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ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Fax: +41 22 749 09 47
Email: copyright@iso.org
Website: www.iso.org

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Foreword

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Nuclear energy — Guidance to the evaluation of measurement uncertainties of impurity in uranium solution by linear regression analysis

1 Scope

This document provides a method for evaluation of the measurement uncertainty arising when an impurity content of uranium solution is determined by a regression line that has been fitted by the "method of least squares". It is intended to be used by chemical analyzers.

Simple linear regression, hereinafter called "basic regression", is defined as a model with a single independent variable that is applied to fit a regression line through n different data points (x_i, y_i) (i = 1,..., n) in such a way that makes the sum of squared errors, i.e. the squared vertical distances between the data points and the fitted line, as small as possible. For the linear calibration, "classical regression" or "inverse regression" is usually used; however, they are not convenient. Instead, "reversed inverse regression" is used in this document[2].

Reversed inverse regression treats y (the reference solutions) as the response and x (the observed measurements) as the inputs; these values are used to fit a regression line of y on x by the method of least squares. This regression is distinguished from basic regression in that the x_i's (i = 1,..., n) vary according to normal distributions but the y_i's (i = 1,..., n) are fixed; in basic regression, the y_i's vary but the x_i's are fixed.

The regression line fitting, calculation of combined uncertainty, calculation of effective degrees of freedom, calculation of expanded uncertainty, reflection of reference solutions' uncertainties in the evaluation result, and bias correction are explained in order of mention. Annex A presents a practical example of uncertainty evaluation. Annex B provides a flowchart showing the steps for uncertainty evaluation. In addition, Annex C explains the use of weighting factors for handling non-uniform variances in reversed inverse regression.

NOTE 1 In the case of classical regression, the fitted regression line is inverted prior to actual sample measurement[3]. In the case of inverse regression, the roles of x and y are not consistent with the convention that the variable x represents the inputs, whereas the variable y represents the response. For these reasons, the two regressions are excluded from this document.

NOTE 2 The term "reversed inverse regression" was suggested taking into account the history of regression analysis theory. Instead, it can be desirable to use some other term, e.g. "pseudo-basic regression".

2 Normative references

There are no normative references in this document.

3 Terms and definitions

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

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at http://www.electropedia.org/

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3.1
calibration
fitting of a regression line of *y* on *x* through *n* data points using the method of least squares

Note 1 to entry: The *n* data points are typically obtained by measuring *n* different reference solutions. After the fitting, the fitted regression line is used as a measurement formula for determining the physical or chemical quantity of a sample.

3.2
calibration quality control factor
factor that is used to check the adequacy of the fitted regression line from the aspect of calibration quality

3.3
calibration uncertainty
uncertainty due to such possible variations of the slope and intercept supposing that the regression line fitting is repeated according to the same procedure using a "new set of *n* different reference solutions" each time

Note 1 to entry: In this case, the fitted regression line will be different each time, i.e. the slope and intercept of the fitted regression line will vary.

3.4
combined uncertainty
uncertainty obtained by combining the *calibration uncertainty* (3.3) and the *random uncertainty of sample measurement* (3.9) according to the error propagation rule

3.5
effective degrees of freedom
degrees of freedom calculated by Welch-Satterthwaite approximate formula

3.6
expanded uncertainty
multiplication of the combined uncertainty u_y by a coverage factor k given depending on the effective degrees of freedom of the *combined uncertainty* (3.4)

Note 1 to entry: The probability that the true value of the physical or chemical quantity will be within ± the "final expanded uncertainty" from the determined and bias-corrected value is "exactly" or "approximately" 95 %; in most cases, "approximately" is more suitable expression.

3.7
predicted *y* value
y value of a point on the fitted regression line

Note 1 to entry: The predicted *y* value given by the regression line formula $y = a + bx$ indicates the physical or chemical quantity that will be determined in response to the light or current signal intensity "*x*" measured by instrument. The square root of the estimate for the variance of the predicted *y* value is treated as the calibration uncertainty in this document.

3.8
prediction interval
possible vertical distance between the additional data point and the previously fitted regression line after a regression line has been fitted using a set of *n* data points

Note 1 to entry: Another data point is additionally produced by measuring "a new reference solution".

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3.9
random uncertainty of sample measurement
<ICP-AES> possible uncertainty that may arise during such a sample measurement supposing that the intensity of the light with a specific wavelength emitted from a sample is measured to determine the sample's impurity content following the regression line fitting

Note 1 to entry: This uncertainty is typically estimated based on multiple measurements of the sample and should not be inferred from the mean squared error.

3.10
uncertainty
concept corresponding to the square root of "variance (or estimate for that variance)" that is handled mainly in statistics

3.11
weighting factors
numbers by which the variances are multiplied in weighted least squares (WLS) regression

Note 1 to entry: OLS (ordinary least squares) regression handles the uniform variances. However, in WLS regression, the variances are assumed to be non-uniform and the weighting factors are used to handle the non-uniform variances.

Note 2 to entry: Let $\sigma_{x1}^2,\ldots, \sigma_{xn}^2$ be the variances of the variables $x_1,\ldots, x_n$ respectively. Then, in OLS regression, $\sigma_{x1}^2 = \cdots = \sigma_{xn}^2$ $(= \sigma_x^2)$, whereas, in WLS regression, typically $\sigma_{x1}^2 \neq \cdots \neq \sigma_{xn}^2$. However, even in the case of WLS regression, the equality $w_1\sigma_{x1}^2 = \cdots = w_n\sigma_{xn}^2$ $(= \sigma_x^2)$ can be established by utilizing the weighting factors w_i's $(i = 1,\ldots, n)$.

4 Principle

In practice, a single regression line fitting will be run for calibration. Nevertheless, supposing that the regression line fitting is repeated using a "new set of n different reference solutions" each time, the slope and intercept of the fitted regression line will be different each time; as a result, it can be observed that the predicted y value varies according to an approximately normal distribution. Such a possible variation of the predicted y value is the cause of the calibration uncertainty that arises during the regression line fitting. In this regard, there is a helpful statistical theory. With the aid of that theory, although calibration experts do not repeat the regression line fitting, they can estimate the variance of the predicted y value using only one set of n data points that have been used for a regression line fitting. In practical calibrations, the square root of such an estimated variance of the predicted y value is treated as the calibration uncertainty, and its degrees of freedom is $n - 2$.

Two components contribute to the uncertainty of the physical or chemical quantity determined by the fitted regression line. One is the calibration uncertainty previously mentioned and the other is the random uncertainty of sample measurement. The two uncertainties are combined and then the effective degrees of freedom of the combined uncertainty is calculated. The effective degrees of freedom, V_{eff}, is obtained by substituting the degrees of freedom of the calibration uncertainty and the degrees of freedom of the random uncertainty together into Welch-Satterthwaite approximate formula.

As the next step, the expanded uncertainty is obtained by multiplying the combined uncertainty u_y by a coverage factor k that is given depending on the effective degrees of freedom of the combined uncertainty.

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