

# Estimation of the uncertainty bands of regression line for correlated data of variable $Y$ using the GUM rules

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## Abstract

The estimation of the accuracy of the linear regression method used for measurements based on the GUM recommendations is considered. The impact of correlation and autocorrelation of the variable  $Y$  data together with type A and type B uncertainties, not provided in statistical literature about regression methods, is discussed. The theoretical backgrounds are given. The simulated examples of determining the uncertainty bands of the regression line fitted to the measured points with different cases of correlated values and absolute and relative uncertainties of type A and type B of the dependent variable  $Y$  are considered.

**Keywords:** measurement; autocorrelation; regression line; type A and type B uncertainty bands.

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## Introduction

The estimation of the accuracy of measurement results and instrumentation used in national metrology services, science, industry and many other fields is now conducted according to the uncertainty terms recommended in the international GUM Guide [1–3]. It is also described in a few books and other literature. In the literature on the linear regression method, e.g. [4–5], the accuracy of its straight-line parameters is statistically estimated only from the measured data and from their random uncertainties in the experiment. The impact of type B uncertainty obtained from the Maximal Permissible Error (MPE) of the used instruments on the uncertainty bands of the straight-line, when a measurement result is obtained using the regression method, and their use over an acceptable period and conditions of the validation data is not considered [4, 6–10]. Even in the latest research works on the regression method based on the Bayes, suggested for the new version of the GUM (GUM 2), the impact of type B uncertainty on the accuracy of the regression function was not separately considered.

The determination of equations for the borders of the uncertainty bands of the regression line for the uncorrelated  $y$ -ordinates of the measured points was analysed earlier in [7–9]. The equations of the regression line uncertainty of the autocorrelated and correlated coordinates of the variable  $Y$ , based on works [6–9], are presented below. In the estimation

of the accuracy, the influence of type B uncertainty is also included.

## 1. Linear regression method for correlated data of variable $Y$

The linear regression method is used below for a dependent random variable  $Y(x, y)$  to determine a straight-line  $y = ax + b$  and borders of its expanded uncertainty band  $\pm U_{y,95}$ . This line is determined according to the specified criterion for measuring  $y_i$ -ordinates (for  $i = 1, \dots, n$ ) of  $n$  tested points  $Q_i(y_i, x_i)$  – see Fig. 1, i.e.:

$$y = ax + b \pm U_{y,95}(x). \quad (1)$$

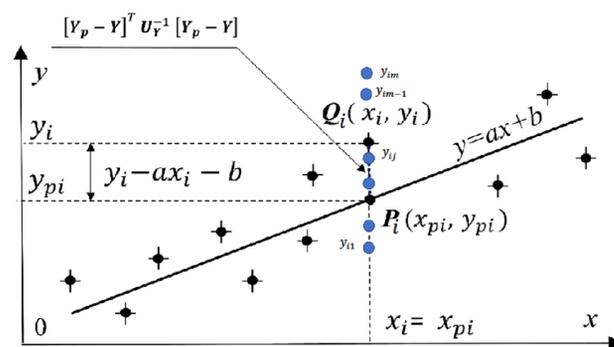


Fig. 1. Regression line for points with measured  $y_i$ -values of variable  $Y$  and known  $x_i$ -values

For most scientific and technological experiments, it can be assumed that the measured results of  $y_i$  for

the dependent variable  $Y(x)$  are random, and the  $x_i$ -values (for  $i = 1, \dots, n$ ) of an independent variable  $X(x)$  are known and precisely determined. Then according to the GUM [1], the  $y_i$ -values have combined uncertainties  $u(y_i) = \sqrt{u_{iA}^2 + u_{iB}^2}$ , and  $u(x_i) = 0$ .

If for every given  $x_i$ , the  $y_i$ -values are stable during the experiment, it is enough to measure them once. If they are randomly changed, then can be measured repeatedly as  $(y_{i1}, \dots, y_{ij}, \dots, y_{im})$  to find the best estimators of the  $y_i$ -values and their uncertainties  $u(y_i)$ .

To describe the accuracy of correlated values  $y_i, \dots, y_n$ , the covariance matrix is used:

$$U_Y = \begin{bmatrix} u^2(y_1) & \cdots & \rho_{y_1n} u(y_1) u(y_n) \\ \vdots & \ddots & \vdots \\ \rho_{y_1n} u(y_1) u(y_n) & \cdots & u^2(y_n) \end{bmatrix}, \quad (2)$$

where  $\rho_{y_{ij}}$  is the correlation coefficient of  $y_i, y_j$  of the variable  $Y$ ; and  $u(y_i), u(y_j)$  are their uncertainties,  $i, j = 1, \dots, n$ .

For a regression line of real data, the correlation of the  $y$ -ordinates of close points is usually much stronger than that of distant points. The elements with the highest values of the correlation coefficients are located around the main diagonal of the  $U_Y$  covariance matrix, and other elements can be treated as equal to zero.

For the least squares' criterion of such a variable  $Y$ , the multivariate Gauss distribution is used:

$$f(\mathbf{Y}) = \frac{1}{(2\pi)^{n/2} \sqrt{\det(U_Y)}} \exp\left(-\frac{1}{2} [\mathbf{Y}_p - \mathbf{Y}]^T U_Y^{-1} [\mathbf{Y}_p - \mathbf{Y}]\right), \quad (3)$$

where  $\mathbf{Y} = [y_1, \dots, y_i, \dots, y_n]^T$  is the  $n$ -dimensional vector of the  $y_i$ -ordinates of the measured points (observed points),  $\mathbf{Y}_p$  is the vector  $y_{ip}$  of their parallel projections to the regression line in the  $0Y$ -direction (fitted points),  $U_Y^{-1}$  is the inverse of the covariance matrix.

A solution to the linear vector equation is:

$$\mathbf{Y}_p = a \mathbf{X}_p + b \mathbf{1} = a \mathbf{X}_p + b, \quad (4)$$

where  $\mathbf{X}_p$  is the cut-off vector  $x_i$  of the measured points,  $\mathbf{1} = [1, \dots, 1]^T$  is the unit vector size of  $n$ .

If the variable  $Y$  is only measured, then the target function  $P = f(\mathbf{Y}) \rightarrow \max$  is applied. This will occur for a minimum of the criteria function  $SK(a, b)$

$$SK(a, b) = -\ln(f(\mathbf{Y})) \rightarrow \min. \quad (5)$$

It is assumed that the sum of the normalized squares of the distance of the measured points with coordinates  $(x_i, y_i)$  for  $i=1, 2, \dots, n$  from the specified points  $(x_i, y_{pi})$  on a regression straight-line (Fig. 1) will reach a minimum of zero of the sum of the squares of the sub-derivatives after the parameters  $a$  and  $b$  of this line. In general, i.e. when the values of both

coordinates are measured, the sets of the values  $y_i$  and  $x_i$  may be autocorrelated, as well as the ordinates  $y_i$  and  $x_i$  of the measured points may be correlated. Then the determination of the linear regression method requires two covariance matrices,  $U_Y$  and  $U_X$ , for both random variables  $Y$  and  $X$ .

When the  $x_i$ -values of the measured points do not have a random dispersion, they are defined precisely, and their uncertainty  $u(x_i) = 0$  and the equation resulting from criterion (5) is simplified, i.e.

$$SK = \Delta \mathbf{Y}^T U_Y^{-1} \Delta \mathbf{Y} = [\mathbf{Y}_p - \mathbf{Y}]^T U_Y^{-1} [\mathbf{Y}_p - \mathbf{Y}]. \quad (6)$$

Dependencies of the coordinates of points  $P_i$  lying on the regression line  $y = ax + b$  with abscissas  $x_{pi} = x_i$  and  $y_{pi}$ -ordinates are described by the vector equation

$$\mathbf{Y}_p = a \mathbf{X}_p + b. \quad (7)$$

The distance of the measured point  $Q_i$  from point  $P_i$  is equal to the coordinate differences between these two points (see Fig. 1). In the regression method with parallel projections of the measured points  $Q_i$  in the  $0y$ -direction on a designated straight-line, the measured point  $Q_i$  is therefore at the distance of  $y_{pi} - y_i = ax_i + b - y_i$  from point  $P_i$ .

The formulas of the regression line are simpler due to the use of auxiliary parameters

$$S = \mathbf{1}^T U_Y^{-1} \mathbf{1} = \sum_{i=1}^n \sum_{j=1}^n [U_Y^{-1}]_{ij}, \quad (7a)$$

$$S_x = \mathbf{X}^T U_Y^{-1} \mathbf{1} = \mathbf{1}^T U_Y^{-1} \mathbf{X}, \quad (7b)$$

$$S_{xx} = \mathbf{X}^T U_Y^{-1} \mathbf{X} = \mathbf{X}^T U_Y^{-1} \mathbf{X}, \quad (7c)$$

$$S_{xy} = \mathbf{X}^T U_Y^{-1} \mathbf{Y} = \mathbf{Y}^T U_Y^{-1} \mathbf{X}, \quad (7d)$$

$$S_y = \mathbf{Y}^T U_Y^{-1} \mathbf{1} = \mathbf{1}^T U_Y^{-1} \mathbf{Y}, \quad (7e)$$

$$S_{yy} = \mathbf{Y}^T U_Y^{-1} \mathbf{Y} = \mathbf{Y}^T U_Y^{-1} \mathbf{Y}. \quad (7f)$$

Then for  $\mathbf{X}_p = \mathbf{X}$  and  $\mathbf{Y}_p = a \mathbf{X}_p + b$  equation (6) takes the form:

$$SK = [a \mathbf{X} + b - \mathbf{Y}]^T U_Y^{-1} [a \mathbf{X} + b - \mathbf{Y}] = a^2 S_{xx} + 2ab S_x - 2a S_{xy} + b^2 S - 2b S_y + S_{yy}. \quad (8)$$

The condition for minimizing expression (8) as the sum of the squares of the distance of  $n$  points  $Q_i$  from the regression line in the  $0y$ -direction (Fig. 1) results from the solution for the system of two equations for its partial derivatives with respect to the parameters

$a$  and  $b$  of the regression line, i.e.  $\frac{\partial SK}{\partial a} = 0, \frac{\partial SK}{\partial b} = 0$ :

$$\begin{cases} a S_{xx} + b S_x = S_{xy} \\ a S_x + b S = S_y \end{cases}. \quad (9)$$

Solving the system of equations (9) we get:

$$a = \frac{SS_{xy} - S_x S_y}{SS_{xx} - (S_x)^2} = \frac{\Delta_a}{\Delta}; \quad b = \frac{S_y S_{xx} - S_x S_{xy}}{SS_{xx} - (S_x)^2} = \frac{\Delta_b}{\Delta}, \quad (10a, b)$$

where  $\Delta_a = SS_{xy} - S_x S_y$ ,  $\Delta_b = S_y S_{xx} - S_x S_{xy}$  and  $\Delta = SS_{xx} - (S_x)^2$ .

The criterion  $SK_{\min}$  from (5) will be met by parameters  $a$  i  $b$  where:

$$SK_{\min} = -aS_{xy} - bS_y + S_{yy}. \quad (11)$$

The borders of the uncertainty band  $U(y)$  lies symmetrically on both sides of the regression line. They will be determined considering the uncertainties  $u_a$  of slope  $a$  and the uncertainty  $u_b$  of intercept  $b$ . The parameters  $a$ ,  $b$  from formulas (10a, b) are correlated. The partial derivatives of the regression straight-line parameters are:

$$\mathbf{c} = \frac{\partial S_{xy}}{\partial \mathbf{Y}} = \mathbf{U}_Y^{-1} \mathbf{X}, \quad \mathbf{d} = \frac{\partial S_y}{\partial \mathbf{Y}} = \mathbf{U}_Y^{-1} \mathbf{1}. \quad (12a, b)$$

The sensitivity matrix for parameters  $a$ ,  $b$  has the form  $\mathbf{AB} = [\mathbf{A}, \mathbf{B}]$  of the elements defined by:

$$\mathbf{A} = \frac{\partial a}{\partial \mathbf{Y}} = \frac{S\mathbf{c} - S_x \mathbf{d}}{\Delta}; \quad \mathbf{B} = \frac{\partial b}{\partial \mathbf{Y}} = \frac{S_{xx} \mathbf{d} - S_x \mathbf{c}}{\Delta}. \quad (13a, b)$$

The covariance matrix of parameters  $a$ ,  $b$  follows from the matrix equation for the variance propagation, i.e.:

$$\mathbf{U}_{ab} = \mathbf{ABU}_Y \mathbf{AB}^T = \begin{bmatrix} \mathbf{AU}_Y \mathbf{A}^T & \mathbf{AU}_Y \mathbf{B}^T \\ \mathbf{AU}_Y \mathbf{B}^T & \mathbf{BU}_Y \mathbf{B}^T \end{bmatrix}, \quad (14)$$

where  $\rho_{ab}$  is the correlation coefficient between parameters  $a$  and  $b$ .

As the matrix  $\mathbf{U}_Y^{-1}$  is symmetrical,  $\mathbf{U}_Y = \mathbf{U}_Y^T$ , and  $\mathbf{U}_Y \mathbf{U}_Y^{-1} = \mathbf{U}_Y^{-1} \mathbf{U}_Y = \mathbf{I}$  – the unit matrix, then:

$$\begin{aligned} u_a^2 &= \mathbf{AU}_Y \mathbf{A}^T = \frac{S}{\Delta}, \\ u_b^2 &= \mathbf{BU}_Y \mathbf{B}^T = \frac{S_{xx}}{\Delta}, \\ \rho_{ab} u_a u_b &= \mathbf{AU}_Y \mathbf{B}^T = -\frac{S_x}{\Delta}. \end{aligned} \quad (14a-c)$$

The standard uncertainty of the regression line  $y = ax + b$  for one-dimensional variable  $Y$  can be obtained from the formula:

$$\begin{aligned} u_{ab}^2(y(x)) &= \begin{bmatrix} \frac{\partial y}{\partial a} & \frac{\partial y}{\partial b} \end{bmatrix} \mathbf{U}_{ab} \begin{bmatrix} \frac{\partial y}{\partial a} & \frac{\partial y}{\partial b} \end{bmatrix}^T = \\ &= [x, 1] \begin{bmatrix} u_a^2 & \rho_{ab} u_a u_b \\ \rho_{ab} u_a u_b & u_b^2 \end{bmatrix} \begin{bmatrix} x \\ 1 \end{bmatrix}. \end{aligned} \quad (15)$$

and after both multiplications:

$$u_{ab}^2(y(x)) = u_a^2 x^2 + 2x \rho_{ab} u_a u_b + u_b^2 = \frac{1}{S} + \frac{S}{\Delta} \left( x - \frac{S_x}{S} \right)^2. \quad (15a)$$

This equation determines type A uncertainty of the variable  $Y$  as a function of two correlated quantities  $ax$  and  $b$ . In the GUM [1], the function of combined uncertainty  $u(y)$  is the geometric sum of the functions of type A and B uncertainties:

$$u(y) = \sqrt{u_{ab}^2(y) + u_B^2(y)}. \quad (16)$$

Formula (16) is used, where the  $y_i$ -coordinates of all points are measured using the same instrument and under the same conditions. In these cases, it is not necessary to separately consider type B uncertainties for  $y_i$  of each measured point, and  $u_{regA}(y) = u_{ab}(y)$ . The function of type B uncertainty, i.e.  $u_B(y)$  in the  $y$ -range of the regression line, shall be determined from the Maximum Permissible Error,  $E_{\max} \%$ , of the meter. It is the standard deviation of uniformly distributed errors with a width of  $\pm E$ , which is

$$u_B(y) = u_B(y_0) + (y - y_0) E_{\max} / \sqrt{3}. \quad (16a)$$

In most cases of measurement practice  $u_B(y_0) \ll u_B(y - y_0)$ .

The parameters  $a$ ,  $b$  of a regression line depend on the  $y_i$ -coordinates of  $n$  measured points. The effective number of the degrees of freedom is  $n-2$ . The expanded uncertainty  $U_p$  of a regression line, e.g. when the confidence level is about  $P=0.95$ , is determined multiplying the combined uncertainty  $u(y)$  by the coverage factor  $k_{0.95}$ . For few  $n$  of points, the Student's  $t$ -distribution is used, and

$$U_{0.95} = k_{0.95} u(y) = t_{0.95, n-2} \sqrt{u_{ab}^2(y) + u_{By}^2}. \quad (17)$$

In rare cases, the  $y_i$ -coordinates and some or all controlled points are measured with different measures and/or under different influenced conditions. Then the sequence of numerical operations in determining the expanded uncertainty is

$$u_i = \sqrt{u_{Ai}^2 + u_{Bi}^2}, \quad i = 1, \dots, n, \quad (17a)$$

$$u_{ab} = u_{ab}(ax + b), \quad (17b)$$

$$U_y(ax + b) = t_{0.95, n-2} u_{ab}(ax + b). \quad (17c)$$

Therefore, equation (1) of the regression line with its expanded uncertainty band finally is:

$$y = ax + b \pm k_{0.95} \sqrt{u_{ab}^2(y) + u_b^2(ax + b)}. \quad (18)$$

The regression straight-line parameters for the correlated values of the variable  $Y$  and their special cases for the data of the uncorrelated values of the variable  $Y$  are summarized together as Table 1 in [9].

## 2. Kinds of correlation for measured ordinates of measured points

**2.1. Points with uncorrelated ordinates and equal uncertainties**

For the same value of absolute uncertainties  $u_i = u$  of  $y_i$  of the measured points, the covariance matrix is:

$$U_Y = u^2 R_Y, \tag{19}$$

where the correlator  $R_Y$  is a square symmetrical matrix size  $n \times n$ , elements of which are the correlation coefficients  $\rho_{y_{ij}}$  between the values  $y_i$  and  $y_j$  for  $i, j = 1, \dots, n$ .

In this case, for given correlation coefficients, the equation for a regression line will always be the same, since the values of the parameters  $a$  i  $b$  from formulas (9a,b) do not depend on the uncertainty  $u$ , but only on the correlator matrix. The regression line for the points with given coordinates and the same relative uncertainties  $y_i$  of all points gets other parameters than for the same absolute uncertainties. For all unknown but equal absolute uncertainties  $u$ , the estimator of the variance  $\hat{u}^2$  is defined as a minimum of the distance squares of divided by  $n-2$  degrees of freedom:

$$\begin{aligned} \hat{u}^2 &= u^2 \frac{-aS_{xy} - bS_y - S_{yy}}{n-2} = \\ &= \frac{-aX^T R_Y^{-1} Y - bY^T R_Y^{-1} \mathbf{1} + Y^T R_Y^{-1} Y}{n-2}. \end{aligned} \tag{20}$$

**2.2. Correlation in a series of repeated measurements of  $y_i$  of single points with the same  $x_i$**

In a series of  $m$  repeated measurements  $y_{i1}, \dots, y_{ik}, \dots, y_{im}$  ( $k = 1, \dots, m$ ) of the  $y_i$ -ordinate of a single point with abscissa  $x_i$ , the autocorrelation may occur. With the same values of uncertainties  $\sigma_{ik} = \sigma = \text{const}$  for each of the obtained  $y_{ik}$ -ordinate values and their correlated results with the correlation coefficients, from  $\rho_{i1}$  for the adjacent points to  $\rho(i, m-1)$  for the farthest points, the local covariance matrix size  $m \times m$  is obtained, given in equation (21)

$$U_{y_i} = \sigma^2 \begin{bmatrix} 1 & \rho_{i1} & \rho_{i2} & \dots & \dots & \rho_{im-1} \\ \rho_{i1} & 1 & \rho_{i1} & \rho_{i2} & \dots & \dots \\ \rho_{i2} & \rho_{i1} & 1 & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \rho_{i2} \\ \dots & \dots & \dots & \dots & 1 & \rho_{i1} \\ \rho_{im-1} & \dots & \dots & \rho_{i2} & \rho_{i1} & 1 \end{bmatrix}. \tag{21}$$

In the covariance matrix  $U_{y_i}$ , the greatest positive correlation occurs for the terms close to the mean  $y_i$ -value. Real type A uncertainty  $u_{y_i}$  of this point is greater than from the classical formula for  $m$  repeated measurements of  $y_i$ .

In estimating the uncertainty  $u_{A_i}$  of the mean value of the results of  $y_{im}$  of the point with abscissa  $x_i$ , instead of the number of measurements  $m$ , the effective number  $n_{\text{ieff}} < m$  must be used described by the following formula [5, 6]:

$$n_{\text{ieff}} = \frac{m}{1 + 2 \sum_{k=1}^{m-1} \frac{m-k}{m} \rho_{ik}}, \tag{22}$$

where  $m$  is the number of autocorrelated measurements,  $\rho_{ik}$  is the value of the autocorrelation function for the measurements of  $y_{ik}$ .

If the results of repeated measurements of the tested point  $Q_i$  are correlated with the coefficient  $\rho_{ik} = \rho$ , then the effective number of measurements of this series is:

$$n_{\text{ieff}} = \frac{m}{1 + \rho(m-1)}. \tag{22a}$$

Table 1 shows an example of the effective uncertainties  $u_{y_i}$  for  $m$ -fold measurements of the  $y_i$ -ordinate of the tested point with abscissa  $x_i$  and for three values of the correlation coefficient  $\rho$  between the measurements.

In each of the three series,  $m = 20$  measurements with the same uncertainty  $\sigma_i$  were performed.

Table 1

Effective uncertainties of a measurement series of  $y_i$  with three correlation coefficients

Correlation coefficient	$\rho$	$\rho=0$	$\rho=0.5$	$\rho=1$
Effective number of measurements	$n_{\text{ieff}}$	$n_{\text{ieff}} = m = 20$	$n_{\text{ieff}} = \frac{2m}{m+1} = 1.9$	$n_{\text{ieff}} = 1$
Effective uncertainties of a series of $m$ measurements of $y_i$	$\frac{\sigma_i}{\sqrt{n_{\text{ieff}}}}$	$0.22\sigma_i$	$0.72\sigma_i$	$\sigma_i$

Table 1 shows that with the increase in the correlation coefficient  $\rho$ , the standard uncertainty of the series increases because the effective number of measurements decreases from 20 to 1.9, and 1 for the correlation coefficients of 0, 0.5 and 1, respectively. The effective uncertainty for uncorrelated observations will be about 5 times less than when they are fully correlated.

$$U_Y = \sigma^2 \begin{bmatrix} 1 & \rho_1 & \dots & \rho_k & \dots & \rho_{n-1} \\ \rho_1 & 1 & \dots & \dots & \dots & \dots \\ \dots & \dots & 1 & \dots & \dots & \rho_k \\ \rho_k & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & 1 & \rho_1 \\ \rho_{n-1} & \dots & \rho_k & \dots & \rho_1 & 1 \end{bmatrix}$$

### 2.3. Correlation between ordinates of various measured points

Let us determine the covariance matrix describing measurements of the variable  $Y$  points with correlated ordinates. For example if  $y_i, y_j$  of two points  $Q(x_i, y_i), Q(x_j, y_j)$  are measured with the same uncertainties  $u_i = u_j = u = \text{const}$ , the autocorrelation function can also be used. In matrix (21), the uncertainty  $\sigma$  of separate measurements in a series is replaced by the effective uncertainty  $u$  of the measured points. Autocorrelation is a symmetrical function rapidly decreasing from the maximum value to zero, and its initial arms can be approximated with a straight line [5]. Usually, it is enough to consider only the neighbouring values of the measured ordinates  $y_{i-1}, y_i, y_{i+1}$  of the points with a known abscissa  $x_{i-1}, x_i, x_{i+1}$ , i.e.  $\rho_1 = \rho$  and  $\rho_k = 0$  for  $i = 2, \dots, n-1$ . For  $n$  equally remote points and of the same uncertainties  $u$  and correlation coefficients  $\rho$ , the covariance matrix  $U_Y$  (23) with its size  $n \times n$  gets all correlation coefficients  $\rho_k = \rho$  for  $i = 1, \dots, n-1$ . When the autocorrelation influence is negligible, the matrix  $U_Y$  reduces to the main diagonal:

The main equations for the regression straight-line parameters and its uncertainty band for the correlated values of the variable  $Y$  are given together in the left column of Table 2, and special cases for the uncorrelated data of the variable  $Y$  are summarized in the right column.

### 3. Numerical examples

Simulated numerical examples and their relations will be provided.

#### 3.1. Regressions line and uncertainty bands for the same value of absolute or of relative uncertainty

Table 3 shows the coordinates of 10 measured points with the same uncertainty values.

The values  $y_i$  are the averages of multiple measurements of the  $y_i$ -ordinates of each point with abscissa  $x_i$ . To identify the effects of individual factors, simplified cases will be analysed. It was assumed that absolute uncertainties  $u_i$  or relative uncertainties  $\delta_{ui}$  of the  $y$ -ordinate values for all points are the same and their abscissas  $x_i$  are constant and known exactly. To compare the results with the results obtained for uncorrelated  $y_i$ -ordinates, the same data of points were

Table 2

Parameters of regression line for autocorrelated and uncorrelated variable  $Y$

<b>Parameter*</b>	<b>measured:</b> $Y = [y_1, \dots, y_i, \dots, y_n]^T$ with uncertainty $u_i(y_i) \neq 0$ ; <b>known:</b> $X = [x_1, \dots, x_i, \dots, x_n]^T$ , $u_i(x_i) = 0$	
<b>Variable <math>Y</math></b>	<b>Correlated</b>	<b>Uncorrelated</b>
<b>Covariance matrix <math>U_Y</math> and its inverse</b>	$U_Y = \begin{bmatrix} u_1^2 & \dots & \rho_{y_1 n} u_1 u_n \\ \vdots & \ddots & \vdots \\ \rho_{y_1 n} u_1 u_n & \dots & u_n^2 \end{bmatrix}, U_Y^{-1}$	$U_Y = \begin{bmatrix} u_1^2 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & u_n^2 \end{bmatrix}, U_Y^{-1} = \begin{bmatrix} u_1^{-2} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & u_n^{-2} \end{bmatrix}$ $U_Y, U_Y^{-1}$ only diagonal elements
<b>Criterion</b>	$SK = [Y - aX - b]U_Y^{-1}[Y - aX - b] \rightarrow \min$	$SK = \sum_{i=1}^n (y_i - ax_i - b)^2 u_i^{-2} \rightarrow \min$
<b>Regression line parameters</b>	Slope $a = \frac{SS_{xy} - S_x S_y}{SS_{xx} - (S_x)^2} = \frac{\Delta_a}{\Delta}$ , abscissa $b = \frac{S_y S_{xx} - S_x S_{xy}}{SS_{xx} - (S_x)^2} = \frac{\Delta_b}{\Delta}$ , where $\Delta = SS_{xx} - (S_x)^2$ , $\Delta_a = SS_{xy} - S_x S_y$ , $\Delta_b = S_y S_{xx} - S_x S_{xy}$ .	

		$\Delta = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n (v_j z_j - v_j z_i)^2 \lambda_i^{-2} \lambda_j^{-2} \ast_1$	$\Delta = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n (x_i - x_j)^2 u_i^{-2} u_j^{-2}$
Auxiliary parameters	$S$	$[1, \dots, 1] U_Y^{-1} [1, \dots, 1]^T = \sum_{i=1}^n \sum_{j=1}^n [u_y^{-1}]_{ij}$	$\sum_{i=1}^n u_i^{-2} \quad \text{or} \quad \sum_{i=1}^n \delta_i^{-2} y_i^{-2}$
	$S_x$	$X^T U_Y^{-1} [1, \dots, 1]^T = [1, \dots, 1] U_Y^{-1} X$	$\sum_{i=1}^n x_i u_i^{-2} \quad \sum_{i=1}^n \delta_i^{-2} x_i y_i^{-2}$
	$S_{xx}$	$X^T U_Y^{-1} X$	$\sum_{i=1}^n x_i^2 u_i^{-2} \quad \sum_{i=1}^n \delta_i^{-2} x_i^2 y_i^{-2}$
	$S_y$	$Y^T U_Y^{-1} [1, \dots, 1]^T = [1, \dots, 1] U_Y^{-1} Y$	$\sum_{i=1}^n y_i u_i^{-2} \quad \sum_{i=1}^n \delta_i^{-2} y_i^{-1}$
	$S_{xy}$	$X^T U_Y^{-1} Y = Y^T U_Y^{-1} X$	$\sum_{i=1}^n x_i y_i u_i^{-2} \quad \sum_{i=1}^n \delta_i^{-2} x_i y_i^{-1}$
	$S_{yy}$	$Y^T U_Y^{-1} Y$	$\sum_{i=1}^n y_i^2 u_i^{-2} \quad \sum_{i=1}^n \delta_i^{-2} \quad \text{where: } u_i = \delta_i y_i$
Sensitivity Matrix $AB$	$AB = [A, B],$		$[AB^T]_i = [a_i, b_i]$
	$A = \frac{\partial a}{\partial Y} = \frac{S U_Y^{-1} X - S_x U_Y^{-1} [1, \dots, 1]^T}{\Delta},$ $B = \frac{\partial b}{\partial Y} = \frac{S_{xx} U_Y^{-1} [1, \dots, 1]^T - S_x U_Y^{-1} X}{\Delta}$		$a_i = \frac{\partial a}{\partial y_i} = \frac{1}{u_i^2} \frac{S x_i - S_x}{\Delta},$ $b_i = \frac{\partial b}{\partial y_i} = \frac{1}{u_i^2} \frac{S_{xx} - S_x x_i}{\Delta}.$
Covariance matrix $U_{ab}$	$U_{ab} = \begin{bmatrix} u_a^2 & \rho_{ab} u_a u_b \\ \rho_{ab} u_a u_b & u_b^2 \end{bmatrix} = AB U_Y AB^T, \quad u_a^2 = \frac{S}{\Delta}, \quad u_b^2 = \frac{S_{xx}}{\Delta}, \quad \rho_{ab} u_a u_b = -\frac{S_x}{\Delta}.$		
Type A uncertainties of regression line $y=ax+b$	Standard	$u_{ab}^2 = u_a^2 x^2 + 2x \rho_{ab} u_a u_b + u_b^2, \quad x_{min} = -\frac{\rho_{ab} u_b}{u_a}, \quad u_{ab min}^2 = (1 - \rho_{ab}^2) u_b^2$ or $u_{ab}^2 = \frac{1}{S} + \frac{S}{\Delta} \left( x - \frac{S_x}{S} \right)^2, \quad x_{min} = \frac{S_x}{S}, \quad u_{ab min}^2 = \frac{1}{S}.$	
	Expanded	$U_{ab} = t_{0.95, n-2} u_{ab}$	
The same uncertainty $u_i = u$ of $y_i$ of all points	Matrix $U_Y$ is replaced by correlator $R$ $U_Y = u^2 R_Y \quad \text{and} \quad U_Y^{-1} = u^{-2} R_Y^{-1}$		$u_a^2 = \frac{u^2}{\sum_{i=1}^n (x_i - \bar{x})^2}, \quad u_b^2 = \frac{1}{n} + \frac{u^2 \bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$ $\rho_{ab} u_a u_b = -\frac{u^2 \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2}$ where $\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i$ $u_{ab}^2(x) = u^2 \left( \frac{1}{n} + \frac{(x - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right)$
Variance estimator	$\widehat{u^2} = \frac{-a X^T R_Y^{-1} Y - b Y^T R_Y^{-1} [1, \dots, 1]^T + Y^T R_Y^{-1} Y}{n - 2}$		$\widehat{u^2} = \frac{-a \sum_{i=1}^n x_i y_i - b \sum_{i=1}^n y_i + \sum_{i=1}^n y_i^2}{n - 2}$
Type B uncertainty	$u_b(y) = u_b(y_0) + (y - y_0) E_{\max} / \sqrt{3}$		

Coordinates of measured points and equal absolute and relative uncertainties of  $y_i$ 

Symbol	Coordinates of points $(x_i, y_i)$ and uncertainties of $y_i$									
	1	2	3	4	5	6	7	8	9	10
$x_i$	1	2	3	4	5	6	7	8	9	10
$y_i$	2	1	4	3	6	5	8	7	10	11
$u(y_i)$	0.5									
$\delta(y_i)$	5%									
$u_{\rho}(y_i)$	0.01(1+y)%									
Regression line	for $u_i=u$ : $y=1.48x - 0.067$					for $\delta_{u_i}=\delta$ : $y = 0.978x - 0.463$				

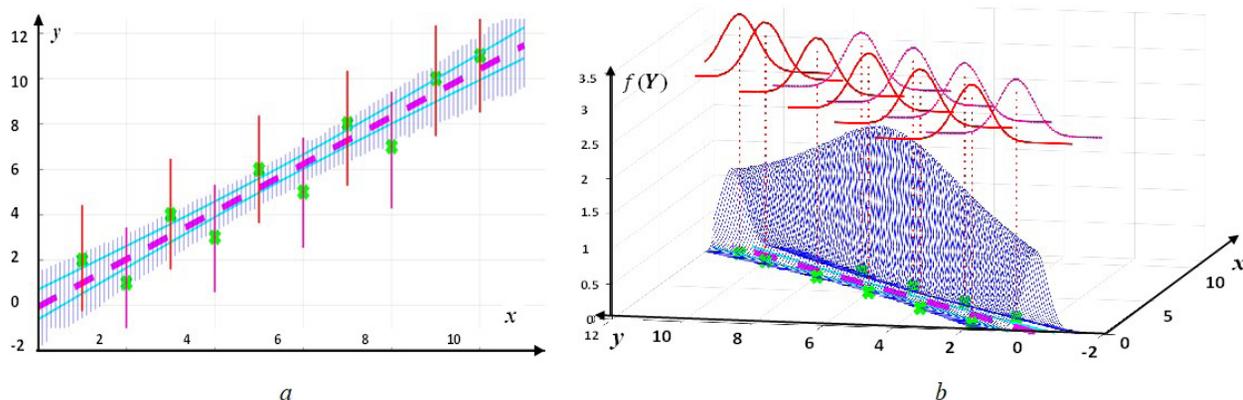


Fig. 2. *a* – Graphs of regression line with band of its expanded type A uncertainty; *b* – Gaussian probability density distributions (pdf-s) with uncertainty  $u = 0.5$  equal for all measured points and pdf-s  $f(y)$  of  $y$ -uncertainties along regression line in 3D view

used as for Experiment I, which is given in our papers [7–9]. All that is illustrated by Fig. 2*a, b*.

Fig. 2*a* shows the line and its uncertainty band (blue lines) determined by the linear regression method for the data from Table 2 when the correlation is absent. It also shows the uncertainty of the ordinates of the measured points (red lines). The figure shows that 95% of the expanded uncertainty region changes along the regression line such that its width decreases from the initial value to a minimum near the centre of the regression line, and then widens back to the original initial size.

At the top in Fig. 2*b*, there are the graphs of Gaussian probability density distributions (pdf – red

curves) for the ordinates of the measured points located on both sides of the regression line. The pdf of the  $y_i$ -ordinates are for 95% coverage with standard deviation  $u = 0.5$ . Below, the probability density curves for  $y$  around the regression line inside its uncertainty band (blue 3D solid) are shown. In the middle of the range of the regression line, pdf is the narrowest and therefore is the highest. The maximum (narrowest) pdf occurs for the minimum uncertainty bandwidth in the middle part of the straight line. When moving away from this maximum in the opposite directions, the maximum value of the pdf function decreases, and the distribution widens as the uncertainty band boundaries move away from each other.

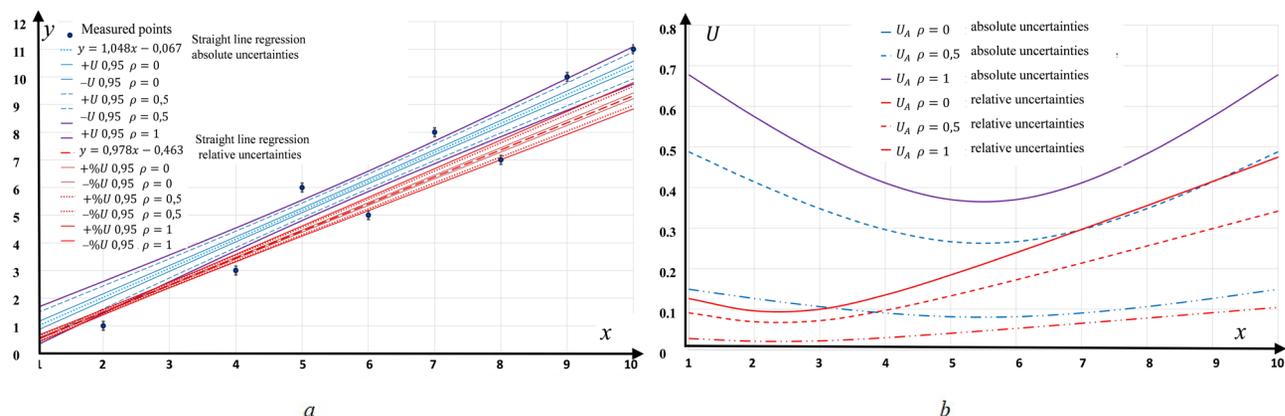


Fig. 3. *a* – Regression lines with expanded type A uncertainty bands; *b* – half height of bands of uncertainty  $U_A$  for three values of correlation coefficient  $\rho$  for series of 10 points from Table 2 measured 20 times each

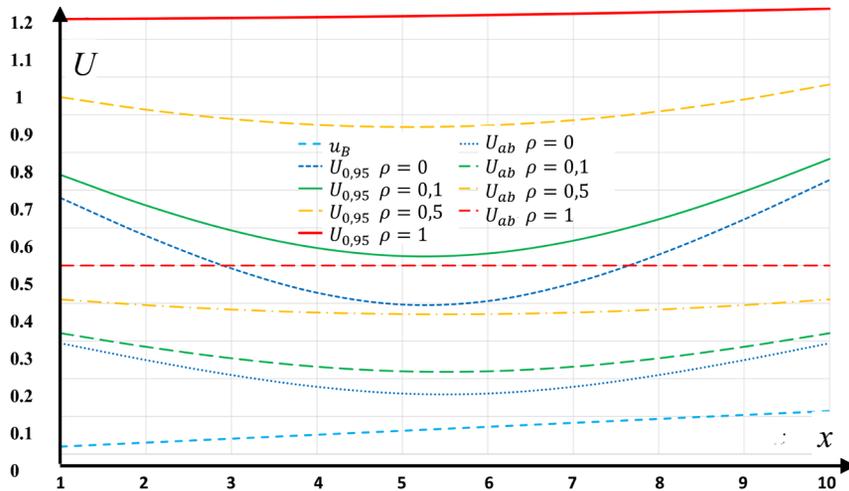


Fig. 4. Uncertainty bands for regression line  $y=1.048x-0.067$  for correlated and uncorrelated measurement points for three covariance matrixes  $U_Y(21)$  for  $u=0.5$ ,  $\rho_k = \rho$  for  $i=1, \dots, 9$ ,  $\rho=0$ ,  $\rho=0.1$ ,  $\rho=0.5$  and  $\rho=1$  with type B uncertainty

Fig. 3a shows two regression lines with their extended type A uncertainty bands  $\pm U_{0.95}$  calculated for the ordinates  $(x_i, y_i)$  of 10 points from Table 3 measured 20 times each with equal absolute uncertainties  $u_i=u$  (blue line  $y=1.048x-0.067$  runs above) or with equal relative uncertainties  $\delta_{u_i}=\delta_u$  (red line  $y=0.978x-0.463$  running below) and for three different correlation coefficients for  $y_i$ .

Fig. 3b shows functions of their  $U_{0.95}$ . With the increase in the correlation coefficient between the results of repeated measurement observations, the expanded uncertainty  $U_A$  increases [5, 6].

In section 2.2, it was shown that the effective number of observations of a sample with 20 measurements for the autocorrelation coefficients 0, 0.5 and 1 decreased from 20 to 1.9 and to 1. The narrowest uncertainty band is obtained for non-correlated observations, i.e. for  $\rho=0$ . If such measurements are made for the  $y_i$ -ordinates of all 20 measurements with the same uncertainty, then for the correlation coefficient  $\rho=1$ , the uncertainty band of the regression line is over four times wider than when the correlation is absent. Negative coefficients  $\rho$  do not occur in these measurements.

### 3.2. Influence of the correlation coefficient value between $y_i$ -ordinates on the uncertainty band

Fig. 4 compares two regression lines and uncertainty bands for the covariance matrix  $U_Y(21)$  with parameters  $u_i=0.5$ ,  $\rho=(0.6; 0.5; 0.4; 0.2; 0.1)$  and  $\rho=0$  for others. The regression line for correlated points is  $y=0.981x+0.417$ .

There is a significant increase (over 30%) in the width of an uncertainty band, when the points described by the covariance matrix are autocorrelated. On the other hand, type B uncertainty has a greater impact on the width of a band determined without correlation than on a band determined with correlation because with the data of Experiment I considered here, an increase in uncertainty by 1% is negligible.

The regression lines and their absolute uncertainty bands for full correlation ( $\rho=0.99 \approx 1$ ) of the measured  $y_i$ -ordinates of the points with the covariance matrix  $U_Y = u^2 [1]$  and when the correlation is absent ( $\rho=0$ ) are given in Fig. 5.

It is shown that with full correlation, i.e. for  $\rho=1$ , the hyperbolic boundaries of the uncertainty band become straight lines parallel to the regression line. The band constriction in the middle of the regression line

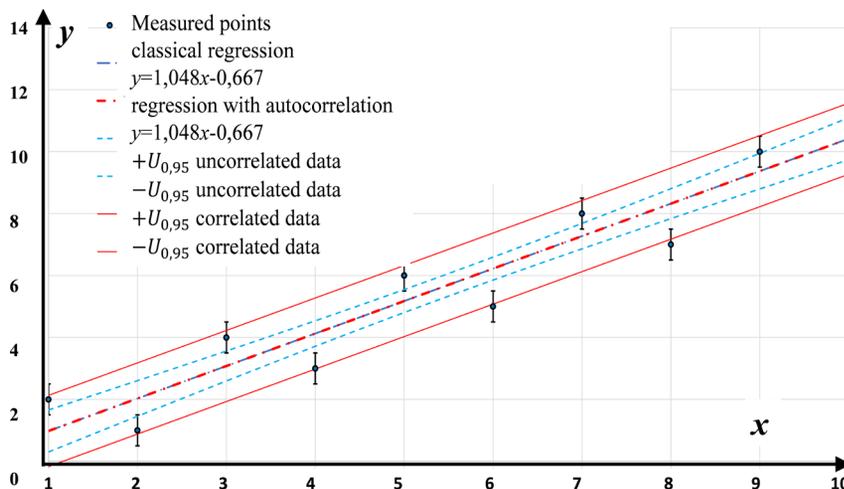
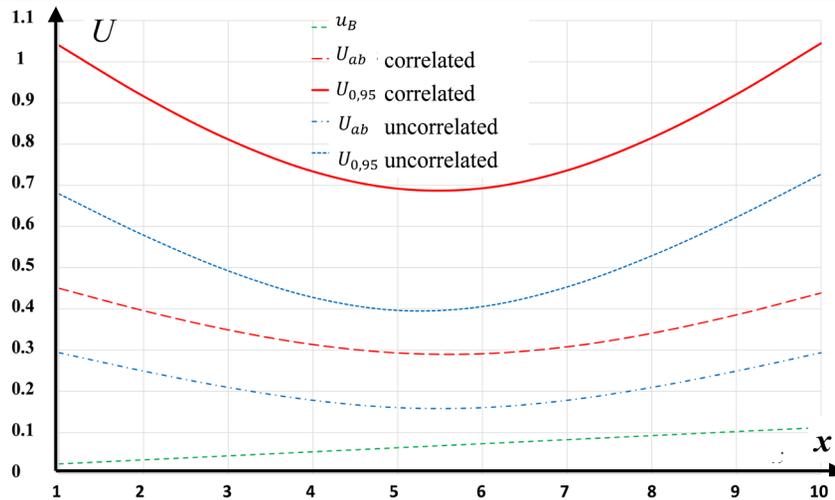


Fig. 5. Regression lines and uncertainty bands for measurement points with uncertainties marked at uncorrelated and correlated points with  $\rho \approx 1$  for covariance matrix  $U_Y$


 Fig. 6. Uncertainties for uncorrelated and correlated  $y_i$  of points with covariance matrix  $U_Y$  (21)

range disappear. The parameters of this regression line do not change with the increases of equal coefficients in the covariance matrix.

The graphs in Fig. 6 concern the courses of uncertainty  $U_{ab}$  (type A) and uncertainty  $u_B$  for the regression line obtained for the same values of the correlation coefficients between the  $y_{ik}$ -coordinates of each of the repeatedly measured points of  $x_i = \text{const}$ , i.e. according to their covariance matrix (21). With the presence of positive correlation, an increase in the width of the uncertainty band is observed.

### 3.3. Comparison of regression lines for constant absolute or relative uncertainties of measured $y_i$

In Fig. 7a, b the regression lines with uncertainty bands for the correlated and uncorrelated  $y_i$ -ordinates, measured with relative uncertainty  $\delta=1\%$ , were compared.

For small and the same values of correlation coefficients, such a straight line (Fig. 7a) deviates from their direction for the same ordinates without

$$U_Y(x) = \begin{bmatrix} u_{y_1}^2 & \rho_{y_1 y_2} u_{y_1} u_{y_2} \\ \rho_{y_1 y_2} u_{y_1} u_{y_2} & u_{y_2}^2 \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial a} & \frac{\partial y_1}{\partial b} \\ \frac{\partial y_2}{\partial a} & \frac{\partial y_2}{\partial b} \end{bmatrix} \begin{bmatrix} u_a^2 & \rho_{ab} u_a u_b \\ \rho_{y_1 y_2} u_{y_1} u_{y_2} & u_b^2 \end{bmatrix} \begin{bmatrix} \frac{\partial y_1}{\partial a} & \frac{\partial y_2}{\partial a} \\ \frac{\partial y_1}{\partial b} & \frac{\partial y_2}{\partial b} \end{bmatrix} = \begin{bmatrix} u_a^2 x_1^2 + 2x_1 \rho_{ab} u_a u_b + u_b^2 & u_a^2 x_1 x_2 + (x_1 + x_2) \rho_{ab} u_a u_b + u_b^2 \\ u_a^2 x_1 x_2 + (x_1 + x_2) \rho_{ab} u_a u_b + u_b^2 & u_a^2 x_2^2 + 2x_2 \rho_{ab} u_a u_b + u_b^2 \end{bmatrix}, \quad (23)$$

where  $\frac{\partial y_i}{\partial a} = x_i$ ,  $\frac{\partial y_i}{\partial b} = 1$  and  $i = 1, 2$ .

For two points with ordinates  $y_1, y_2$ , variances  $u_{y_1}^2, u_{y_2}^2$  and correlation coefficient  $\rho_{y_1 y_2}$  are

$$u_{y_1}^2 = u_a^2 x_1^2 + 2x_1 \rho_{ab} u_a u_b + u_b^2, \quad (23a, b)$$

$$u_{y_2}^2 = u_a^2 x_2^2 + 2x_2 \rho_{ab} u_a u_b + u_b^2$$

$$\rho_{y_1 y_2} = \frac{u_a^2 x_1 x_2 + (x_1 + x_2) \rho_{ab} u_a u_b + u_b^2}{u_{y_1} u_{y_2}}. \quad (24)$$

$$u_c^2(x) = u_{ab}^2 + u_B^2 = (u_a^2 + a^2 \delta_B^2) x^2 + 2(\rho_{ab} u_a u_b + a \delta_B (u_{B0} + \delta_B (b - y_0))) x + u_b^2 + (u_{B0} + \delta_B (b - y_0))^2. \quad (25)$$

correlation. Its slope was reduced from 0.978 to 0.869. The boundaries of the uncertainty band slightly widen for absolute uncertainties, and the boundaries of the band for relative uncertainties remain practically unchanged. The linearly increasing type B uncertainty  $u_B$  causes a disturbance of the symmetry of the limits of the expanded uncertainty  $U_{0,95}$  band in relation to the centre of the regression line and a shift towards higher values of the independent variable  $x$ . As a result, this uncertainty bandwidth increases with  $x$ , for both correlated and uncorrelated measuring points.

### 3.4. Correlation of the variable $Y$ values within the uncertainty band

Apart from the correlation between the  $y_i$ -ordinates of the measured points  $Q_i(x_i, y_i)$ , the  $y_i$ -values of points  $P_i(x_i, y_i)$  on the regression line  $y = ax + b$  (see Fig. 1) are also correlated with each other. This is because the covariance matrix of its two points  $y_i = ax_i + b$  (for  $i = 1, 2$ ) is determined by the variance propagation equation:

If the regression line describes the characteristic of the tested instrument, measurement device or process, and under variable influencing conditions, the unknown part of systematic errors cannot be eliminated, then type B uncertainty  $u_B$  should also be evaluated. It is assumed that the values of  $u_B$  result from maximum permissible errors  $E_{\max}$  of the applied digital meters as a linear function  $u_B(y) = u_{B0} + \delta_B (y - y_0)$  [1], or  $u_B(x) = u_{B0} + \delta_B (b - y_0) + \delta_B ax$ .

The combined uncertainty  $u_c$  of the regression line is larger than type A uncertainty  $u_{ab}$  and is described by the formula

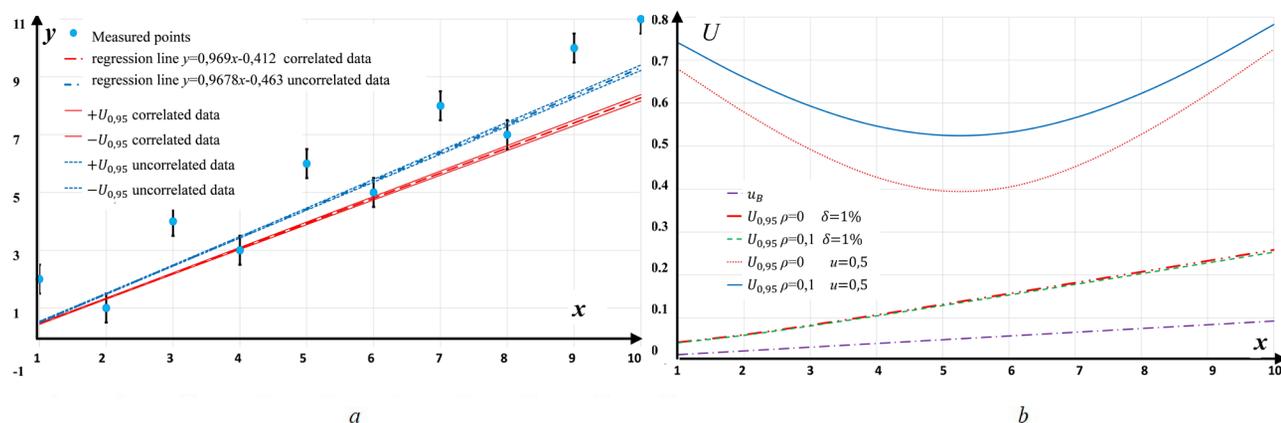


Fig. 7. Cases of equal relative uncertainty  $\delta=1\%$  for uncorrelated and correlated  $y_i$  of points for covariance matrix  $U_Y$  (21) with  $\delta=1\%$ ,  $\rho_k=0.1$  for  $i = 1, \dots, 9$ : a – regression lines; b – uncertainty  $U_{0.95}$  together with type B uncertainty

Then with the influence of type B uncertainties, the effective values of variances  $u_{aC}^2$ ,  $u_{bC}^2$  and the correlation coefficient  $\rho_{aBC}$ , will be respectively:

$$u_{aC}^2 = u_a^2 + a^2 \delta_B^2, \quad u_{bC}^2 = u_b^2 + (u_{B0} + \delta_B (b - y_0))^2 \quad (26a,b)$$

$$\rho_{aBC} = \frac{\rho_{ab} u_a u_b + a \delta_B (u_{B0} + \delta_B (b - y_0))}{u_{aC} u_{bC}}. \quad (26c)$$

Variances of the combined uncertainty in points  $x_i$  for  $i=1,2$  ( $u_{B0} = \delta_B = \delta$  for  $y_0=0$ ) are:

$$u_{yCi}^2 = (u_a^2 + a^2 \delta^2) x_i^2 + 2x_i (\rho_{ab} u_a u_b + a \delta^2 (1+b)) + u_b^2 + \delta^2 (1+b)^2. \quad (27)$$

Fig. 8 shows absolute  $U$  and relative uncertainty bands  $\delta_U = U/y$  of the regression line. They are obtained from (27) for absolute  $u=0.5$  and relative 1% uncertainties, and the correlation coefficient  $\rho_k = 0.3$  for  $i = 1, \dots, 9$  with a linearly increasing type B uncertainty  $u_{B0} = \delta_B = \delta$  for  $y_0=0$ .

In the uncertainty band narrowing area, the uncertainty for the correlated  $y_i$ -values increases almost twice as compared to the uncorrelated  $y_i$  with the same absolute uncertainties, and the influence of type B uncertainty makes the uncertainty bands slightly asymmetric. The resulting relative uncertainties decrease from several dozen percent at the beginning of the regression line to less than 10% at the end of its range. For relative uncertainties, the bands of correlated and uncorrelated variables almost coincide. They are slightly greater for the values of uncorrelated variables than for correlated variables. The initial relative values linearly increase to the level below 3, while relative values do not exceed the level of 2–3%. The influence of a linearly increasing type B uncertainty is practically imperceptible.

The correlation coefficient  $\rho_{C_{y_1 y_2}}$  between the variables  $y_1$  and  $y_2$  from (24) of the regression line, considering the influence of type B uncertainty (27), has the form

$$\rho_{C_{y_1 y_2}} = \frac{(u_a^2 + a^2 \delta_B^2) x_1 x_2 + (x_1 + x_2) (\rho_{ab} u_a u_b + a \delta_B (u_{B0} + \delta_B (b - y_0))) + u_b^2 + (u_{B0} + \delta_B (b - y_0))^2}{u_{yC1} u_{yC2}}. \quad (28)$$

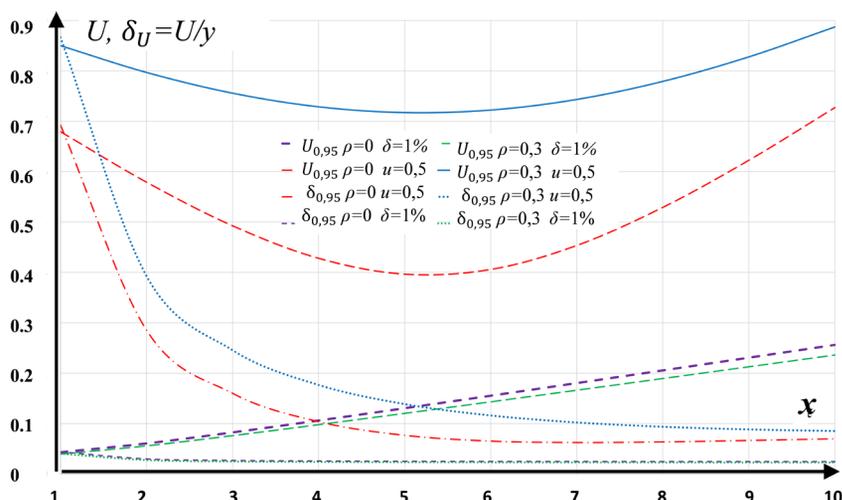


Fig. 8. Absolute  $U$  and relative uncertainty bands  $\delta_U = U/y$  of the regression line

Due to the linear dependency of  $y$  from  $x$ , these variables are fully correlated, which means that the same correlation coefficient as (28) have both variables  $x_1$  and  $x_2$ .

#### 4. Conclusions

The type A uncertainty bands of the regression line determined from measurements, similarly as for uncorrelated variables, run hyperbolically, and their cut-offs are symmetrical as to this line.

For the same value of relative uncertainties, the limits of the uncertainty band of the regression line are split hyperbolas with tangents diagonal to the line. In the middle part of the band, there is a constriction of width  $S$  depending on the parameters of the covariance matrix. With full correlation, i.e. for  $\rho=1$ , the hyperbolic boundaries of the uncertainty band become straight lines parallel to the regression line.

With the increase in the correlation coefficient between the ordinates of the tested points, the slope of the regression line decreases significantly. The ordinates of points within the uncertainty band are correlated more strongly if they are closer, and their

correlation coefficient tends to 1. This is applied to the entire range of  $y$ .

The accuracy of the regression line parameters improves with repeated measurements of the  $y$ -ordinate value of each point with the same abscissa  $x_i$ . The results of observations in such a series are close to each other, and it is necessary to consider the impact of their autocorrelation. For a given point, the local covariance matrix, or the formula for the effective number of measurements can be used – see works of Warsza and Zieba [4, 5].

Type B uncertainty is evaluated heuristically from the maximum permissible error  $E$  (MPB) of the meter. For the uniform distribution of errors with a range  $2E$ , the uncertainty  $u_B$  is the standard deviation  $E/\sqrt{3}$ . Usually, the error  $E$  linearly depends on  $(y - y_0)$  inside the measured range  $y_{\max} - y_0$  (e.g. for digital instruments).

The  $u_B$  uncertainty is summed up geometrically with type A uncertainty of the regression line obtained from measurements. The resultant combined and expanded uncertainty bands widen with the increase of  $y$  and  $x$ .

## Оцінка смуг невизначеності лінії регресії для корельованих даних змінної $Y$ з використанням правил GUM

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#### Анотація

Розглянуто оцінювання невизначеності вимірювань при побудові калібрувальної залежності засобів вимірювання за допомогою вимірювального експерименту, у ході якого вимірюються значення змінної  $Y$  спільно з вимірюванням абсциси  $X$ . Стаття обмежується дослідженням найпростішого випадку – лінійної регресії, але з урахуванням даних невизначеності вимірювань типу А і типу В та з урахуванням кореляції й автокореляції між ними. Отримано вирази для сумарної стандартної та розширеної невизначеностей у кожній точці вимірювань. Залежність відхилень вимірених значень ординати  $Y$  від значень абсциси  $X$  являє собою досліджувану смугу невизначеності. Наведено основні співвідношення для випадку відсутності невизначеності вимірювання абсциси  $X$ . Розглянуто випадок наявності точок із некорельованими ординатами та однаковими невизначеностями. Досліджено кореляцію в серії повторних вимірювань в одній точці ординати з одним і тим самим значенням абсциси. Наведено співвідношення для оцінювання невизначеності вимірювань за наявності кореляції між ординатами різних вимірених точок. Розглянуто змодельовані чисельні приклади. Розраховано лінію регресії та смуги невизначеності для однакового значення абсолютної або відносної невизначеності. Досліджено вплив значення коефіцієнта кореляції для ординат на діапазон невизначеності. Порівняно лінії регресії для постійних абсолютних або відносних невизначеностей вимірених значень ординати. Розглянуто приклад наявності кореляції значень змінної  $Y$  в діапазоні невизначеності.

**Ключові слова:** вимірювання; автокореляція; лінія регресії; смуги невизначеності типу А та типу В.

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