INTERNATIONAL STANDARD

ISO 24185

First edition
2022-08

Evaluation of the uncertainty of measurements from a stationary autocorrelated process

Évaluation de l'incertitude de mesure d'un processus stationnaire autocorrélé

Reference number
ISO 24185:2022(E)

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Published in Switzerland

Contents

Page

Foreword

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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*.

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Introduction

In metrology, it is common practice that the dispersion or standard deviation of the average of repeated measurements, i.e., the standard uncertainty of the sample mean, is calculated by the sample standard deviation of the measurements divided by the square root of the sample size. The calculated standard uncertainty is an estimator of the standard deviation of the sample mean when the repeated measurements have the same mean and variance and are uncorrelated. However, it often happens that the measurements are correlated. In continuous productions such as in the chemical industry, most process data on quality characteristics are self-correlated over time or autocorrelated. In general, autocorrelation can be caused by the measuring system, the dynamics of the process, or both. In many cases, the data can exhibit a drifting behaviour. In biology, random biological variation, for example, the random burst in the secretion of some substance that influences the blood pressure, can have a sustained effect so that several consecutive measurements are all influenced by the same random phenomenon. In data collection, when the sampling interval is short, autocorrelation, especially positive autocorrelation of the data, is a concern.

When the measurements are from an autocorrelated process, it is inappropriate to evaluate the standard uncertainty of the sample mean as described above. As stated in ISO/IEC Guide 98-3:2008, 4.2.7, “If the random variations in the observations of an input quantity are correlated, for example, in time, the mean and experimental standard deviation of the mean as given in 4.2.1 and 4.2.3 may be inappropriate estimators (C.2.25) of the desired statistics (C.2.23).”

Autocorrelated processes can be classified to be two kinds of processes based on whether they are stationary or nonstationary:

a) Stationary process – a direct extension of an independent and identically distributed (i.i.d.) sequence. An autocorrelated process is stationary if it is in a state of “statistical equilibrium”. This implies that the basic behaviour of the process does not change in time. In particular, a stationary process has a mean and variance that are constants over time;

b) Nonstationary process – a process that is not stationary.

The aim of this document is to provide a method to evaluate the standard uncertainty of the mean of measurements from a stationary process.

Evaluation of the uncertainty of measurements from a stationary autocorrelated process

1 Scope

This document describes a method to evaluate the standard uncertainty for a process mean, arising from observable variation in successive possibly autocorrelated measurements. In this document, the successive measurements are restricted to stationary processes. This document also includes tests for validity of assumptions. The resulting uncertainty is related to that arising from observable measurements while other sources of uncertainty are also considered.

2 Normative reference

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 3534-2, *Statistics — Vocabulary and symbols — Part 2: Applied statistics*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 3534-2 and the following 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/

3.1 Terms

3.1.1
covariance stationary process
weakly stationary process
stationary process
stochastic process characterized by a constant process mean, a constant process variance and an autocovariance function which only depends on the difference of the process indices and does not depend on the process index

3.1.2
autocovariance
internal covariance between members of a sequence of ordered observations

3.2 Abbreviated terms and symbols

3.2.1 Abbreviated terms

i.i.d.	independent and identically distributed
ACF	autocorrelation function

3.2.2 Symbols

T	index set for a stochastic process
X_t	random variable X at time t
$X_{t,\mathrm{A}}$	component of X_t which has the Type A uncertainty component of X_t
e_{B_t}	component of X_t which has zero mean and the Type B uncertainty component of X_t
μ_t	true mean of X_t
μ	true process mean of a stationary process
σ_t	true standard deviation of X_t
σ	true process standard deviation of a stationary process $\{X_t\}$
σ_A	true standard deviation of $X_{t,\mathrm{A}}$ for a stationary process $\{X_t\}$
σ_B	true standard deviation of e_B for a stationary process $\{X_t\}$
u_B	Type B evaluation of the standard uncertainty of $\{X_t\}$
$N\left(\mu,\sigma^2\right)$	normal distribution with mean μ and variance σ^2
$\gamma(t_1,t_2)$	autocovariance between X_{t_1} and X_{t_2}
$\rho(t_1,t_2)$	autocorrelation between X_{t_1} and X_{t_2}
τ	index lag between two process indices
$\gamma(\tau)$	autocovariance of a stationary process at lag τ
$\hat{\gamma}(\tau)$	estimator of $\gamma(\tau)$
$\rho(\tau)$	autocorrelation of a stationary process at lag τ
$\hat{\rho}(\tau)$	estimator of $\rho(\tau)$
$\hat{\sigma}_{\hat{\rho}(i)}$	estimator of standard deviation of $\hat{\rho}(i)$
x_t	a value of X_t at index t
$\bar{x}$	arithmetic mean value of a sequence of x
s_x	sample standard deviation of a sequence of x

4 Stochastic process and time series

4.1 General

A stochastic process $\{X_t; t \in T\}$ is a collection of random variables, where T is an index set[3] of the process. When T represents time, the stochastic process is referred as a time series. When T takes on a discrete set of values, e.g. $T = \{1, 2, ...\}$, the process is said to be a discrete time series. In this document, only discrete time series that are equally spaced in time are considered. A discrete time series $x_1, ..., x_N$ can be viewed as the values taken on by a sequence of random variables of $X_1, ..., X_N$. The sequence of $x_1, ..., x_N$ is called a realization of $X_1, ..., X_N$.

4.2 Autocovariance and autocorrelation of a stochastic process

If $\{X_t; t \in T\}$ is a stochastic process with mean μ_t and standard deviation σ_t at t,

a) for any $t_1, t_2 \in T$, the autocovariance function $\gamma(\cdot)$ is:

$$\gamma(t_1, t_2) = \mathrm{E}\left[\left(X_{t_1} - \mu_{t_1}\right)\left(X_{t_2} - \mu_{t_2}\right)\right]$$

b) for any $t_1, t_2 \in T$, the autocorrelation function $\rho(\cdot)$ is:

$$\rho(t_1, t_2) = \frac{\gamma(t_1, t_2)}{\sigma_{t_1}\sigma_{t_2}}$$

For a stochastic process or a time series, if there exist non-zero $\rho(t_1, t_2)$ for any $t_1 \neq t_2$, then the stochastic process or the time series is called autocorrelated.

4.3 Stationary process

4.3.1 General

As defined in 3.1.1, a stationary process means a weakly stationary or covariance stationary process. A stochastic process is said to be stationary if it is in a state of "statistical equilibrium", See Reference [4], p. 14. Namely, the basic behaviour of such a process does not change with the process index. The stochastic process $\{X_t; t \in T\}$ is said to be covariance stationary or weakly stationary, or stationary, in this document if:

a) $\mathrm{E}[X_t] = \mu$ (constant for all t);

b) the variance $\mathrm{Var}[X_t] = \sigma^2 < \infty$ (i.e., a finite constant for all t);

c) $\gamma(t_1, t_2)$ depends only on lag $\tau = t_1 - t_2$ and does not depend on t. In this case, $\gamma(t_1, t_2)$ is denoted by $\gamma(\tau) = \gamma(t_1, t_2) = \gamma(|t_1 - t_2|)$.

The first two requirements are that the stochastic process has constant mean and constant variance. The third requirement is that the autocovariance function only depends on the lag and does not depend on t. If one or more of these requirements are not met, the process is nonstationary. For a stationary process, the autocovariance function at lag τ is denoted by $\gamma(\tau)$. When the process is a time series, the difference in process indices, $t_1 - t_2$ corresponds to a time difference.

The autocorrelation function (ACF) of a stationary process or a time series at lag τ is given by:

$$\rho(\tau) = \frac{\gamma(\tau)}{\sigma^2}$$

Note that $\rho(0) = 1$.

4.3.2 White noise

A time series is called white noise if:

a) $\{X_t\}$ are identically distributed with a same mean and same finite variance for all t;

b) the autocovariance $\gamma(t_1, t_2) = 0$ when $t_1 \neq t_2$ for any t_1 and t_2.

It follows from b) that all autocorrelations of white noise with non-zero lags are zero. From a) and b), white noise is a special case of a stationary process. When $\{X_t\}$ is white noise with the same distribution for each t, it is an i.i.d. sequence.

4.4 Estimation of the mean, autocovariance, and autocorrelation for a stationary process

4.4.1 Estimation of μ

Given a realization $\{x_t; t=1,2,...,N\}$ of a stationary process $\{X_t\}$, as a common practice the process mean μ is estimated by the arithmetic mean or sample mean $\bar{x} = \frac{1}{N}\sum_{t=1}^{N} x_t$.

4.4.2 Estimation of $\gamma(\tau)$ and $\rho(\tau)$

Given a realization of a stationary process, $\{x_t; t=1,2,...,N\}$, the autocovariance at τ is estimated by:

$$\hat{\gamma}(\tau) = \frac{1}{N}\sum_{t=1}^{N-|\tau|}(x_t - \bar{x})(x_{t+|\tau|} - \bar{x}) \text{ for } \tau = -(N-1),...,-1,0,1,...,(N-1) \text{ and zero for } |\tau| \geq N \text{ [3].}$$

In particular, when $\tau = 0$ $\hat{\gamma}(0)$ is an estimator of the process variance. In practice, the traditional sample variance s_X^2, which uses $N-1$ in the denominator instead of N is often used in place of $\hat{\gamma}(0)$. The corresponding estimator of the autocorrelation called the sample autocorrelation is given by Formula (1):

$$\hat{\rho}(\tau) = \frac{\hat{\gamma}(\tau)}{\hat{\gamma}(0)} = \frac{\sum_{t=1}^{N-|\tau|}(x_t - \bar{x})(x_{t+|\tau|} - \bar{x})}{\sum_{t=1}^{N}(x_t - \bar{x})^2} \tag{1}$$

In practice, to obtain a useful estimate of the autocorrelation function, a practical rule (see Reference [5], p. 32) is $N \geq 50$ and $|\tau| \leq N/4$.

4.5 Tests of autocorrelation of stationary process data

A simple test of whether the process data is independent white noise is given by constructing the sample autocorrelation function (ACF) with a confidence band. The sequence $\hat{\rho}(i)$, for $i = 1,\ldots,N$, of sample autocorrelation values is formed from the values $x_1,\ldots,x_N$. For $i \geq 1$, about 95 % of the $\hat{\rho}(i)$ should fall between the bounds $\pm 1{,}96/\sqrt{N}$.

NOTE This test uses the result that, for large N, the sample autocorrelations, $\{\hat{\rho}(\tau)\}$, of an independent white noise sequence $X_1,\ldots,X_N$ with finite variance are approximately independently and identically normally distributed with zero mean and variance $1/N$ (see Reference [6], p. 222-223 and Reference [5], p. 32-34). This approach is often used to check whether the process data is autocorrelated[6][7].

The variance of a sample autocorrelation is used to check whether the autocorrelation is significantly different from zero. The standard deviation of the sample autocorrelation at lag i is approximated by Reference [8] as given by Formulae (2)and (3):

$$\hat{\sigma}_{\hat{\rho}(1)} = 1/\sqrt{N} \tag{2}$$

and

$$\hat{\sigma}_{\hat{\rho}(i)} = \sqrt{\frac{1+2\sum_{k=1}^{i-1}\hat{\rho}^2(k)}{N}} \quad \text{for } i=2,3,... \tag{3}$$

Based on that,

$$|\,\hat{\rho}(i)\,| > 1,96\sqrt{\frac{1}{N}} \quad \text{for } i=1 \tag{4}$$

and

$$|\,\hat{\rho}(i)\,| > 1,96\sqrt{\frac{1+2\sum_{k=1}^{i-1}\hat{\rho}^2(k)}{N}} \quad \text{for } i=2,3,... \tag{5}$$

is evidence against $\rho(i)=0$ at the $\alpha=0,05$ level for $i=1,2,3,...$. That is, if the inequality in Formula (4) or Formula (5) holds, it indicates that the hypothesis that $\rho(i)=0$ does not hold at the $\alpha=0,05$ level.

Statistical process control procedures as given in ISO 7870-9 can be applied to check whether a sequence of measurements is from a stationary process regarding constant mean and variance.

5 Uncertainty of a sample mean for stationary measurements

In metrology, when $\{x_1,...,x_N\}$ is a realization of the mutually independently and identically distributed random variables, $\{X_1,...,X_N\}$, the standard uncertainty of the sample mean $\bar{x}$ is calculated as:

$$u_{\bar{x}} = \frac{s_x}{\sqrt{N}} \tag{6}$$

where s_x is the sample standard deviation of the measurements (see ISO/IEC Guide 98-3:2008, 4.2.3). However, in many cases, the measurements are autocorrelated. ISO/IEC Guide 98-3:2008, 4.2.7 states “If the random variations in the observations of the input quantity are correlated, for example, in time, the mean and experimental standard deviation of the mean as given in 4.2.1 and 4.2.3 may be inappropriate estimators of the desired statistics.”

For a stationary process, the process mean is estimated by the sample mean:

$$\bar{X}=\frac{X_1+\ldots+X_N}{N}$$

From Reference [8], the variance of $\bar{X}$ is calculated by:

$$\mathrm{Var}[\bar{X}]=\left[1+\frac{2}{N}\sum_{i=1}^{N-1}(N-i)\rho(i)\right]\frac{\sigma^2}{N} \tag{7}$$

where σ is the process standard deviation and $\rho(i)$ is the process autocorrelation at lag i. Note that Formula (6) is a special case of Formula (7) when $\{X_1,...,X_N\}$ is white noise. Given a sequence of stationary measurements $\{x_1,...,x_N\}$, σ and $\rho(i)$ can be estimated by the corresponding sample statistics and the standard uncertainty of $\bar{x}$ is given by:

$$u_{\bar{x}}=\sqrt{1+\frac{2}{N}\sum_{i=1}^{N-1}(N-i)\hat{\rho}(i)}\,\frac{s_x}{\sqrt{N}} \tag{8}$$

where s_x is the sample standard deviation based on $\{x_1,...,x_N\}$, and $\hat{\rho}(i)$ is an estimate of the autocorrelation $\rho(i)$ at lag i. In Formula (8), the significant $\hat{\rho}(i)$ can be determined by Formula (4) or (5). Define

$$N_{\mathrm{c}}=\max\{i\,\|\hat{\rho}(i)|>1,96\hat{\sigma}_{\hat{\rho}(i)}\} \tag{9}$$

which is the maximum value of i for which $|\hat{\rho}(i)|>1,96\hat{\sigma}_{\hat{\rho}(i)}$. The standard deviation, $\hat{\sigma}_{\hat{\rho}(i)}$, is given in Formulae (2) and (3). To have a useful estimate of sample autocorrelation as discussed in 4.4.2, a practical requirement that only those autocorrelations $\hat{\rho}(i)$ with $|i|\le N/4$ are included in Formula (8) is proposed. Combining that with the requirement on the significant autocorrelations, the upper limit in the summation in Formula (8) is replaced by Formula (10):

$$N_{\mathrm{r}}=\min\{N_{\mathrm{c}},[N/4]\} \tag{10}$$

so that only the practically reasonable $\hat{\rho}(i)$ are included, where $[x]$ means the integer part of x. In practice, the standard uncertainty of the average of measurements from a stationary process is calculated from

$$u_{\bar{x}}=\sqrt{1+\frac{2}{N}\sum_{i=1}^{N_{\mathrm{r}}}(N-i)\hat{\rho}(i)}\,\frac{s_x}{\sqrt{N}} \tag{11}$$

Note that since $\mathrm{Var}[\bar{X}]>0$ from Formula (7), $1+\frac{2}{N}\sum_{i=1}^{N-1}(N-i)\rho(i)$ is positive. However, $1+\frac{2}{N}\sum_{i=1}^{N_r}(N-i)\hat{\rho}(i)$ in Formula (11) may be negative. This may happen due to

a) the process being nonstationary,

b) the bias of $\hat{\rho}(i)$ from $\rho(i)$, and

c) the choice of the cut-off point for the upper limit of the summation in Formula (11).

If the process is nonstationary, Formula (11) cannot be used. From b), to reduce the bias of $\hat{\rho}(i)$ from $\rho(i)$, consider increasing the size of data set. Anyway, if $1+\frac{2}{N}\sum_{i=1}^{N_r}(N-i)\hat{\rho}(i)<0$, the use of

Formula (11) is questionable and the assumption of the process stationarity should be checked. However, most autocorrelated measurements in practice are positively autocorrelated. In this case, a negative variance estimate for $\bar{X}$ is unlikely to arise.

For illustration, three practical examples are presented in Annex A.

6 Stationary measurements with Type B evaluation of uncertainty

Until now, the measurement uncertainty is based on the observable measurements only. That is, the uncertainty is based on statistical analysis of data or Type A evaluation only (see ISO/IEC Guide 98-3:2008, 3.3.5). However, in metrology the Type B evaluation of uncertainty, which is not based on statistical analysis of data, cannot be ignored. Assume that for a stationary process $\{X_t\}$, each random variable X_t can be expressed as given by Formula (12):

$$X_t = X_{t,\mathrm{A}} + e_{\mathrm{B}_t} \tag{12}$$

with a Type A evaluation of the random variable $X_{t,\mathrm{A}}$ and a Type B evaluation of the zero-mean random variable e_{B_t}. Components $X_{t,\mathrm{A}}$ and e_{B_t} are statistically independent for all t, and their corresponding standard deviations are σ_A and σ_B, respectively[7]. Thus,

$$\mathrm{Var}[X_t] = \sigma_\mathrm{A}^2 + \sigma_\mathrm{B}^2.$$

The standard uncertainty of $\{X_t\}$ based on Type B evaluation is denoted by u_B, which is an estimate of σ_B. From Reference [8] and Formula (11), the standard uncertainty $u_{\bar{x}}$ of a sequence of stationary measurements $\{x_1, \ldots, x_N\}$ is given by Formula (13):

$$u_{\bar{x}} = \sqrt{\left[1 + \frac{2}{N}\sum_{i=1}^{N_\mathrm{r}}(N-i)\hat{\rho}(i)\right]\frac{s_X^2}{N} + u_\mathrm{B}^2} \tag{13}$$

where N_r is given by Formulae (9) and (10).

7 The case of a weighted mean

In metrology, a weighted mean of a random sample constituting a sequence of values of size N is often used to estimate the mean. That is

$$\bar{X}_w = \sum_{t=1}^{N} w_t X_t$$

where $\{w_t, t = 1,...,N\}$ are constant weights with $w_t \geq 0$ and $\sum_{t=1}^{N} w_t = 1$. Similar to Formula (7), when the process is stationary and the weights are not random,

$$\mathrm{Var}[\bar{X}_w] = \sigma^2 \left[\sum_{i=1}^{N} w_i^2 + 2\sum_{i=1}^{N-1} \rho(i) \sum_{j=1}^{N-i} w_j w_{j+i} \right] \tag{14}$$

Note that when $w_i = 1/N$ for $i = 1,...,N$, Formula (14) becomes Formula (7). From Formula (14), the corresponding standard uncertainty of a sequence of stationary measurements $\{x_1,...,x_N\}$ is obtained by Formula (15):

$$u_{\bar{X}_w}^2 = s_x^2 \left[\sum_{i=1}^{N} w_i^2 + 2\sum_{i=1}^{N_r} \hat{\rho}(i) \sum_{j=1}^{N-i} w_j w_{j+i} \right] \tag{15}$$

For the case in which both Type A evaluation and Type B evaluation of uncertainty are presented, with the same assumption as made in Formula (12), see Formula (16):

$$\bar{X}_w = \sum_{t=1}^{N} w_t X_{t,\mathrm{A}} + e_{\mathrm{B}_t} \tag{16}$$

When the weights are known, similar to Formula (14) the uncertainty of the weighted mean is given by Formula (17):

$$u_{\bar{X}_w}^2 = s_x^2 \left[\sum_{i=1}^{N} w_i^2 + 2\sum_{i=1}^{N_\mathrm{r}} \hat{\rho}(i) \sum_{j=1}^{N-i} w_j w_{j+i} \right] + u_\mathrm{B}^2 \tag{17}$$

Annex A
(informative)

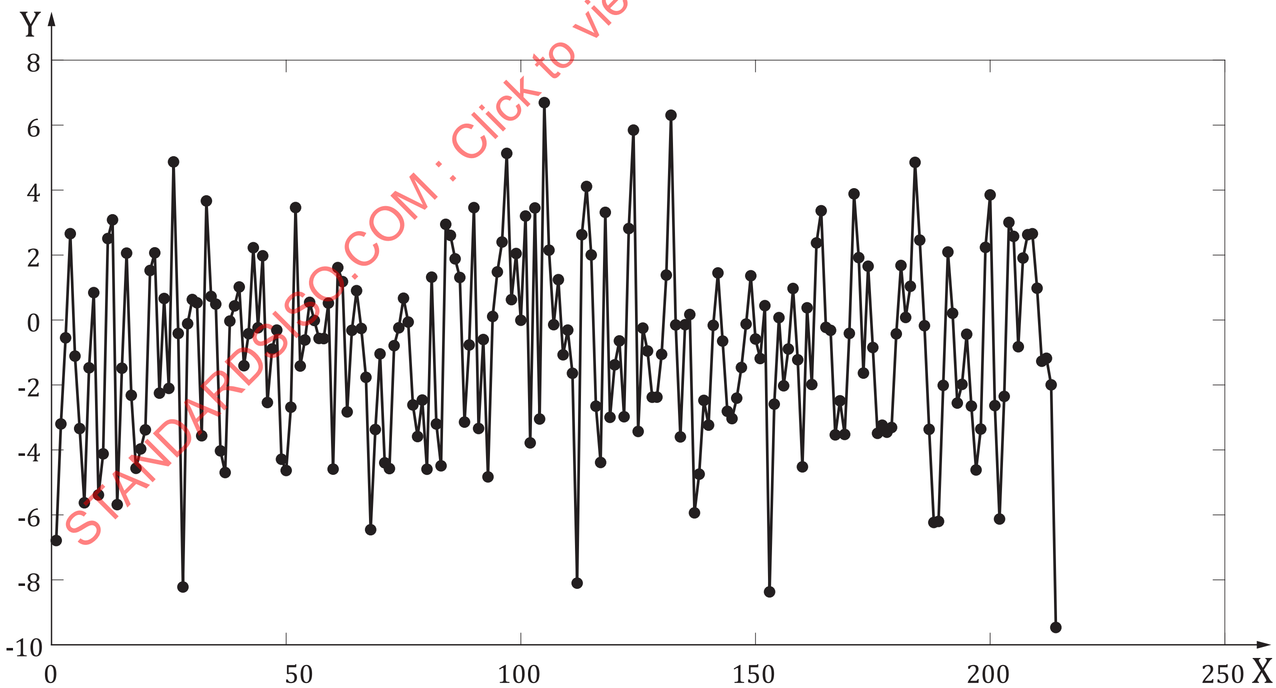
Three practical examples

A.1 General

For illustration of the method, three practical examples are presented. The measurement data as time series are plotted. Successive points are joined by straight lines to facilitate visualization. For each time series, the corresponding autocorrelations are presented by autocorrelation function (ACF) plots[3]. In each ACF plot, assuming the time series is white noise an approximate 95 % confidence band is given by two broken lines. In addition, when the time series is a stationary process an approximate 95 % confidence band constructed by two solid lines is shown to demonstrate whether each autocorrelation is significantly different from zero.

A.2 Example 1

A study was made of the voltage difference of two Josephson voltage standards. There are 214 pressure-adjusted voltage measurements taken at equal time intervals. From the data, shown in Figure A.1, it is reasonable to treat the process as stationary. In addition, appropriate process control procedures in ISO 7870-9 are applied to the data indicating the mean and variance of the process may be treated as constants, respectively.



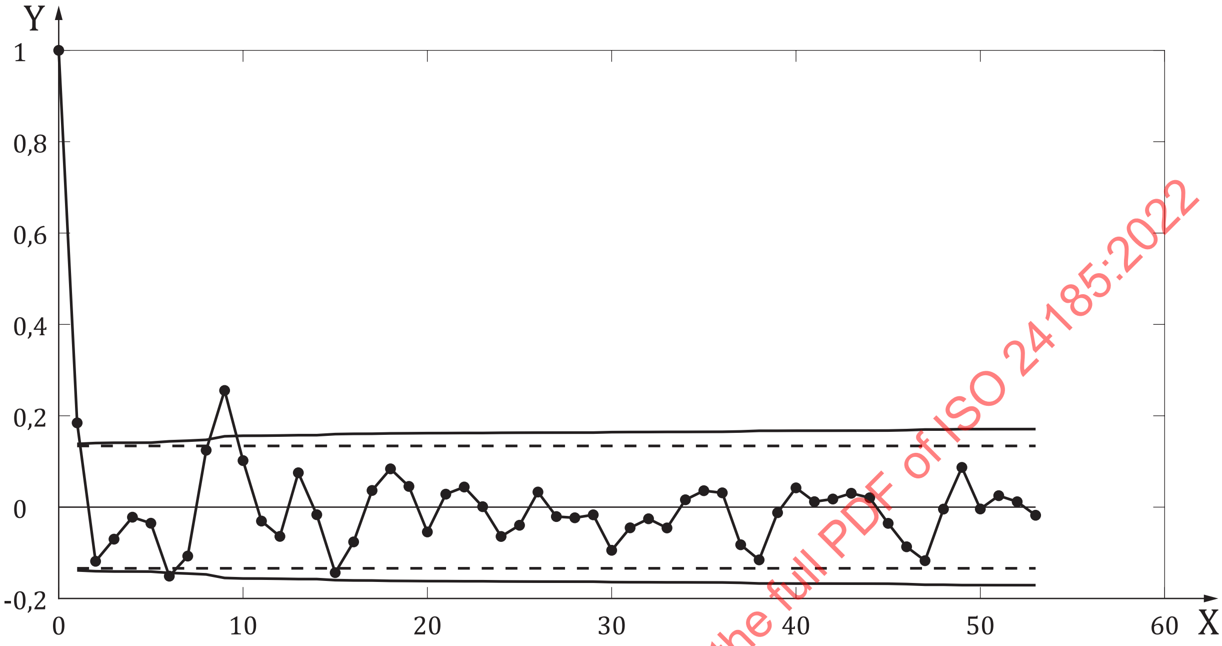
Key

X measurement number

Y voltage difference (nV)

Figure A.1 — Series of voltage differences of two Josephson voltage standards

In the ACF plot, assuming the time series is white noise, an approximate 95 % confidence band given by two broken lines (based on 4.5) is shown in Figure A.2. The measurements are autocorrelated because the autocorrelation of lags 1, 6, 9 and 15 are outside the broken-line band with limits of $\pm 1{,}96/\sqrt{214}$. Thus, it is inappropriate to treat the measurements as an i.i.d. sequence. The sample mean $\bar{x} = -0{,}869$ nV. The sample standard deviation $s_x = 2{,}888$ nV.



Key

X lag

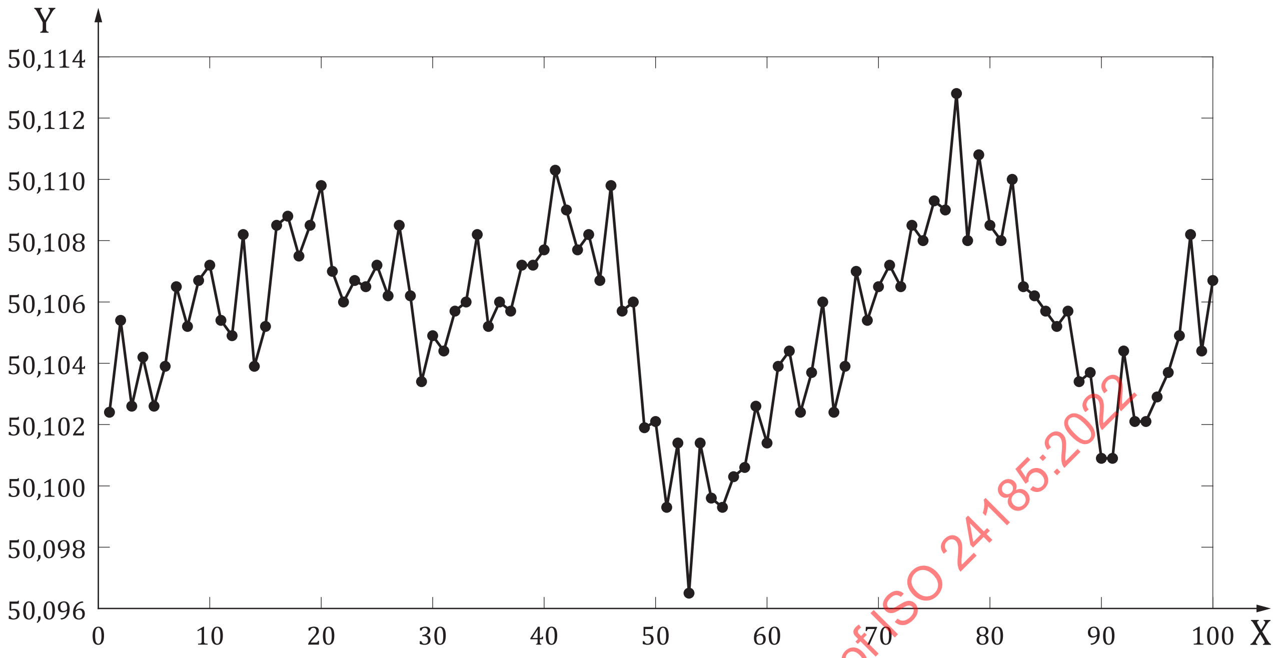
Y autocorrelation

Figure A.2 — ACF plot of voltage difference measurements, assuming the time series is white noise a 95 % confidence band (broken lines), and a 95 % confidence band (solid lines) for significant autocorrelations

On the other hand, the second band shown by two solid lines based on Formulae (4) and (5) for the autocorrelations which are significantly different from zero indicates the autocorrelations of lags 1, 6, and 9 are significantly different from zero and the significant autocorrelation with largest index is at lag 9. From Formulae (9) and (10), $N_r = N_c = 9$. If it is assumed that the data are not autocorrelated, from Formula (6), the standard uncertainty of the mean would be 0,197 nV. Since the measurements are determined to be autocorrelated, Formula (11) is used to calculate the standard uncertainty of the mean: $u_{\bar{x}}$ = 0,208 nV, which is 5,4 % larger than 0,197 nV. This result demonstrates the importance to check whether measurement data are autocorrelated.

A.3 Example 2

A temperature reading is taken every minute by a thermocouple immersed in a thermal bath[9]. There are 100 measurements in all as shown in Figure A.3. Appropriate process control procedures in ISO 7870-9 are applied to the data indicating the mean and variance of the process may be treated as constants.



Key

X time (minute)

Y temperature (°C)

Figure A.3 — Time series of temperature readings

In the ACF plot, assuming the time series is white noise, an approximate 95 % confidence band demonstrated by two broken lines (based on 4.5) is shown in Figure A.4. The measurements are autocorrelated because the autocorrelation of lags 1-7 and 11-24 are outside the broken-line band with limits of $\pm 1{,}96/\sqrt{100}$. Thus, it is inappropriate to treat the measurements as white noise. The sample mean $\bar{x} = 50{,}105\,43\ °\mathrm{C}$. The sample standard deviation $s_x = 0{,}002\,90\ °\mathrm{C}$.