

Statistical Analysis on Uncertainty for Autocorrelated Measurements and its Applications to Key Comparisons

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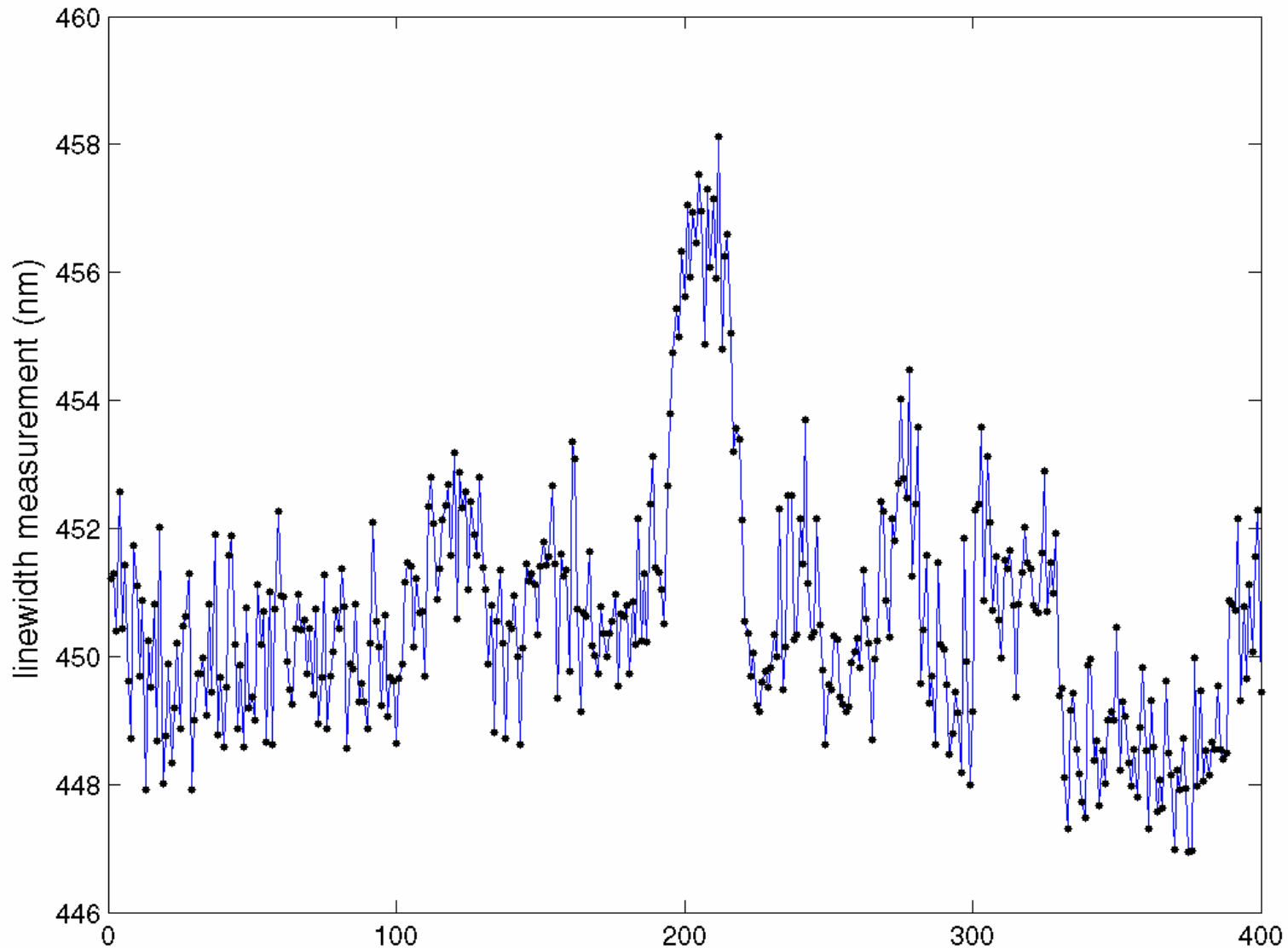
1. Introduction

In metrology, for given repeated measurements, $\{X_1, \dots, X_n\}$ of size of n

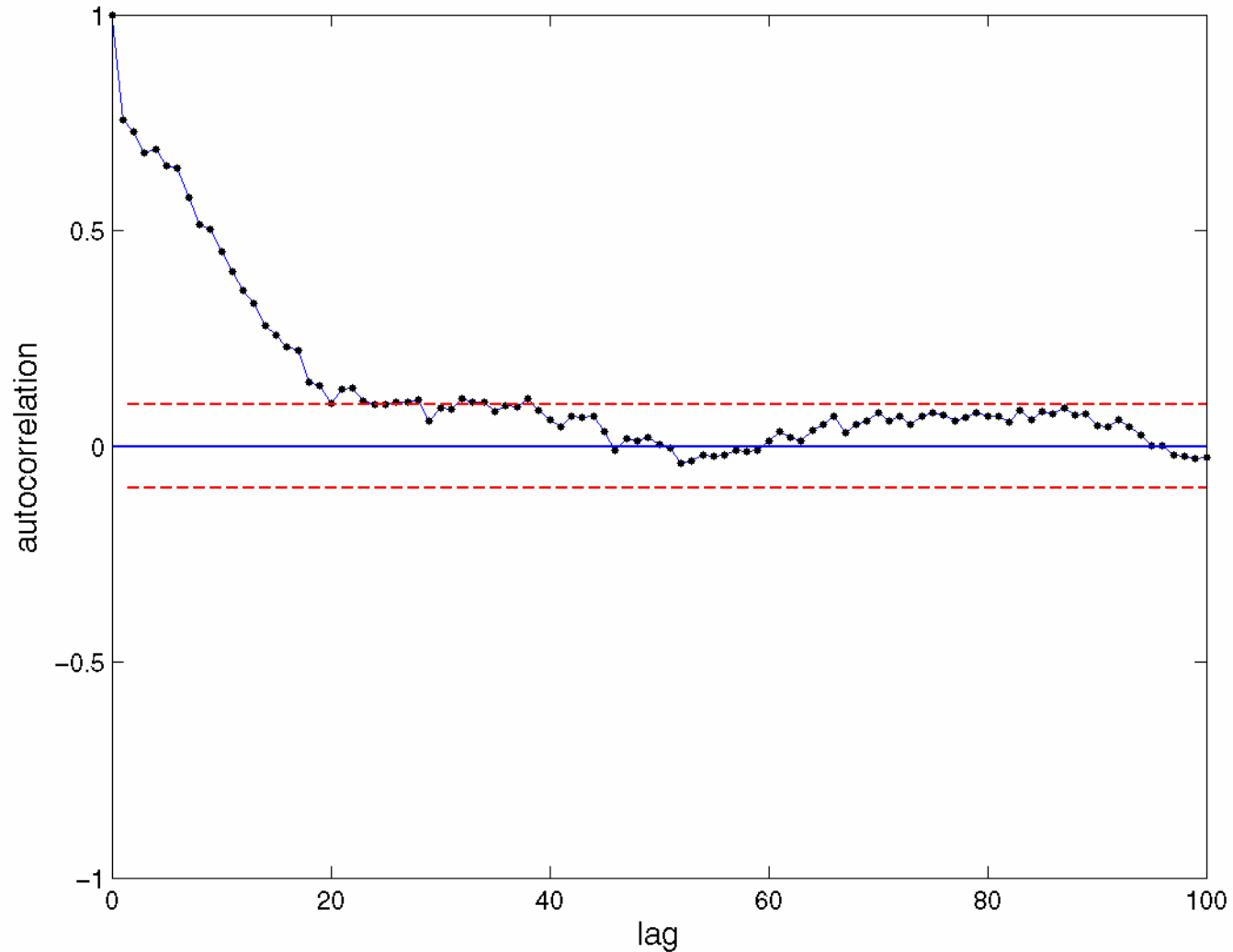
$$u_{\bar{X}} = \frac{S_X}{\sqrt{n}}$$

Here we assume that $\{X_1, \dots, X_n\}$ have same mean and variance and are uncorrelated. However the condition of uncorrelatedness does not always hold. In many cases measurements are autocorrelated or self-correlated. Here are two examples.

The figure shows 400 linewidth measurements for a nominally 500 nm line by a SEM.



This shows the ACF plot of the linewidth measurements with a 95% confidence band for WN.



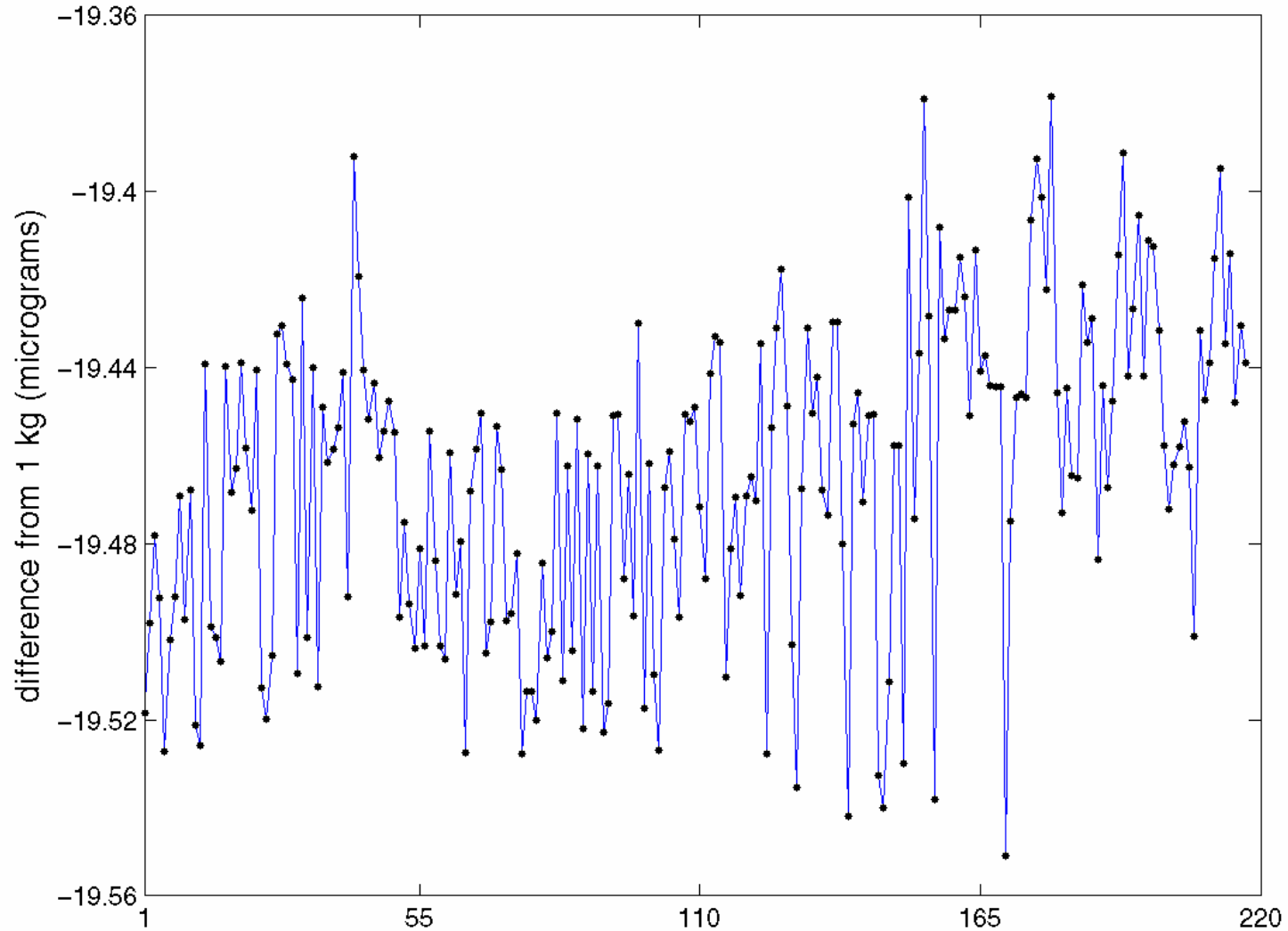
The ACF plot is a plot for the sample autocorrelations, which measures the autocorrelation of the data.

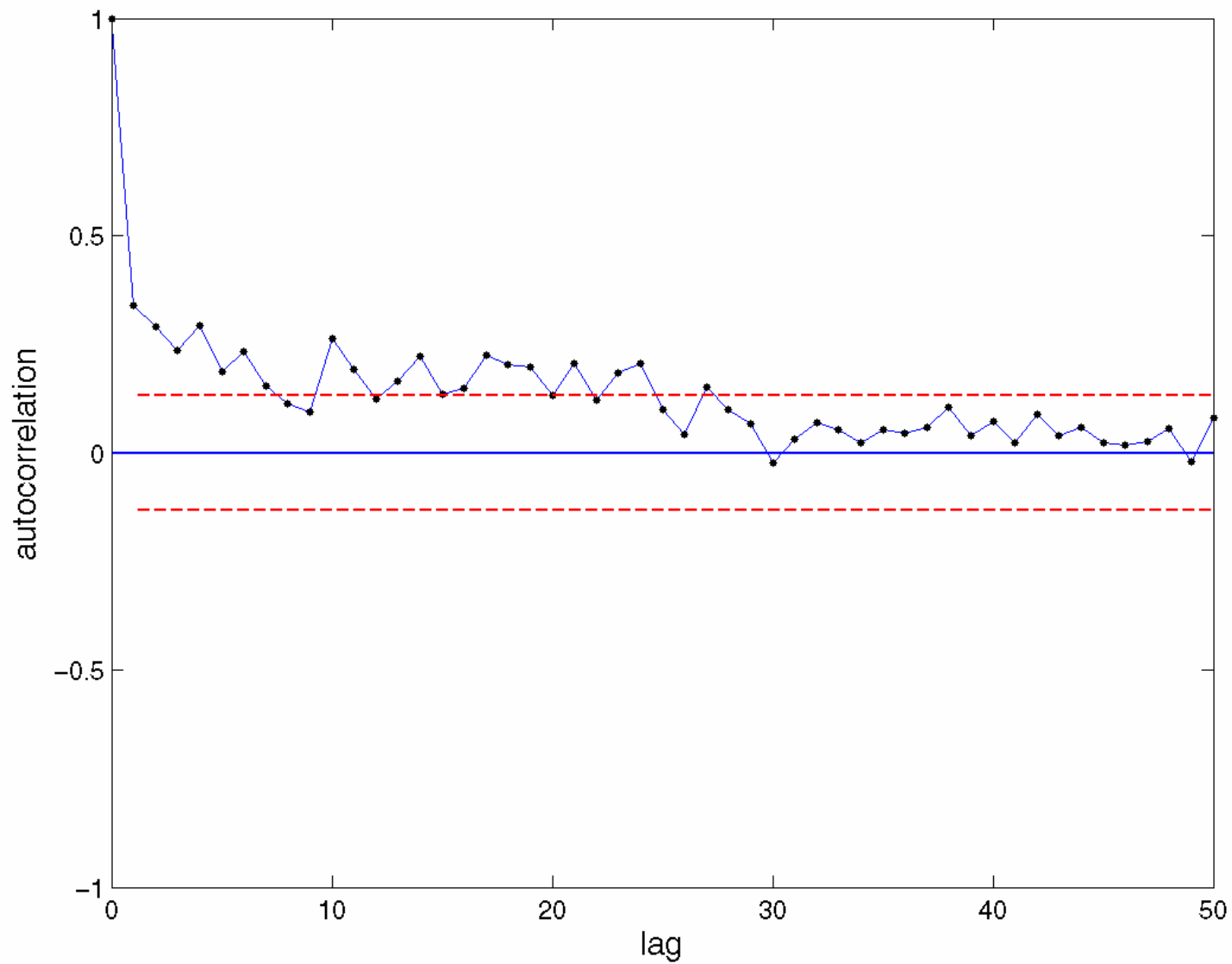
The confidence band is centered at zero and with limits of

$\pm 1.96/\sqrt{n}$ with $n = 400$ The confidence band is for the autocorrelations of an uncorrelated sequence or white noise. Namely, if the data are statistically independent, then its sample autocorrelation has a mean of zero and an approximate standard deviation of $1/\sqrt{n}$

Obviously, the linewidth measurements are autocorrelated and thus the uncertainty given in the above may not be appropriate to use.

High precision weight measurements with differences from the 1kg check standards.





The ACF plot shows the autocorrelations and a 95% confidence band for white noise. Obviously, the measurements are autocorrelated and thus the traditional approach to calculate the uncertainty of the average of measurements is not appropriate.

If the mean is estimated by a weighted mean, $\bar{X}_w = \sum_{i=1}^n w_i X_i$ then when the uncertainty of the weighted mean is calculated, the traditional approach

$$u_{\bar{X}_w} = \sqrt{\sum_{i=1}^n w_i^2} \sigma_X$$

is also not appropriate. Thus, appropriate approaches are needed to calculate the corresponding uncertainties. For autocorrelated processes, an important class is the one of stationary processes. We propose a practical approach to compute the uncertainty of the average of the measurements from a stationary process.

2. Stationary processes

A discrete time series $\{X_t, t = 1, 2, \dots\}$ is (weakly) stationary if

$$(1) \quad E[X_t] = \mu$$

$$(2) \quad \text{Var}[X_t] = \sigma_X^2 < \infty$$

$$(3) \quad \text{Cov}[X_t, X_{t+\tau}] = R(\tau)$$

$R(\tau)$ is the autocovariance of $\{X_t\}$ at lag of τ . $R(0) = \sigma_X^2$

The autocorrelation is defined as $\rho(\tau) = R(\tau)/R(0)$

When the measurements are from a stationary process, they have the same mean and variance for all t .

Examples of stationary processes

(1) White noise ---- mean=0 and $\rho(\tau) = 0$ for all $\tau \neq 0$

(2) First order autoregressive process (AR(1))

$$(X_t - \mu) = \phi(X_{t-1} - \mu) + a_t$$

When $|\phi| < 1$ the process is stationary. $\rho(k) = \phi^k$ when
 $k \geq 0$

(3) Moving average process (MA(q))

$$X_t - \mu = a_t - \theta_1 a_{t-1} - \dots - \theta_q a_{t-q}$$

$$\rho(k) = 0 \quad \text{when} \quad |k| > q$$

3. Uncertainty of a sample mean for stationary measurements

For the sample mean $\bar{X} = \frac{X_1 + \dots + X_n}{n}$ when $\{X_t\}$ is stationary

$$\text{Var}[\bar{X}] = \left[1 + \frac{2 \sum_{i=1}^{n-1} (n-i) \rho(i)}{n} \right] \frac{\sigma_X^2}{n}$$

where σ_X^2 is the variance of $\{X_t\}$. When the measurements are uncorrelated,

$$\text{Var}[\bar{X}] = \frac{\sigma_X^2}{n}$$

When $\{X_t\}$ is an AR(1) process

$$\text{Var}[\bar{X}] = \frac{n - 2\phi - n\phi^2 + 2\phi^{n+1}}{n^2 (1 - \phi)^2} \sigma_X^2$$

The uncertainty of the sample mean is given by

$$u_{\bar{X}}^2 = \left[1 + \frac{2 \sum_{i=1}^{n-1} (n-i) \hat{\rho}(i)}{n} \right] \frac{S_X^2}{n}$$

where

$$S_X^2 = \frac{1}{n-1} \sum_{k=1}^n (X_k - \bar{X})^2$$
$$\hat{\rho}(i) = \frac{\sum_{k=1}^{n-i} (X_k - \bar{X})(X_{k+i} - \bar{X})}{\sum_{k=1}^n (X_k - \bar{X})^2}$$

Two issues in using the above estimator:

- (1) When i is close to n the number of product in the numerator is small and the estimate $\hat{\rho}(i)$ will not be good.
- (2) Since $\hat{\rho}(i) \rightarrow 0$ when $i \rightarrow \infty$ we need to consider if any $\hat{\rho}(i)$ is statistically significant from zero.

For (1), a rule of thumb: $\hat{\rho}(i)$ can only be used when $n \geq 50$ and $i \leq n/4$ Thus, we only use these $\hat{\rho}(i)$ with $i \leq n/4$

For (2), by Wold Decomposition Theorem, a realization of a stationary process can be approximated by a finite order MA process

$$X_t - \mu = a_t - \sum_{k=1}^q \theta_k a_{t-k}$$

Based on that, for a set of time series data, the order of the corresponding MA model, q needs to be found to have all $\hat{\rho}(i)$ in the uncertainty formula significantly different from zero.

For an MA(q) process and a sufficiently large n , $\hat{\rho}(i)$ for $i > q$ is approximately normally distributed with a mean of zero and a variance of

$$\sigma_{\hat{\rho}(i)}^2 \approx \frac{1 + 2 \sum_{k=1}^q \rho^2(k)}{n}$$

In particular, when $\{X_i\}$ is an uncorrelated sequence with same mean and variance,

$$\sigma_{\hat{\rho}(i)}^2 \approx \frac{1}{n}$$

which was used to build a confidence band of ACF for white noise.

In practice for $i > q$ an estimator of $\sigma_{\hat{\rho}(i)}^2$ is

$$\hat{\sigma}_{\hat{\rho}(i)}^2 = \frac{1 + 2 \sum_{k=1}^q \hat{\rho}^2(k)}{n}$$

Since $\hat{\rho}(i)$ are asymptotically normally distributed with $E[\hat{\rho}(i)] \approx 0$ for $i > q$

$$|\hat{\rho}(i)| > 1.96 \sqrt{\frac{1 + 2 \sum_{k=1}^q \hat{\rho}^2(k)}{n}}$$

is evidence against MA(q) at the $\alpha = 0.05$ level. Namely, if an MA(q) is to be considered, $\hat{\rho}(i)$ should remain within the limits for $i > q$

Thus, a cut-off lag is given by

$$n_c = \max \{ i \mid |\hat{\rho}(i)| > 1.96\hat{\sigma}_{\hat{\rho}(i)} \}$$

Thus, the upper limit in the summation in the uncertainty formula is replaced by

$$n_r = \min \{ n_c, [n/4] \}$$

To warranty that only reasonable good $\hat{\rho}(i)$ are included. Thus, the uncertainty of the average of measurements from a stationary process can be calculated by

$$u_{\bar{X}}^2 \approx \left[1 + \frac{2 \sum_{i=1}^{n_r} (n-i) \hat{\rho}(i)}{n} \right] \frac{S_X^2}{n}$$

A factor or a ratio is

$$r = 1 + \frac{2 \sum_{i=1}^{n_r} (n-i) \hat{\rho}(i)}{n}$$

4. Confidence intervals for the mean value

Central Limit Theorem: When $\{X_1, \dots, X_n\}$ are statistically independent and identically distributed with μ and σ_X^2 when n is large enough

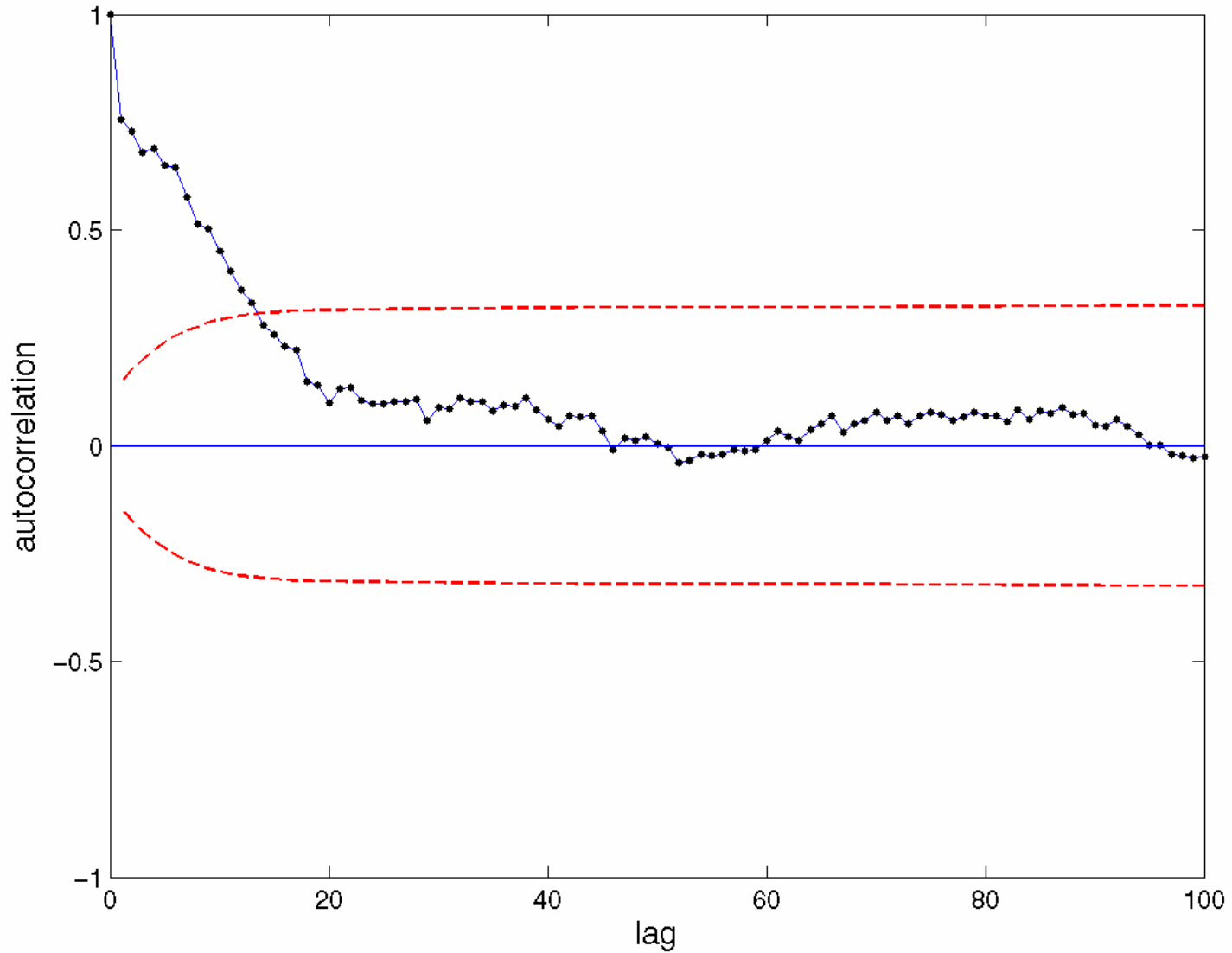
$$\bar{X} \approx N\left(\mu, \frac{\sigma_X^2}{n}\right)$$

For a stationary process, CLT still holds when some regular conditions are met. Thus, when n is large enough, the 95% confidence limits are

$$\bar{X} \pm 1.96u_{\bar{X}}$$

For the first example, $n = 400$ and $n_r = 13$ the $u_{\bar{X}} = 0.3776$ which is much larger than 0.0964, the uncertainty based on independence assumption. R, the ratio = 3.9.

ACF plot of linewidth measurements with a 95 % confidence band



Since $\bar{X} = 450.62$ a 95 % confidence band of the mean is

$$450.62 \pm 1.96 \times 0.38 = 450.62 \pm 0.74$$

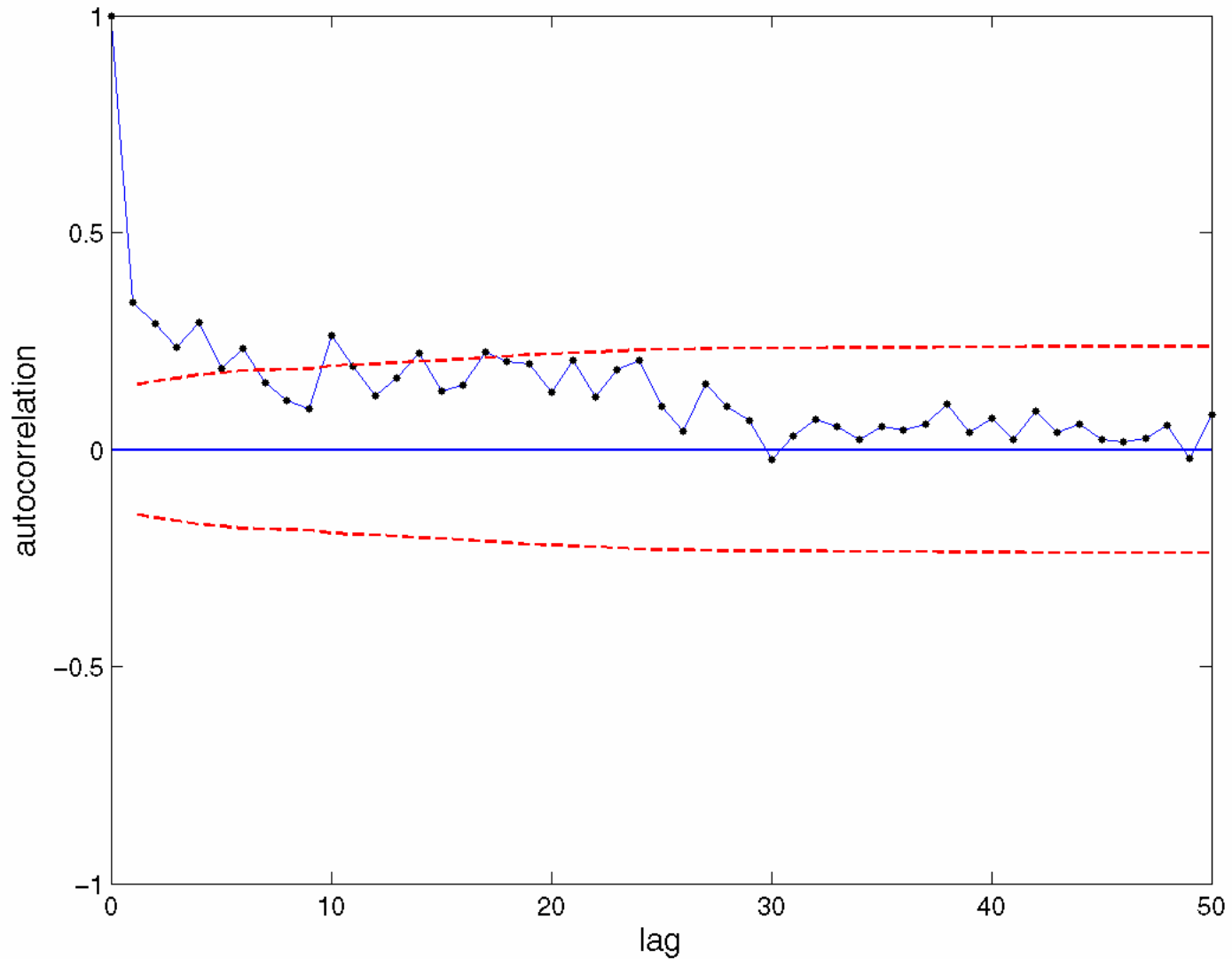
For the second example of the weights measurements, $n=217$.

$$n_r = n_c = 17$$

$u_{\bar{X}} = 0.0067$ which is much larger than 0.0024, the uncertainty based on independence assumption. R, the ratio is 2.8. A 95 % confidence band is given by

$$-19.4645 \pm 1.96 \times 0.0067 = -19.4645 \pm 0.0131$$

ACF plot of the weights measurements with a 95 % confidence band



5. Applications to Key Comparisons

For a Key Comparison, if the measurements by any lab are autocorrelated, then the Type A uncertainty for the lab should be determined based on the autocorrelations assuming the data are from a stationary process.

If there are more than one traveling standard and the measurements by any lab are autocorrelated, then the Type A uncertainty for this standard and this lab needs to be determined based on the corresponding autocorrelations.

If the Type A uncertainty of any lab is obtained by combining all traveling standards, then the calculation should be based on the autocorrelation structures of measurements for all standards.

6. Discussions and conclusions

When repeated measurements are autocorrelated, it is not appropriate to use the traditional approach to calculate the uncertainty of the average of the measurements. We propose a practical approach to calculate the uncertainty when the data are from a stationary process.

(1) The result can be extended to the case of a weighted mean.

$$\bar{X}_w = \sum_{i=1}^n w_i X_i$$

When $\{X_t\}$ is stationary, it can be shown that

$$Var[\bar{X}_w] = \sigma_X^2 \left\{ \sum_{i=1}^n w_i^2 + 2 \sum_{i=1}^{n-1} \rho(i) \left[\sum_{j=1}^{n-i} w_j w_{j+i} \right] \right\}$$

The corresponding uncertainty can be calculated.

(2) We assume that time series data were collected at equally spaced (time) interval. However, in practice a time series dataset often contains more or less missing values. In time series analysis, various attempts have been made to deal with such a kind of case. Therefore, in metrology once the measurements are determined to be autocorrelated, it is very important to make sure the data are collected at equal time interval.

(3) An autocorrelated process or a time series can be non-stationary such as a random walk:

$$X_t = X_{t-1} + a_t$$

with $X_0 = 0$ and $\{a_t\}$ white noise. It is obvious that

$$X_t = \sum_{i=1}^t a_i$$

Thus,

$$\text{Var}[X_t] = t \sigma_a^2$$

If measurements are from a non-stationary process using the average value and the corresponding variance to characterize the measurement standard may be misleading.