a stated domain of applicability.

In any particular instance, numerical values for the inputs (p, n, the x_i, the s_i and P) would be provided. Figure 11 in ISO 13528:2005 is a specific instance of a graph produced by plotting the points (x_i, s_i), $i = 1, \ldots, p$. It also shows the boundaries of confidence regions corresponding to a significance level P, for $P = 0{,}001, 0{,}01, 0{,}05$.

EXAMPLE 2 ISO/TS 28037:2010, Determination and use of straight-line calibration functions

Clause 9 of ISO/TS 28037:2010[12] is concerned with obtaining estimates a and b of the parameters A and B in a straight-line calibration function $Y = A + BX$ relating variables X and Y. Measured values (data points) x_i and y_i of X and Y are available, as are associated standard uncertainties $u(y_i)$ and covariances $\text{cov}(y_i, y_j)$ associated with each pair (y_i, y_j), $i = 1, \ldots, m$, $j = 1, \ldots, m, j \neq i$. Uncertainties associated with the x_i are regarded as negligibly small in this clause of ISO/TS 28037:2010, as are other covariances. The specification in this case is as follows:

a) Software inputs

m	number of data points,
x_i	measured value of X-coordinate of the ith data point, $i = 1, \ldots, m$,
y_i	measured value of Y-coordinate of the ith data point, $i = 1, \ldots, m$,
$u(y_i)$	standard uncertainty associated with y_i, $i = 1, \ldots, m$, and
$\text{cov}(y_i, y_j)$	covariance associated with pair (y_i, y_j), $i = 1, \ldots, m, j = 1, \ldots, m, j \neq i$.

b) Software outputs

a	estimate of A,
b	estimate of B,
$u(a)$	standard uncertainty associated with a,
$u(b)$	standard uncertainty associated with b, and
$\text{cov}(a, b)$	covariance associated with a and b.

c) Outputs obtained from inputs using algorithm given in subclause 9.2.2 of ISO/TS 28037:2010.

NOTE A software implementation is provided at http://standards.iso.org/iso/ts/28037/ .

d) Inputs and outputs and relevant intermediate values relate to the various (sub)clauses and quantities as follows:

Items in a) and b) and how items in b) are obtained from those in a) are described in subclauses 9.1 and 9.2 of ISO/TS 28037:2010.

e) Performance of the software

The software obtains results having adequate numerical accuracy for practical calibration problems, by the use of stable numerical methods (see 6.2). The software reproduces the data products (figures, tables and other numerical results) in ISO/TS 28037:2010 in accordance with Clause 3.

5 Software support

5.1 Support for software implementation

5.1.1 The Committee should consider any software aspects relevant to an ISO publication with which it is concerned and the consequent categories of support to be provided. Categories of support for the task in hand relate to the following:

0 no support;

1 general-purpose software provided by a third party;

2 specific software provided by a third party;

3 stand-alone software accompanying the ISO publication, that is, software that can be run by the user of the ISO publication;

4 sample code included in the ISO publication for extension or generalization by users or third parties;

5 an algorithm (step-by-step procedure) for implementation as software by users or third parties.

The categories of support to be provided in any particular case should be stated in the Scope of the relevant ISO publication, and the Committee should be prepared to provide such support.

NOTE 1 The “third party” is the provider of the software, the first party being the user of the ISO publication, and the second party the Committee involved in preparing the publication.

NOTE 2 Instances of 2 and 3 are given in 5.1.3 Example.

5.1.2 The following information should be given in the relevant ISO publication where appropriate:

a) domain of applicability of the software;

b) numerical accuracy expected in the outputs from application of the software. A measure of the sensitivity of the outputs to changes in the inputs can also be given. Also see 6.2.4;

NOTE The numerical accuracy in general depends on the input data and is specific to that data.

c) any results to be provided by the software in addition to the outputs. Such results may be those of intermediate calculations;

d) execution time and memory requirements of the software.

EXAMPLE The time to compute a median for N input data is comparable to that required to sort N floating-point numbers using a fast sorting algorithm.

The Committee should consider which of a) to d) apply to the relevant ISO publication, and in terms of these the appropriate categories of support in 5.1.1.

NOTE 1 Since execution time in d) depends on many factors, including hardware and programming language, this time can be stated in a relative sense.

NOTE 2 Software performance issues are considered in 6.2.

