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Interval Estimators of the Centre and Width of a Two-Dimensional Microstructure

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In metrology it is used to estimate the stipulated quantity as a mean and its uncertainty. This procedure is legitimate when the evaluated data are symmetrically distributed and the distribution is (at least approximately) known. But there exist many evaluating treatments in which the evaluated values are non-symmetrically distributed. In this case it is mathematically correct to use an interval estimator for the stipulated (measured) quantity i.e. to evaluate the (1-α)-confidence interval for the (true) stipulated (measured) quantity. This (random) interval covers with probability 1-α the (true) stipulated quantity. In the paper are presented interval estimators for some parameters of two-dimensional structures.

Keywords: confidence interval, evaluating of measured data, fitting by a regression line

1. Introduction

THE TYPICAL photoelectric signal from a two-dimensional cross section of interest of a reflective microline (grating line) is in Fig.1. The edges $^{(1)}x$, $^{(2)}x$, the centre x_S and width w of the structure should be estimated for a given (nonrandom) threshold F.

Measurements $Y_1, Y_2, Y_3, \ldots, Y_n$, of the photoelectric signal in (exact) points $x_1, x_2, x_3, \ldots, x_n$ are considered to be normally distributed, independent and with equal standard deviations. The parts of the photoelectric signal, adherent to the structure edges (for given threshold F) are supposed to be linear. So we fit the expected linear parts of the photoelectric signal by regression lines. In this case the stipulated quantities (structure's edge and center coordinate or structure's width), calculated by the inverse transformation from regression line, are non-symmetrically distributed.

Let us denote $y_1, y_2, y_3, \ldots, y_n$ the realizations of $Y_1, Y_2, Y_3, \ldots, Y_n$ and $a+bx$ the appropriate regression line. The estimators of the regression coefficients $\hat{a}$, $\hat{b}$ and their standard deviations $s_{\hat{a}}, s_{\hat{b}}$ are determined from pairs of measured values $\{x_i, y_i\}_{i=1}^{n}$ using standard procedures (see e.g. [3]). A common estimator of the x value for assigned level F (threshold) of the electric signal is

$$\hat{x} = \frac{F - \hat{a}}{\hat{b}}.$$

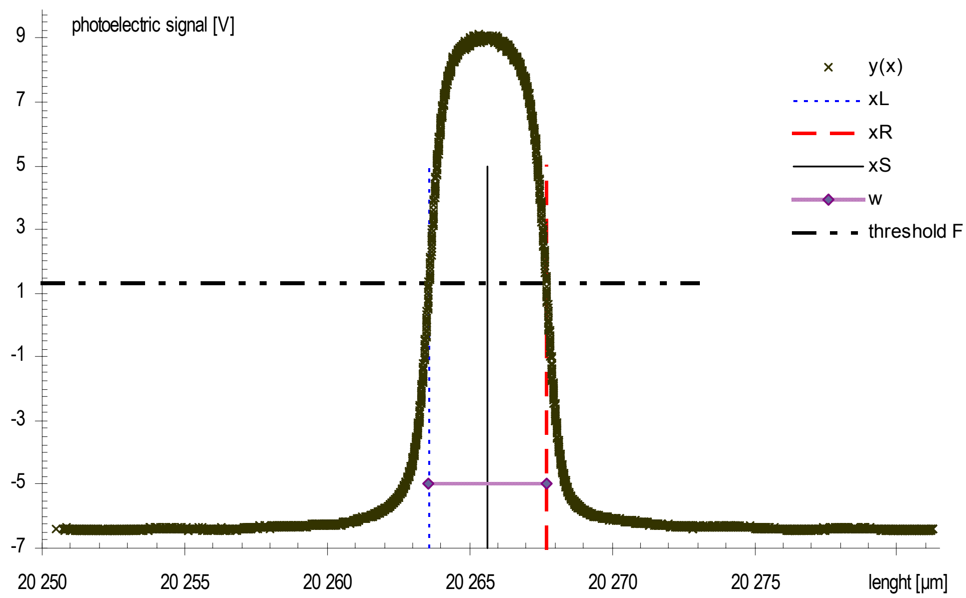

Fig.1. Photoelectric signal from a reflective microline [4].

Using the Law of propagation on uncertainty (see [2]) we obtain the standard deviation (in fact the estimate of the standard deviation) of the estimator $\hat{x}$ as

$$s_{\hat{x}} = \frac{1}{\hat{b}}\sqrt{\frac{s^2}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}\left(\sum_{i=1}^{n} x_i^2 - 2\hat{x}\sum_{i=1}^{n} x_i + n\left(\hat{x}\right)^2\right)}$$

where $$s^2 = \frac{1}{n-2}\left(\sum_{i=1}^{n} y_i^2 - \frac{\left(\sum_{i=1}^{n} y_i\right)^2}{n} - \hat{b}\left(\sum_{i=1}^{n} x_i y_i - \frac{\sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n}\right)\right) \quad (1)$$

In deriving the (1-α)-confidence interval for x arise difficulties caused by the generally nonsymmetrical distribution of $\hat{x}$ and so this confidence interval cannot be determined in the usual way as $\left(\hat{x} - ks_{\hat{x}},\, \hat{x} + ks_{\hat{x}}\right)$.

The wanted (1-α)-confidence interval for x can be determined by the below described procedure.

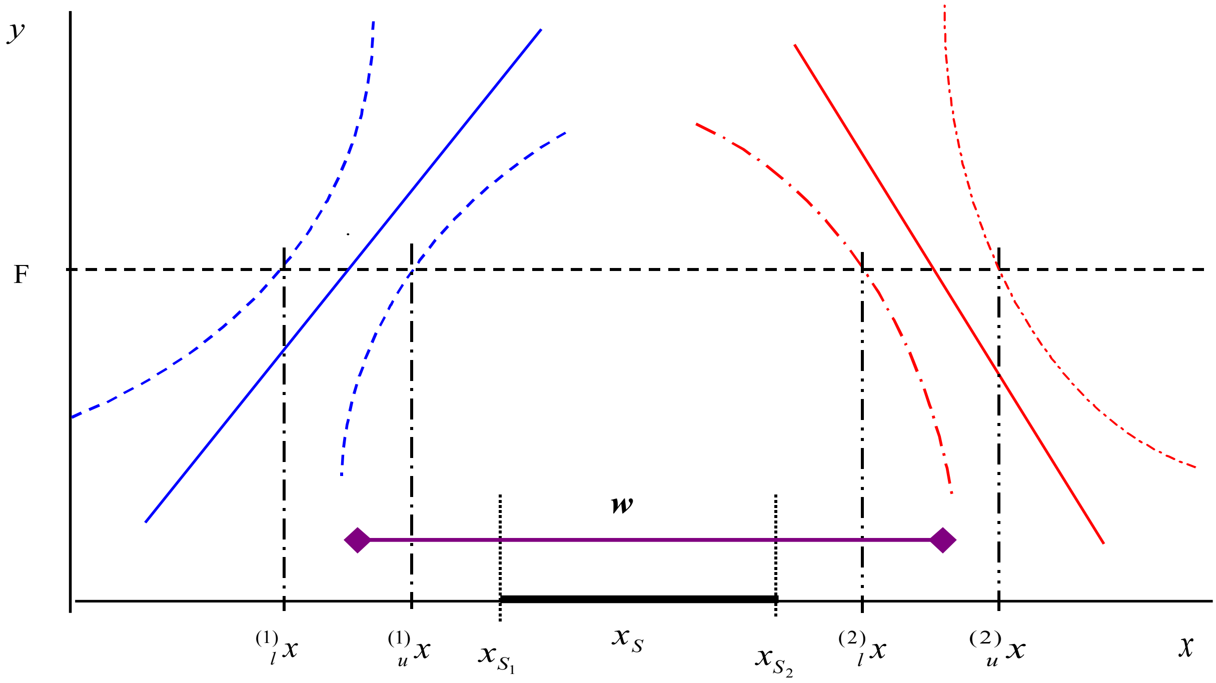

Fig.2 The confidence intervals for the structure edges $\left({}^{(1)}_{l}x, {}^{(1)}_{u}x\right)$, $\left({}^{(2)}_{l}x, {}^{(2)}_{u}x\right)$

2. Subject & Methods

The (1-α)-confidence interval for the edge coordinate x

The regression lines (blue for the left edge, red for the right edge) with the relevant confidence bounds are in Fig.2. According to [1], p. 509-512, in the case of sufficiently steep edges of the structure and small s (what is here also assumed), the (1-α)-confidence interval for x is $({}_l x,\, {}_u x)$ according to Fig.2. For its boundaries ${}_l x$, ${}_u x$ and given (errorless, nonrandom) value of the photoelectric signal (threshold) F it holds

$$F = \hat{a} + \hat{b}\,{}_l x - s d_x\left[t_{n-2}\left(1-\frac{\alpha}{2}\right)\right],$$

$$F = \hat{a} + \hat{b}\,{}_u x + s d_x\left[t_{n-2}\left(1-\frac{\alpha}{2}\right)\right]$$

with $$d_x = \sqrt{\frac{1}{n}\left(1 + \frac{\left(nx - \sum_{i=1}^{n} x_i\right)^2}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}\right)},$$

and $t_{n-2}\left(1-\frac{\alpha}{2}\right)$ is the $\left(1-\frac{\alpha}{2}\right)$-quantile of the Student t-distribution with n-2 degrees of freedom, s is given in (1).

Solving both preceding equations the bounds ${}_l x$ and ${}_u x$ are

$${}_l x = \frac{-B}{2A} - \frac{\sqrt{B^2 - 4AC}}{2A}, \quad {}_u x = \frac{-B}{2A} + \frac{\sqrt{B^2 - 4AC}}{2A} \quad (2)$$

for $$A = \hat{b}^2 - \frac{ns^2\left[t_{n-2}^2\left(1-\frac{\alpha}{2}\right)\right]}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2},$$

$$B = 2\left(\frac{s^2\left[t_{n-2}^2\left(1-\frac{\alpha}{2}\right)\right]\sum_{i=1}^{n} x_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} - \hat{b}\left(F - \hat{a}\right)\right),$$

$$C = \left(F - \hat{a}\right)^2 - \frac{s^2}{n}\left[t_{n-2}^2\left(1-\frac{\alpha}{2}\right)\right]\left(1 + \frac{\left(\sum_{i=1}^{n} x_i\right)^2}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}\right).$$

The bounds ${}_l x$ and ${}_u x$ are evaluated for the left (upper index is (1)) and the right (upper index (2)) structure's edges.

The (1-α)-confidence interval for the line center coordinate x_S

By determining the structure's center and width for given (errorless, nonrandom) F in analyzed cross section it is necessary to use the x values from two confidence intervals $\left({}^{(1)}_{l}x, {}^{(1)}_{u}x\right)$ and $\left({}^{(2)}_{l}x, {}^{(2)}_{u}x\right)$ that correspond to the structure's edges, see Fig.2.

Using Bonferroni's inequality (see e.g. in [3]) for the structure's center x_S it is valid

$$P\left\{x_S \in \left(\frac{{}^{(1)}_{l}x + {}^{(2)}_{l}x}{2}, \frac{{}^{(1)}_{u}x + {}^{(2)}_{u}x}{2}\right)\right\} \geq 1 - 2\alpha,$$

i.e.

$$\left(x_{S_1} = \frac{{}^{(1)}_{l}x + {}^{(2)}_{l}x}{2}, \quad x_{S_2} = \frac{{}^{(1)}_{u}x + {}^{(2)}_{u}x}{2}\right) \tag{3}$$

is the at least (1-2α)-confidence interval for the structure's center.

The (1-α)-confidence interval for the line width w

For the structure's width w is similarly true

$$P\left\{w \in \left({}^{(2)}_{l}x - {}^{(1)}_{u}x, \ {}^{(2)}_{u}x - {}^{(1)}_{l}x\right)\right\} \geq 1 - 2\alpha,$$

and that is why

$$\left(w_1 = {}^{(2)}_{l}x - {}^{(1)}_{u}x, \ w_2 = {}^{(2)}_{u}x - {}^{(1)}_{l}x\right) \tag{4}$$

is the least (1-2α) - confidence interval for the structure's wide w.

3. Conclusion

For the nonsymmetrical distribution of measured (calculated) data it is not correct to estimate the true value by the mean and the uncertainty. This could occur when a regression line fits the measured data and for the estimation of the wanted quantity the inverse transformation is applied.

In this case, e.g. in measuring the geometry of two-dimensional micro structures, the proper interval estimator of the true coordinates of the structure's edges, center and the structure's width should be evaluated in the following manner.

For a chosen (errorless) value (threshold) F of quantity y (e.g. photoelectric signal in the length comparator) and $\alpha \in (0,1)$, the (1-α)-confidence interval for the structure's edge is (${}_l x$, ${}_u x$) where ${}_l x$, ${}_u x$ are given in (2), the (1-2α)-confidence interval for the structure's center is given in (3), and the (1-2α)-confidence interval for the structure's width is given in (4). This approach assumes, of course, another reasoning not only in nanometrology.

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