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RESEARCH ARTICLE

A New Algorithm for Generalization of Least Square Method for Straight Line Regression in Cartesian System for Fully Correlated Both Coordinates

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Abstract

This work presents the estimation of parameters and uncertainty of straight regression line using the least square method when both coordinates in Cartesian System XOY are affected by errors and fully correlated. The maximalization of the likelihood multivariate Gaussian function as equivalent of minimalization of objection function is derived for common vector variable Z included $\boldsymbol{X}$ and $\boldsymbol{Y}$ vectors random variable vectors of coordinates of measurement points. In this way all kind of possible correlations are taken into account within the metrological literature, there exist some works taking them into account. The core of the presentation is the mathematical manipulation based on linear algebra matrixes and vectors with elements of functional analysis. Any novelty claimed in this field will be carefully demonstrated. The problem is reduced to the determination of numerical one-dimensional characteristic e.g. objection function as function of slope a of straight regression line. The algorithm allows to determine numerically the covariance matrix $\boldsymbol{U}_{ab}$ and the coverage corridor for straight line regression. The implementation of the numerical method is applied in scripts Plot_G.txt and U_ab.txt running in MATLAB environment. Finally, the comparison of results based on the previous published tests are carried out.

Key Words: *Linear algebra; Uncertainty; Covariance matrix; Weighted total least squares method*

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1. Introduction

Methods of using least square fit for linear regression are well-known and have been widely applied since the works of C.F. Gauss and A.M Legendre dating to the eighteenth century. These methods are used in many engineering disciplines including: econometrics, social science, astronomy, geodetics, chemistry, climate science, biology but most important, in metrology. Least square method can be found as first publication by Pearson in 1901, also by Deming (1943), York (1966) with exact analytic solutions [1], of Golub and van Loan in which they introduced the errors-in-variables (EIV) models [2], Lybanon 1984 with method of effective variances and exact solutions for heteroscedasticity case [3], (Neri 1989) with special and proposed data for simulations [4], Krystek (2011) and Anthon [5] with special algorithm with correlation x and y coordinates with exact solutions of specific case using parametrization algorithm, publication by A.R. Amiri-Simkooei and Jazaeri using algorithm based on the Lagrange multipliers (2014) [6,7] and also many others [8-23].

Within the past few decades we had a lot of publications in the highest journals in the USA, Canada, Chine, Europe in this area of least square methods. It is not possible to give a complete list of them in literature references, but they can be partially found in the works published in the references section.

The numerical algorithm for WTLS (Weighted Total Least Square) method is very useful in metrology and that is why all known algorithm have been already implemented in a series of software developed by several NMIs: for example from NIST USA, NPL Great Britain, PTB Germany PTB , INRIM Italy and many others [18].

The proposed method is under development and maximum achieved accuracy on Person data with York weights is almost eight digits after point. It is to early to make a comparison with other implementation with advanced and sophisticated algorithm. In general three testing cases from article of A.R. Amiri-Simkooei and Jazaeri using algorithm based on the Lagrange multipliers are used in order to compare accuracy of calculations [6,7], but some cases with analytical solution of the problem also are demonstrated.

The proposed method is addressed to any carried out experiment when two data set of two coordinates x and y with covariances matrix are experimentally determined, e.g. measured. Based on the above data putting in EXCEL, the method implemented in MATLAB scripts Plot_G.txt and U_ab.txt is very fast and with high accuracy numerically determines the characteristics of the objective function in the parameter of straight regression line: a-slope and also b-intercept within the desired range of its variability. In this way, it allows you in relatively short time to assess whether there is a minimum of objective function and the least square method has the possibility to apply. The proposed method resolves problem of generalized of least square method e.g. WTLS so in the specific cases of covariances matrixes for Weighted Least Square (WLS) and Ordinary Least Square (OLS) method are also solved to. The overall breakdown is WTLS followed by WTS and OLS. From the linear algebra point of view this will reflect when the covariance matrix includes: non-diagonal elements, exactly diagonal elements or it is a identity matrix multiplied by a constant variance, respectively.

Since 1993 we used in our metrological works Guide for Expression of Uncertainty (GUM) and also supplements: one for propagation of distribution-Monte Carlo Methods, and also with supplement 2 describing methods estimating uncertainty on multivariate variables. So we will use the concept of defined uncertainty according to the GUM. JCGM100:2008, Evaluation of measurement data - Guide to the expression of uncertainty in measurement. + Supplement 2. Extension to any number of output quantities. JCGM102:2011.

The works include: estimating parameters of straight regression line, assumption for straight line regression, derivation of effective inverse covariance matrix, analyzing two extreme cases with domination of covariances matrixes $\boldsymbol{U}_X$ or $\boldsymbol{U}_Y$ with analytical solutions, consequences of the new approach and finally the new algorithm, some testing cases, summary and conclusions.

Most of parts of this work was presented during Joint Virtual Workshop of ENBIS and MATHMET Mathematical and Statistical Methods for Metrology MSMM 2021 in Turyn in Italy, (ID 78) which took place at 31 May-1 June 2021 the presentation was titled Generalization of least square method for straight line regression-A new approach [24].

2. Estimating Parameters of Straight Regression Line

In the figure 1 we have marked the measuring points M_i with coordinates x_i, y_i i=1,...,n, and plotted the straight regression line and the coverage corridor in cartesian system Y0X. If assume there is a regression of y on x with only coordinates y affected by errors, this corridor looks similar even when the second coordinates x is also affected by errors or any possible coordinates are correlated.

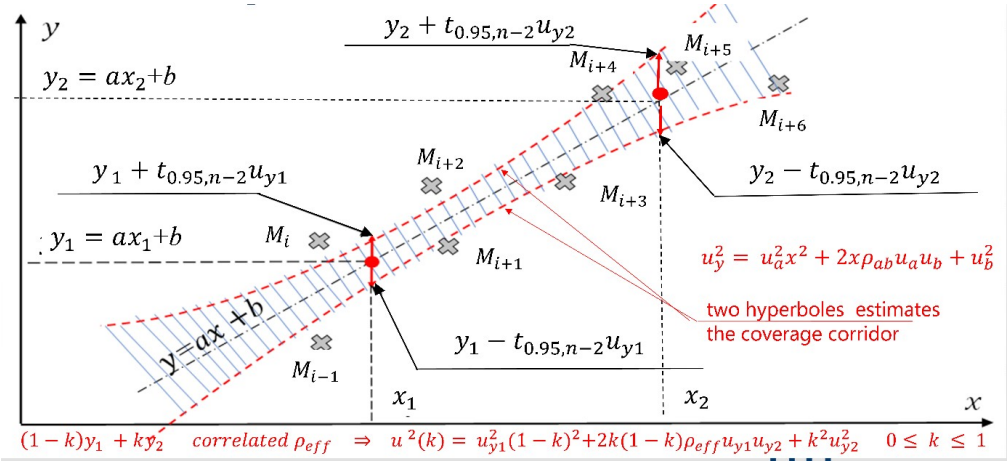


Figure 1: *Solution for straight line regression y on x problem in Cartesian XOY system. The coverage corridor between two hyperboles determining the standard/expanded uncertainties for y output quantity for every values of independent variables x.*

From metrological point of view we should determine standard/extended uncertainty at selected points for example: x_1 and x_2 From GUM it means the standard deviation of distribution of sum of two correlated distributions: for slope of straight line regression $a{\cdot}x$ (x – is treated as factor) and for intercept of straight line regression b. When the uncertainties of the variable y are much smaller than uncertainties of variable of x or close to zero, the uncertainty relating to variable x is transferred to the coverage corridor for the variable y in this accepted system. Therefore, the above model can be used for both variables that are error-affected and correlated in any way. Variance -

the square of standard uncertainty is the variance of the sum of the two correlated mentioned distributions ax and b where the mean values a and b determine for slope and intercept, respectively. On the other hand, the interval limits by expanded uncertainty for the two selected points x_1 *and* x_2 coordinates require a extension factor/coefficient to be set, which in this case is equal to the inverse of cumulative distribution function for student distribution for 95 % of probability and n-2 degree of freedom.

This form of variance is equivalent to a linear or quasi-linear sum of two weighted correlated random variables $(1-k)\,y_1+k\,y_2$,which it was presented at MATHMET conference in 2019 in Lisbon- see bottom of figure 1 [25].

So, the finding of straight regression line coverage corridor is very important as well as finding uncertainties for slope U_a and for intercept U_b and correlation coefficients ρ_{ab} e.g. elements of covariance matrix $\boldsymbol{U}_{ab}$. It is similar to the determining mean value and standard or expanded uncertainty. In contrary to very precision numerical method of propagation of distribution e.g. the Monte-Carlo method [26] to find the coverage corridor w applied the propagation of uncertainties in the form of a matrix equation using the linear model where all output quantities are sums of input quantities with corresponding sensitivity coefficients. Because the elements of covariance matrix $\boldsymbol{U}_{ab}$ are necessary for the determination of confidence curves describing by two hyperboles the method of linearizing of the model for performance multivariate function is used. In such model with multivariate random variables the uncertainty of one variable is extended to the covariance matrix. The covariance matrix propagation equation means that the transformations of the covariance matrix of input $\boldsymbol{U}_{in}$ to the output covariance matrix are $\boldsymbol{U}_{out}$ carried out using of a sensitivity matrix $\boldsymbol{C}$-Jacobian matrix whose elements are the first partial derivatives of the transform function $\boldsymbol{U}_{out} = \boldsymbol{C}\boldsymbol{U}_{in}\boldsymbol{C}^T$ [1]. This is the most general expression for the propagation of variances from one set of variables onto another. The estimation of expanded uncertainty at the output of the system requires to determine the area of the confidence region (coverage region) with a given probability so the extended coefficient (coverage factor) $k_{0,95}$ is required. Thus, in order to determine the coverage corridor and thus to determine the expanded uncertainty for these two points, it is necessary to know not only the parameters a and b of straight line regression, but also the $\boldsymbol{U}_{ab}$ covariance matrix. The matrix law of the propagation of uncertainty results in a correlation coefficient between the coordinates y_1 and y_2 are given:

$$\boldsymbol{U}_{y_{12}}=\begin{bmatrix}\frac{\partial y_1}{\partial a} & \frac{\partial y_1}{\partial b}\\ \frac{\partial y_2}{\partial a} & \frac{\partial y_2}{\partial b}\end{bmatrix}\boldsymbol{U}_{ab}\begin{bmatrix}\frac{\partial y_1}{\partial a} & \frac{\partial y_2}{\partial a}\\ \frac{\partial y_1}{\partial b} & \frac{\partial y_2}{\partial b}\end{bmatrix}=\begin{bmatrix}x_1 & 1\\ x_2 & 1\end{bmatrix}\boldsymbol{U}_{ab}\begin{bmatrix}x_1 & x_2\\ 1 & 1\end{bmatrix} \tag{1}$$

Where covariances matrixes are defined as:

$$\boldsymbol{U}_{ab}=\begin{bmatrix}u_a^2 & \rho_{ab}u_a u_b\\ \rho_{ab}u_a u_b & u_b^2\end{bmatrix},\ \boldsymbol{U}_{y_{12}}=\begin{bmatrix}u_{y_1}^2 & \rho_{y12}u_{y_1}u_{y_2}\\ \rho_{y12}u_{y_1}u_{y_2} & u_{y_2}^2\end{bmatrix} \tag{1 a,b}$$

After simply matrix multiplication we have (i=1,2)

$$u_{y_i}^2 = x_i^2 u_a^2 + 2 x_i \rho_{ab} u_a u_b + u_b^2, \qquad \rho_{y1,2} = \frac{u_a^2 x_1 x_2 + \rho_{ab} u_a u_b (x_1 + x_2) + u_b^2}{u_{y_1} u_{y_2}} \tag{2 a,b}$$

3. Assumption for Straight Line Regression

As a result of repeated measurement at each measuring points of the values of both coordinates, we can determine the mean value, uncertainty for each coordinates, and also determine the experimental correlation coefficients of each pairs of the M_i and $M_j$considered measuring points.It can be taken into account autocorrelation for a random variable, x_i and x_j, and $y_i$and ,y_j as well as cross-correlation for x_i and y_j, x_j and y_i, x_i and y_i, x_j and y_j coordinates see figure 2.

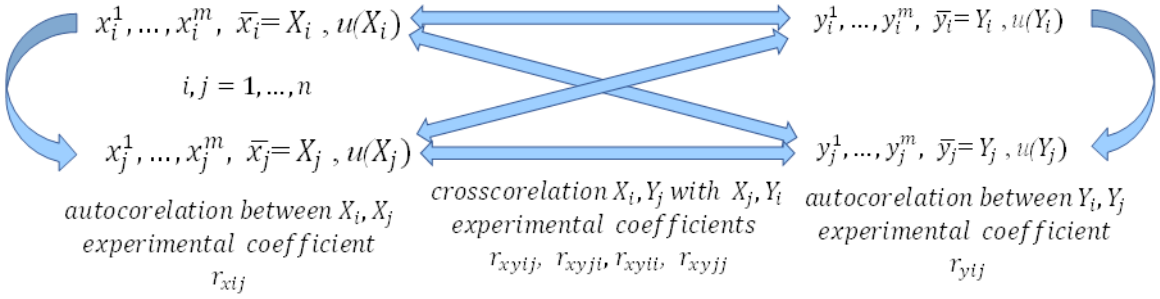


Figure 2: *Any possible correlations between measurement data of chosen pairs measurements points* M_i *and* M_j.

By adopting Gaussian distributions as input at any measurements points, we get joint density distributions inside the coverage corridor at the corresponding P_i and P_j points lying on a straight regression line to which errors are determined from the measuring points. The resulting distributions at P_i and P_j points along the *y* define the individual confidence intervals-see figure 3 Our task is from input quantities obtain output quantities *a*, *b* and the covariance matrix $\boldsymbol{U_{ab}}$.

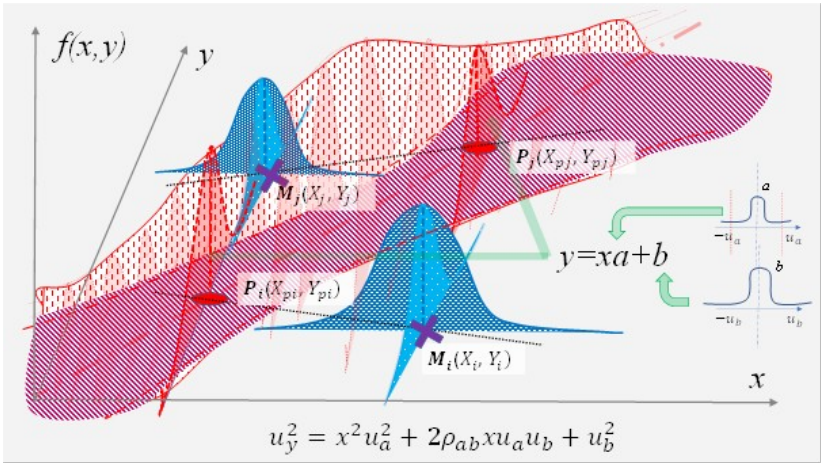


Figure 3: *Joint probability multivariate distribution f(x, y) according with (5) along straight line regression and two probability one dimensional distribution at the two projecting points* P_i *and* P_j *laying on the*

straight line regression corresponding to the two measurement points M_i and M_j with probability distribution along x and y. The projecting points distributions are always a sum of two random correlated variables a multiplicated by factor x with standard uncertainty xu_a and variables b with standard uncertainty u_b.The variance (square of standard uncertainty) is as given at the bottom of figure.

Now, from two n–dimensional vectors random variables: $\boldsymbol{X}=[X_1,\ldots,X_n]^T$, $\boldsymbol{Y}=[Y_1,\ldots,Y_n]^T$, we create mean vector of new common vector random variable 2 x n- dimensional – multivariate variable $\boldsymbol{Z}$ to take into account any cross correlation between both coordinates,

$$\boldsymbol{Z}=[\boldsymbol{X}^{\boldsymbol{T}},\boldsymbol{Y}^{\boldsymbol{T}}]^T=[X_1,\ldots,X_n,Y_1,\ldots,Y_n]^T=[Z_1,\ldots,Z_{2n}]^T \tag{3}$$

Where mean vector is

$$\boldsymbol{Z}_{\boldsymbol{P}}=[X_{P1},\ldots,X_{Pn},Y_{P1},\ldots,Y_{Pn}]^T=[Z_{P1},\ldots,Z_{P2n}]^T, \tag{3 a,b}$$

where and $z_i^k=x_i^k$, i=1,…,n, $z_j^k=y_j^k$, $j=n+1,\ldots,2n, k=1,\ldots,m$. In our derivations we applied very useful vector equation of straight line regression in vector representation which can be expressed as:

$$\begin{bmatrix} Y_{P1} \\ \ldots \\ Y_{Pn} \end{bmatrix}=a\begin{bmatrix} X_{P1} \\ \ldots \\ X_{Pn} \end{bmatrix}+b\begin{bmatrix} 1 \\ \ldots \\ 1 \end{bmatrix} <=> \quad \boldsymbol{y_P}=a\,\boldsymbol{X_P}+\boldsymbol{b}, \quad \boldsymbol{b}=b\begin{bmatrix} 1 \\ \ldots \\ 1 \end{bmatrix} \tag{4}$$

We put vector random variable to the likelihood for a Gaussian joint density multivariate function and from maximizing likelihood obtain minimizing condition for objective function. The common covariance matrix $\boldsymbol{U_Z}$ is a typical covariance matrix size of $2n$ x $2n$ for **Z**-random vector variable size of $2n$. The likelihood for a Gaussian joint density multivariate function is expressed as

$$\mathrm{L}((\boldsymbol{\Delta Z})=f(\boldsymbol{\Delta Z})=\frac{1}{(2\pi)^n\sqrt{det(\boldsymbol{U_Z})}}\exp\left(\frac{-1}{2}\boldsymbol{\Delta Z}^T\boldsymbol{U_Z^{-1}}\boldsymbol{\Delta Z}\right) \tag{5}$$

Where the vector of errors is defined as: $\boldsymbol{\Delta Z}=\boldsymbol{Z}-\boldsymbol{Z_p}=[\boldsymbol{\Delta X}^{\boldsymbol{T}},\boldsymbol{\Delta Y}^{\boldsymbol{T}}]^{\boldsymbol{T}}$, and covariance matrix $\boldsymbol{U_Z}$ can be described as

$$\boldsymbol{U_Z}=\begin{bmatrix} u^2(Z_1) & \cdots & \rho_{n1}u(Z_1)u(Z_{2n}) \\ \vdots & \ddots & \vdots \\ \rho_{1n}u(Z_1)u(Z_{2n}) & \cdots & u^2(Z_{2n}) \end{bmatrix} \tag{6}$$

and determinant of $\boldsymbol{U_Z}$ must be greater than zero:$det(\boldsymbol{U_Z})>0$. In (6) the standard deviation $\sigma(Z_i)$ are replaced by uncertainties $u(Z_i)$ and correlation coefficients ρ_{ij} are estimated by experimental correlation coefficients r_{ij}

$$r_{ij}=\frac{\sum_{k=1}^{m}\left(z_i^k-Z_i\right)\left(z_j^k-Z_j\right)}{\sqrt{\sum_{k=1}^{m}\left(z_i^k-Z_i\right)^2}\sqrt{\sum_{k=1}^{m}\left(z_j^k-Z_j\right)^2}} \quad \text{and} \quad i,j=1,\ldots,2n. \tag{7}$$

The maximum likelihood means the minimum of the objective function:

$$\mathrm{L}(\boldsymbol{\Delta Z}) \rightarrow max \Leftrightarrow G(\boldsymbol{\Delta Z})=\boldsymbol{\Delta Z}^T\boldsymbol{U}_Z^{-1}\boldsymbol{\Delta Z} \rightarrow min \tag{8}$$

Hence, the two equations of system are obtained:

$$\begin{cases} G(\boldsymbol{\Delta Z})=\boldsymbol{\Delta Z}^T\boldsymbol{U}_Z^{-1}\boldsymbol{\Delta Z} \rightarrow min \\ \boldsymbol{Y}_p=a\,\boldsymbol{X}_p+\boldsymbol{b} \end{cases} \tag{9 a,b}$$

where the covariance and inverse of the covariance matrixes can be partitioned to the parts of size n x n**:**

$$\boldsymbol{U}_Z=\begin{bmatrix} \boldsymbol{U}_X & \boldsymbol{U}_{XY} \\ \boldsymbol{U}_{XY}^T & \boldsymbol{U}_Y \end{bmatrix}, \qquad \boldsymbol{U}_Z^{-1}=\begin{bmatrix} \boldsymbol{V}_{11} & \boldsymbol{V}_3 \\ \boldsymbol{V}_3^T & \boldsymbol{V}_{22} \end{bmatrix} \tag{10 a,b}$$

So, the units of $\boldsymbol{U}_Z$ matrix are not uniform in general because $\boldsymbol{U}_X,\boldsymbol{U}_{XY}\left(\boldsymbol{U}_{XY}^T\right),\boldsymbol{U}_Y$ size of n x n have different units: square of unit x, product of units x y and square of unit y, respectively. The matrix $\boldsymbol{U}_{XY}$ is not a covariance matrix because it does not have a diagonal with square of uncertainties. The matrix $\boldsymbol{U}_{XY}$ should be called as covariance parts where all elements have the same form . In general, $\rho_{ij}u(X_i)u(Y_j)i,j=1,\ldots,n$ $\rho_{ij}u(X_i)u(Y_j)\neq\rho_{ji}u(X_j)u(Y_i)$ and the matrix $\boldsymbol{U}_{XY}$ do not need to be symmetrical $\boldsymbol{U}_{XY}^T\neq\boldsymbol{U}_{XY}$ at all**,** although both $\boldsymbol{U}_{XY}^T$ and $\boldsymbol{U}_{XY}$ have the same diagonal elements. Also, both vectors $\boldsymbol{z}$ and $\boldsymbol{z}_p$, have two units: part of $\boldsymbol{X}$ has unit of x and part of $\boldsymbol{Y}$ has a unit of y. Analogically the four parts of $\boldsymbol{U}_Z^{-1}$ have a different units. The matrixes $\boldsymbol{V}_{11},\boldsymbol{V}_3(\boldsymbol{V}^T_3),\boldsymbol{V}_{22}$, have inverse of square of unit x, inverse of product of units x y and inverse of square of unit y, respectively.

4. Derivation of Effective Inverse Covariance Matrix

This is mathematical description of our task and as we see the symmetric matrix $\boldsymbol{U}_z$ has to be partitioned with different units as well as inverse matrix has to be partitioned to four element with different units. The objective function can be described as:

$$\begin{aligned} G(\boldsymbol{\Delta Z},a,b)=G(\boldsymbol{\Delta X},\boldsymbol{\Delta Y},a,b) &= [\boldsymbol{\Delta X}^T,\boldsymbol{\Delta Y}^T]\boldsymbol{U}_Z^{-1}\begin{bmatrix}\boldsymbol{\Delta X}\\ \boldsymbol{\Delta Y}\end{bmatrix} = [\boldsymbol{\Delta X}^T,\boldsymbol{\Delta Y}^T]\begin{bmatrix}\boldsymbol{V}_{11} & \boldsymbol{V}_3\\ \boldsymbol{V}_3^T & \boldsymbol{V}_{22}\end{bmatrix}\begin{bmatrix}\boldsymbol{\Delta X}\\ \boldsymbol{\Delta Y}\end{bmatrix} = \\ &= \boldsymbol{\Delta X}^T\boldsymbol{V}_{11}\boldsymbol{\Delta X}+\boldsymbol{\Delta X}^T\boldsymbol{V}_3\boldsymbol{\Delta Y}+\boldsymbol{\Delta Y}^T\boldsymbol{V}_3^T\boldsymbol{\Delta X}+\boldsymbol{\Delta Y}^T\boldsymbol{V}_{22}\boldsymbol{\Delta Y} = \\ &= \boldsymbol{\Delta X}^T\boldsymbol{V}_{11}\boldsymbol{\Delta X}+2\boldsymbol{\Delta X}^T\boldsymbol{V}_3\boldsymbol{\Delta Y}+\boldsymbol{\Delta Y}^T\boldsymbol{V}_{22}\boldsymbol{\Delta Y} \end{aligned} \tag{11}$$

This leads to the objective function which consists of three elements:

1 First autocorrelation x - domination of $\boldsymbol{U}_X$ matrix with the ability to solve problems by subjugating mathematical formulas for regression x on y :

$$\Delta X^T V_{11} \Delta X \gg 2\Delta X^T V_3 \Delta Y + \Delta Y^T V_{22} \Delta Y \quad \text{then} \quad U_z^{-1} = V_{11} \approx U_X^{-1};$$

2 The middle cross correlation between x and y - the second element is corresponding for cross correlation and occurs only when both above elements are considered non-zero $V_3 \neq 0$, and therefore requires invertible of U_Z matrix. If the middle element is zero, the invertible matrix U_z^{-1} is composed by independently invertible two matrixes the U_X^{-1} and U_Y^{-1}.

3 Third autocorrelation y - responsible for the dominance of the U_Y matrix – regression y on x with autocorrelation y :

$$\Delta Y^T V_{22} \Delta Y \gg 2\Delta X^T V_3 \Delta Y + \Delta X^T V_{11} \Delta X \text{ then } U_z^{-1} = V_{22} \approx U_Y^{-1}$$

From vector equation of straight line regression for projecting points we obtain:

$$Y_p = a X_p + b \Rightarrow Y_p - Y + Y = a X_p - a X + a X + b \tag{12}$$

Defining the new vector $E = Y - aX - b$, the error vector ΔY can be expressed as:

$$\Delta Y = a \Delta X + E \tag{13}$$

Substitution of the error vector ΔY leads to expression for objective function as follows

$$G(\Delta X, a, b) = \Delta X^T V_{11} \Delta X + \Delta X^T V_{33} \Delta Y + \Delta Y^T V_{22} \Delta Y =$$
$$= \Delta X^T V_{11} \Delta X + \Delta X^T V_3 [a\Delta X + E] + [a\Delta X + E]^T V_3^T \Delta X + [a\Delta X + E]^T V_{22} [a\Delta X + E] =$$
$$= \Delta X^T V_{11} \Delta X + a \Delta X^T V_{33} \Delta X + 2E^T V_3^T \Delta X + a^2 \Delta X^T V_{22} \Delta X + 2a E^T V_{22} \Delta X + E^T V_{22} E \tag{14}$$

Where $V_{33} = V_3 + V_3^T$ is a symmetric matix.

The final expression for objective function is:

$$G(\Delta X, a, b) = \Delta X^T V \Delta X + 2E^T \left(V_3^T + a V_{22}\right) \Delta X + E^T V_{22} E \tag{15}$$

where $V = V(a) = V_{11} + a V_{33} + a^2 V_{22}$, V - symmetric matrix, has a real eigenvalues λ_{Vi} with normalized orthogonal eigenvectors R_i, i=1,...,n and

$$V R_i = \lambda_{Vi} R_i, \qquad R_i R_j = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \tag{16}$$

This expression (15) will be minimized analytically by looking for a local minimum for error vector ΔX- we have hyper parabolic/quadratic dependence, and next minimizing for local minimum for variable b to finally expressed the function $G(a)$ as one dimensional dependence on a. If matrix V is diagonal like for noncorrelated case it is possible to express (15) as sum of quadratic form. Orthogonal matrix $H^T = H^{-1}$ is composed of normalized eigenvectors $H = [R_1, \ldots, R_n]$ and $H^{-1} H = H H^{-1} = \mathbf{I}$ and also matrix V can be diagonalized in the following way:

$$\boldsymbol{H}^{-1}\boldsymbol{V}\boldsymbol{H}=\begin{bmatrix}\lambda_{V1} & 0 & 0\\ 0 & \dots & 0\\ 0 & 0 & \lambda_{Vn}\end{bmatrix} \tag{17}$$

The same possibility of expression of objection function as sum of quadratic form we obtain if we apply a mathematic trick to insert two times an identity matrix to diagonalize matrix V. Consequently, it is always possible to present this expression:

$$G(\boldsymbol{\Delta X},a,b)=\left(\boldsymbol{H}^{T}\boldsymbol{\Delta X}\right)^{T}\boldsymbol{H}^{-1}\boldsymbol{V}\boldsymbol{H}\left(\boldsymbol{H}^{T}\boldsymbol{\Delta X}\right)+2\left(\boldsymbol{H}^{T}\boldsymbol{\Delta X}\right)^{T}\boldsymbol{H}^{-1}\left(\boldsymbol{V}_{3}+a\boldsymbol{V}_{22}\right)\boldsymbol{E}+\boldsymbol{E}^{T}\boldsymbol{V}_{22}\boldsymbol{E} \tag{18}$$

in the form of sums of quadratic forms:

$$G(\boldsymbol{\Delta X},a,b)=\sum_{i=1}^{n} h x_i^2\lambda_{Vi}+2h x_i h VE_i+\boldsymbol{E}^{T}\boldsymbol{V}_{22}\boldsymbol{E} \tag{19}$$

where $\boldsymbol{\Delta X}$ is linearly transformed (by translation, rotation) to the new n-dimensional vector $\boldsymbol{hx}=\boldsymbol{H}^{T}\boldsymbol{\Delta X}$. and hVE_i are elements of $\boldsymbol{H}^{-1}(\boldsymbol{V}_{3}+a\boldsymbol{V}_{22})\boldsymbol{E}$ vector. The minimum of G in the case of all eigenvalues $\lambda_{Vi}>0$, i=1,..,n, is reached when all quadratic forms have minimum and therefore matrix $\boldsymbol{V}$ must be positive definite**.** If all the eigenvalues of matrix $\boldsymbol{V}$ are positive, i.e. the $\boldsymbol{V}$ matrix is positive define, then objective function takes the minimum value when for each square form reaches the minimum. It occurs for the vertex of hyper parabola of (19) - we have a special expressions for parabola, that is, we can differentiate function G due to the error vector $\boldsymbol{X}-\boldsymbol{X}_{p}$ and therefore due to the vector- that is, choose such a set of points $\boldsymbol{X}_{p}$ on a regression that minimizes locally objective function. Automatically we obtain expression of error vector for $\Delta\boldsymbol{X}$ and for $\Delta\boldsymbol{Y}$ on above minimizing condition. There is no need to parameterize and search the vector $\boldsymbol{X}_{p}$ set to minimize the objective function.

The condition for minimum of $G(\boldsymbol{\Delta X},a,b)$ due to $\boldsymbol{\Delta X}$ ($\boldsymbol{X}$- constant vector of coordinates x)

$$\frac{\partial G(\Delta\boldsymbol{X},a,b)}{\partial\boldsymbol{\Delta X}}=\frac{\partial G\left(\boldsymbol{X}-\boldsymbol{X}_{p},a,b\right)}{\partial\left(\boldsymbol{X}-\boldsymbol{X}_{p}\right)}=\frac{\partial G\left(-\boldsymbol{X}_{p},a,b\right)}{\partial\left(-\boldsymbol{X}_{p}\right)}=\boldsymbol{0} \tag{20}$$

Hence, $\boldsymbol{\Delta X}_{\boldsymbol{vertex}}^{\boldsymbol{T}}=-\boldsymbol{E}^{T}(\boldsymbol{V}_{3}^{T}+a\boldsymbol{V}_{22})\boldsymbol{V}^{-1}$ because for quadratic dependence: $g(x)=a_1x^2+b_1x+c_1$ and $a_1>0$ we have the minimum at $x_{vertex}=\frac{-b_1}{2a_1}$. And also from $\boldsymbol{\Delta Y}=a\Delta\boldsymbol{X}+\boldsymbol{E}$, and then $\boldsymbol{\Delta Y}_{\boldsymbol{vertex}}^{\boldsymbol{T}}=\boldsymbol{E}^{T}(\boldsymbol{V}_{11}+a\boldsymbol{V}_{3})\boldsymbol{V}^{-1}$**.** The value of minimum of quadratic form $G(\boldsymbol{\Delta X},a,b)$ from (15), it is at vertex of hyper parabola:

$$G\left(\boldsymbol{\Delta X}_{\boldsymbol{vertex}},a,b\right)=G(\mathrm{a,b})=\boldsymbol{E}^{T}\left(\boldsymbol{V}_{3}^{T}+a\boldsymbol{V}_{22}\right)\boldsymbol{\Delta X}_{\boldsymbol{vertex}}+\boldsymbol{E}^{T}\boldsymbol{V}_{22}\boldsymbol{E} \tag{21}$$

After simplifying we obtain:

$$G(\Delta\boldsymbol{X},a,b)\geq G(\mathrm{a,b})=\boldsymbol{E}^{T}\left[\boldsymbol{V}_{22}-\left(\boldsymbol{V}_{3}^{T}+a\boldsymbol{V}_{22}\right)\boldsymbol{V}^{-1}\left(\boldsymbol{V}_{3}+a\boldsymbol{V}_{22}\right)\right]\boldsymbol{E} \tag{22}$$

The minimum of objective function is given at vertex of hyper parabola for local minimum for error vector of $\boldsymbol{\Delta X}$. In this way the objective function can be expressed as for regression y on x

when we introduce the effective inverse of covariance matrix, which is dependent on slope a as well as matrix $\boldsymbol{V}$.

$$G(a,b)=\left[\boldsymbol{Y}-a\,\boldsymbol{X}-\boldsymbol{b}\right]^{T}\boldsymbol{U}_{\boldsymbol{Yeff}}^{-1}\left[\boldsymbol{Y}-\boldsymbol{a}\,\boldsymbol{X}-\boldsymbol{b}\right] \tag{23}$$

where effective inverse of covariance matrix is given by

$$\boldsymbol{U}_{\boldsymbol{Yeff}}^{-1}=\boldsymbol{V}_{22}-\left(\boldsymbol{V}_{3}^{T}+a\,\boldsymbol{V}_{22}\right)\boldsymbol{V}^{-1}\left(\boldsymbol{V}_{3}+a\,\boldsymbol{V}_{22}\right) \tag{24}$$

where the matrix $\boldsymbol{V}=\boldsymbol{V}(a)=\boldsymbol{V}_{11}+a\,\boldsymbol{V}_{33}+a^{2}\boldsymbol{V}_{22}$ and it is dependent on a.

When the matrix $\boldsymbol{V}_3$ is symmetric e.g. $\boldsymbol{V}_3=\boldsymbol{V}_3^{T}$ then the expression for effective inverse matrix reduces to the form:

$$\boldsymbol{u}_{\boldsymbol{yeff}}^{-1}=\left(\boldsymbol{V}_{11}\boldsymbol{V}_{22}-\boldsymbol{V}_{3}\boldsymbol{V}_{3}\right)\boldsymbol{V}^{-1}=\left(\boldsymbol{V}_{11}\boldsymbol{V}_{22}-0{,}25\,\boldsymbol{V}_{33}\boldsymbol{V}_{33}\right)\boldsymbol{V}^{-1} \tag{24a}$$

5. Domination of Matrix Uy - Regression y on x With Autocorrelation

At this moment we consider, in simply linear algebra way, the regression y on x when matrix $\boldsymbol{U}_{\boldsymbol{X}}$ is zero and all errors are calculate along variable y. The OY direction of measurement error is accepted. Here, $uY_i\neq 0$ and $uX_i=0$ and $\boldsymbol{X}_{\boldsymbol{p}}=\boldsymbol{X}$, $\boldsymbol{\Delta X}=0$, $\boldsymbol{\Delta Y}=\boldsymbol{Y}-\boldsymbol{Y}_{\boldsymbol{p}}=\boldsymbol{Y}-\boldsymbol{a}\,\boldsymbol{X}_{\boldsymbol{p}}-\boldsymbol{b}=\boldsymbol{Y}-\boldsymbol{a}\,\boldsymbol{X}-\boldsymbol{b}$. The covariance matrix have these parts: $\boldsymbol{U}_{\boldsymbol{Z}}=\boldsymbol{U}_{\boldsymbol{Y}},\boldsymbol{U}_{\boldsymbol{Z}}^{-1}=\boldsymbol{U}_{\boldsymbol{Y}}^{-1},\boldsymbol{U}_{\boldsymbol{XY}}=\boldsymbol{U}_{\boldsymbol{X}}=0$.

The objective function becomes:

$$G(a,b)=\boldsymbol{\Delta Y}^{T}\boldsymbol{U}_{\boldsymbol{Y}}^{-1}\boldsymbol{\Delta Y}=\left[\boldsymbol{Y}-a\,\boldsymbol{X}-\boldsymbol{b}\right]^{T}\boldsymbol{U}_{\boldsymbol{Y}}^{-1}\left[\boldsymbol{Y}-a\,\boldsymbol{X}-\boldsymbol{b}\right] \tag{25}$$

Introducing the new universal notation of parameters for universal notation of inverse of covariance matrix $\boldsymbol{U}^{-1}=\boldsymbol{U}_{\boldsymbol{Y}}^{-1}$ in the following manner and use distributive property which holds with respect to multiplication over addition we introduce the new scalar parameters:

$$S=\boldsymbol{1}^{T}\boldsymbol{U}^{-1}\boldsymbol{1}=\sum_{i=1}^{n}\sum_{j=1}^{n}\left[u^{-1}\right]_{ij},$$

$$S_x=\boldsymbol{X}^{T}\boldsymbol{U}^{-1}\boldsymbol{1}=\boldsymbol{1}^{T}\boldsymbol{U}^{-1}\boldsymbol{X},\qquad S_y=\boldsymbol{Y}^{T}\boldsymbol{U}^{-1}\boldsymbol{1}=\boldsymbol{1}^{T}\boldsymbol{U}^{-1}\boldsymbol{Y}$$

$$S_{xx}=\boldsymbol{X}^{T}\boldsymbol{U}^{-1}\boldsymbol{X},\quad S_{xy}=\boldsymbol{X}^{T}\boldsymbol{U}^{-1}\boldsymbol{Y}=\boldsymbol{Y}^{T}\boldsymbol{U}^{-1}\boldsymbol{X},\quad S_{yy}=\boldsymbol{Y}^{T}\boldsymbol{U}^{-1}\boldsymbol{Y} \tag{26 a-f}$$

and $\left[u^{-1}\right]_{ij}$- is the ij- element of inverse covariance matrix $\boldsymbol{U}^{-1}$. The calculations (25) would be started by finding very well known the following sums which be replaced by multiplication transposition vector by inverse of covariance matrix and by vector - this is very important issue. The constant of matrix $\boldsymbol{U}=\boldsymbol{U}_{\boldsymbol{Y}}$ gives possibility to minimize the objective function analytically because of

$$G(\mathrm{a,b})=a^{2}S_{xx}+2ab\,S_x-2\,a\,S_{xy}+b^{2}S-2b\,S_y+S_{yy} \tag{27}$$

In (27) we have quadratic dependence on *a* and *b*, hence the condition for global minimum is equivalent for two local minimum corresponding *a* and *b*:

$$G(a,b)\to min \Rightarrow \frac{\partial G(a,b)}{\partial a}=0,\frac{\partial G(a,b)}{\partial b}=0,\left(S_{xx}>0,S>0\right) \tag{28}$$

Of course when effective inverse covariance matrix depends on *a* the objective function can minimized locally only by intercept *b*. The analytical solution for the two-line equation gives global minimum [24]:

$$\begin{cases} a\,S_{xx}+b\,S_x=S_{xy} \\ a\,S_x+bS=S_y \end{cases} \tag{29 a,b}$$

and solution can be found by determinant method of determinants. Parameters *a* and *b* are given as:

$$a=\frac{\Delta_a}{\Delta},b=\frac{\Delta_b}{\Delta} \tag{30 a,b}$$

where: $\Delta_a=S\,S_{xy}-S_x\,S_y,\Delta_b=S_y\,S_{xx}-S_x\,S_{xy}\wedge\Delta=SS_{xx}-\left(S_x\right)^2.$

The uncertainty: *ua* of slope *a* and *ub* for abscissa (intercept) *b* and correlation coefficient ρ_{ab} of parameters *a, b* can be determined analytically too. The below equation (33) presents the unique solution for regression *y* on *x* with using the old very well known formulas for element of covariance matrix $\boldsymbol{U_{ab}}$ for non corelated case. But they correct in the case of autocorrelation variable *y* described by covariance matrix $\boldsymbol{U_Y}$.

First the sensitive Jacobian matrix $\boldsymbol{C}$ is derived [27]. The sensitive coefficients, equal first spatial derivatives $\frac{\partial S_{xy}}{\partial y_i},\frac{\partial S_y}{\partial y_i}$ of parameters of linear regression, determines vector component of **e** and **f**:

$$e_i=\frac{\partial S_{xy}}{\partial y_i}=\left[\boldsymbol{U_Y^{-1}X}\right]_i,\boldsymbol{f}_i=\frac{\partial S_y}{\partial y_i}=\left[\boldsymbol{U_Y^{-1}1}\right]_i \tag{31a,b}$$

for $i=1,\ldots,n$. In symbolic notation it is: $\boldsymbol{e}=\frac{\partial S_{xy}}{\partial Y}=\boldsymbol{U_Y^{-1}X}=\boldsymbol{X^T U_Y^{-1}},\ \boldsymbol{f}=\frac{\partial S_y}{\partial Y}=\boldsymbol{U_Y^{-1}1}=\boldsymbol{1^T U_Y^{-1}}$.The sensitive matrix **C** for parameters *a, b* can be written as $\mathbf{C}=\left[\boldsymbol{P},\ \boldsymbol{Q}\right]$ and elements of it by:

$$\boldsymbol{P}=\frac{\partial a}{\partial \boldsymbol{Y}}=\frac{S\boldsymbol{e}-S_x\boldsymbol{f}}{\Delta},\qquad \boldsymbol{Q}=\frac{\partial b}{\partial \boldsymbol{Y}}=\frac{S_{xx}\boldsymbol{e}-S_x\boldsymbol{f}}{\Delta} \tag{32a,b}$$

From matrix law of propagation of uncertainty the matrix $\boldsymbol{U_{ab}}$ for *a* and *b* parameters is:

$$\boldsymbol{U_{ab}=C\,U_Y\,C^T}=\begin{bmatrix}\boldsymbol{P\,U_Y\,P^T} & \boldsymbol{P\,U_Y\,Q^T}\\ \boldsymbol{P\,U_Y\,Q^T} & \boldsymbol{Q\,U_Y\,Q^T}\end{bmatrix}=\begin{bmatrix}u_a^2 & \rho_{ab}u_a u_b\\ \rho_{ab}u_a u_b & u_b^2\end{bmatrix} \tag{33}$$

Where: ρ_{ab} is a correlations coefficient for pair *a* and *b*.

Taking advantage of the fact that the $\boldsymbol{U_Y^{-1}}$ is symmetrical as $\boldsymbol{U_Y}$, that is why $\boldsymbol{U_Y}=\boldsymbol{U_Y^T}$, $\boldsymbol{U_Y^{-1}}=\left(\boldsymbol{U_Y^{-1}}\right)^T$ and $\boldsymbol{U_Y^{-1}U_Y}=\boldsymbol{I}$ unit matrix, it yields: $\boldsymbol{e\,U_Y e^T}=\boldsymbol{X^T U_Y^{-1} U_Y}(\boldsymbol{X^T U_Y^{-1}})^T=S_{xx}$, $\boldsymbol{f\,U_Y f^T}=\boldsymbol{1^T U_Y^{-1} U_Y}(\boldsymbol{1^T U_Y^{-1}})^T=S$, and $\boldsymbol{e\,U_Y f^T}=\boldsymbol{f\,U_Y e^T}=\boldsymbol{X^T U_Y^{-1} U_Y}(\boldsymbol{1^T U_Y^{-1}})^T=S_x$ and matrix elements $\boldsymbol{U_{ab}}$ simplify to the form [26]:

$$u_a^2=\boldsymbol{P\,U_Y P^T}=\frac{S}{\Delta};\qquad u_b^2=\boldsymbol{Q\,U_Y Q^T}=\frac{S_{xx}}{\Delta};$$

$$\rho_{ab}u_a u_b=\boldsymbol{P\,U_Y Q^T}=\frac{-S_x}{\Delta} \tag{34 a-c}$$

The parameters of covariances matrix u_a, u_b and ρ_{ab} can be derived analytically and have the same form as for noncorrelated case, but we can remember that we have more general definitions of S, $S_x, S_y, S_{xy}, S_{xx}, S_{yy}$ parameters (26a-f):

$$u_a=\sqrt{S/\Delta};\qquad u_b=\sqrt{S_{xx}/\Delta};\qquad \rho_{ab}=-S_x/\sqrt{S\,S_{xx}} \tag{35 a-c}$$

What is different from classical case e.g. noncorrelated case, that the value Δ may be zero ? In order to demonstrate the possibility of zero set Δ, we use the procedure of diagonalization of matrix $\boldsymbol{U_Y}$. Generalization of patterns for regression *y* on *x* of correlated coordinates *y* can lead to singularity (Δ=0?). The value Δ is calculated for the selected coordinate system of the vector variable $\boldsymbol{X}$ and is equal:

$$\Delta=S\cdot S_{xx}-\left(S_x\right)^2=\boldsymbol{1^T U_Y^{-1} 1\,X^T U_Y^{-1} X}-\left(\boldsymbol{X^T U_Y^{-1} 1}\right)^2 \tag{36}$$

After transformation, using matrix–linear orthogonal operator $\boldsymbol{D^T}=\boldsymbol{D^{-1}}$: $\boldsymbol{1}=\boldsymbol{D\,P}$ and $\boldsymbol{X}=\boldsymbol{D\,W}$ where $\boldsymbol{P}=\boldsymbol{D^{-1}1}$ and $\boldsymbol{W}=\boldsymbol{D^{-1}X}$ n – dimensional vectors and

$$\boldsymbol{D^{-1}U_Y^{-1}D}=\begin{bmatrix}\frac{1}{\lambda_1} & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & \frac{1}{\lambda_n}\end{bmatrix} \tag{37}$$

where λ_i- eigenvalues of matrix $\boldsymbol{U_Y}$, i=1,…,n. and performing algebraic operations, the final formula for Δ is:

$$\Delta=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(p_i w_j-p_j w_i\right)^2\lambda_i^{-1}\lambda_j^{-1} \tag{38}$$

The final form (38) of Δ can be always greater than zero if all eigenvalues of $\lambda_i>0$ for i=1,…,n. It is possible to zero set formula on Δ if at least one eigenvalue is negative. Hence, matrix $\boldsymbol{U_Y^{-1}}$ $\left(\boldsymbol{U_Y}\right)$ should be positive definite and all eigenvalues should be positive $\lambda_i > 0$ to avoid singularity. So we should assume that matrix $\boldsymbol{U_Y}$ can by positive definite.

6. Domination of Matrix Ux - Solution For Regression *x* on *y* With Autocorrelation

At this moment we derive the solution for regression x on y . From mathematical point of view to obtain the case when matrix $\boldsymbol{U}_{\boldsymbol{X}}$ is dominated it enough to be done by swapping $\boldsymbol{X}$ vector with $\boldsymbol{Y}$ vector and introducing new parameters W instead S. This case occurs when $u(X_i)\neq 0$ and $u(Y_i)=0$ and $\boldsymbol{Y}_{\boldsymbol{p}}=\boldsymbol{Y}$, $\boldsymbol{\Delta Y}=\boldsymbol{0}$. Then, the full covariance matrix reduces to $\boldsymbol{U}_{\boldsymbol{Z}}=\boldsymbol{U}_{\boldsymbol{X}}$, $\boldsymbol{U}_{\boldsymbol{Z}}^{-1}=\boldsymbol{U}_{\boldsymbol{X}}^{-1}$ and $\boldsymbol{U}_{\boldsymbol{XY}}=\boldsymbol{U}_{\boldsymbol{Y}}=0$ The equation of projecting points can be written in vector form as:

$$\boldsymbol{X}_{\boldsymbol{p}}=a_x\boldsymbol{Y}_{\boldsymbol{p}}+b_x\boldsymbol{1}=a_x\boldsymbol{Y}+\boldsymbol{b}_{\boldsymbol{x}} \text{ and } \boldsymbol{X}_{\boldsymbol{p}}-\boldsymbol{X}=a_x\boldsymbol{Y}+\boldsymbol{b}_{\boldsymbol{x}}-\boldsymbol{X} \tag{39a,b}$$

Only errors along OX direction are considered and then the objective function becomes:

$$G(a,b)=\boldsymbol{\Delta X}^{\boldsymbol{T}}\boldsymbol{U}_{\boldsymbol{X}}^{-\boldsymbol{1}}\boldsymbol{\Delta X}=\left[\boldsymbol{X}-a_x\boldsymbol{Y}-\boldsymbol{b}_{\boldsymbol{x}}\right]^{\boldsymbol{T}}\boldsymbol{U}_{\boldsymbol{X}}^{-\boldsymbol{1}}\left[\boldsymbol{X}-a_x\boldsymbol{Y}-\boldsymbol{b}_{\boldsymbol{x}}\right] \tag{40}$$

From the mathematical point of view this is exactly the same expression as for y on x case using variable swapping $\boldsymbol{X}\rightarrow\boldsymbol{Y}$ and $\boldsymbol{Y}\rightarrow\boldsymbol{X}$ and replacing the inverse of covariance matrix $\boldsymbol{U}_{\boldsymbol{Y}}^{-\boldsymbol{1}}$ by $\boldsymbol{U}^{-\boldsymbol{1}}=\boldsymbol{U}_{\boldsymbol{X}}^{-\boldsymbol{1}}$. It is similar like the solution for regression y on x also with expression for matrix $\boldsymbol{U}_{\boldsymbol{ab}}$. The subscript index x is used to distinguish from the previous one. The solution to the regression parameters is analogous:

$$a_x=\frac{\Delta_{ax}}{\Delta_x}, \qquad b_x=\frac{\Delta_{bx}}{\Delta_x} \tag{41a,b}$$

where a new notations are of (scalar parameters S are exchanging by W)

$$\Delta_{ax}=W\,W_{yx}-W_x\,W_y,\ \Delta_{bx}=W_x\,W_{yy}-W_y\,W_{yx},\ \Delta_x=W\,W_{yy}-(W_y)^2 \text{ and } \Delta_x\neq 0.$$

Variances u_{ax}^2, u_{bx}^2 and covariance element $\rho_{axbx}u_{ax}u_{bx}$ are determined by analogy as (34a-c):

$$u_{ax}^2=\frac{W}{\Delta_x}, \qquad u_{bx}^2=\frac{W_{yy}}{\Delta_x}, \qquad \rho_{abx}u_{ax}u_{bx}=\frac{-W_y}{\Delta_x} \tag{42a-c}$$

Determining uncertainty for variable y requires the application of the straight line equation:

$$x=a_x y+b_x \tag{43}$$

And now it necessary to carried out the transformation from parameters a_x and b_x to the parameters a and b and also it must be applied the matrix law of propagation of uncertainty. The straight regression line can be transformed into new form fitted to the mode from figure 1.

$$y=\frac{x}{a_x}-\frac{b_x}{a_x} \tag{44}$$

leads to dependencies for the variable y the parameters a, b are given:

$$a=\frac{1}{a_x} \quad \text{and} \quad b=\frac{-b_x}{a_x} \tag{45}$$

The matrix law of propagation of uncertainty as a matrix equation is the following:

$$\boldsymbol{U}_{\boldsymbol{ab}}=\begin{bmatrix} \frac{\partial a}{\partial a_x} & \frac{\partial a}{\partial b_x} \\ \frac{\partial b}{\partial a_x} & \frac{\partial b}{\partial b_x} \end{bmatrix} \boldsymbol{U}_{\boldsymbol{a_x b_x}} \begin{bmatrix} \frac{\partial a}{\partial a_x} & \frac{\partial b}{\partial a_x} \\ \frac{\partial a}{\partial b_x} & \frac{\partial b}{\partial b_x} \end{bmatrix} =$$

$$a_x^{-4}\begin{bmatrix} 1 & 0 \\ -b_x & a_x \end{bmatrix}\begin{bmatrix} u_{ax}^2 & \rho_{abx}u_{ax}u_{bx} \\ \rho_{abx}u_{ax}u_{bx} & u_{bx}^2 \end{bmatrix}\begin{bmatrix} 1 & -b_x \\ 0 & a_x \end{bmatrix} \tag{46}$$

Finally in the case of domination of matrix $\boldsymbol{U}_{\boldsymbol{X}}$ the elements of $\boldsymbol{U}_{\boldsymbol{ab}}$ matrix can be determined and these expression will be used in case 3 for testing of proposed algorithm. After the multiplication and simplification:

$$u_a^2=a^4u_{ax}^2=a^4W/\Delta_x, \qquad u_b^2=a^2\left(b^2W+W_{yy}-2W_yb\right)/\Delta_x,$$

$$\rho_{ab}u_au_b=\frac{a^3\left(bW-W_y\right)}{\Delta_x}, \quad \text{and} \quad \rho_{ab}=\frac{b-\frac{W_y}{W}}{\sqrt{b^2+\frac{W_{yy}}{W}-\frac{2bW_y}{W}}} \tag{47a,b,c,d}$$

7. Characteristic Function *G(a)* for Two Extreme Cases: Domination of Covariance Matrix Ux and Uy

The following are two typical sets of $G(a)$ characteristic function sets for $a < 0$ and $a > 0$ for two extreme cases: domination of matrix $\boldsymbol{U}_{\boldsymbol{Y}}$ and domination of matrix $\boldsymbol{U}_{\boldsymbol{X}}$, where analytical solution for a, b, and $\boldsymbol{U}_{\boldsymbol{ab}}$ are existing (41,42,45,47). In below cases we have always minimum of the objective function. The $G(a)$ in both cases are also analytically determined from (27). The mixed characteristics for more complicated case with cross correlations are expected. In the left side of two plots below we have two parabolas: dependence on quadratic of a, and on the right side we have parabolic dependence on see a^{-1} figure 4.

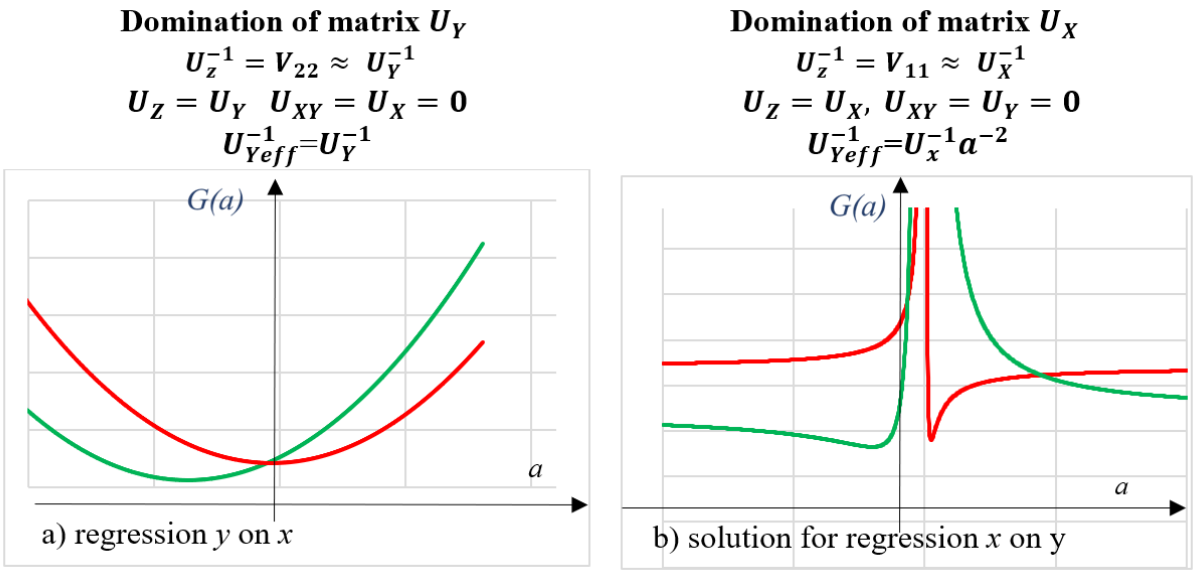


Figure 4: *Characteristic functions G(a) in green line for a < 0 and in red line for a > 0 for two extreme cases: a) two plots of G(a) for regression y on x – domination of matrix* $\boldsymbol{U}_Y$ *b) two plots of G(a) for solution for regression x on y.*

8. Consequences of the New Approach

We define matrix $\boldsymbol{\beta}$ of weight coefficients which can be used for identification of type of regression x on y or y on x. As you can see, there is an unequivocal relationship between the weight coefficients $\boldsymbol{\beta}$ matrix or its inverse and the slope a of straight-line regression. We get a linear matrix dependency for the error vectors in the 0X and 0Y directions. So, from equations for $\boldsymbol{\Delta x}_{vertex}$ and $\boldsymbol{\Delta Y}_{vertex}$ corresponding to the value of the minimum (21) of characteristic function *G(a,b)*, the matrix of weight coefficients („slopes") of crossing lines is defined as:

$$\boldsymbol{\beta} = \frac{\boldsymbol{\Delta Y}_{vertex}}{\boldsymbol{\Delta X}_{vertex}} = -\left(\boldsymbol{V}_{11} + a\boldsymbol{V}_3\right)\left(\boldsymbol{V}_3^T + a\boldsymbol{V}_{22}\right)^{-1} \tag{48a}$$

or inverse matrix

$$\boldsymbol{\beta}^{-1} = \frac{\boldsymbol{\Delta X}_{vertex}}{\boldsymbol{\Delta Y}_{vertex}} = -\left(\boldsymbol{V}_{11} + a\boldsymbol{V}_3\right)^{-1}\left(\boldsymbol{V}_3^T + a\boldsymbol{V}_{22}\right) \tag{48b}$$

From (48) the slope of regression line is determined by matrix $\boldsymbol{\beta}$ and parts of inverse covariance matrix $\boldsymbol{U}_z$

$$a = -\left(\boldsymbol{V}_{11} + \boldsymbol{\beta}\boldsymbol{V}_3\right)\left(\boldsymbol{V}_3^T + \boldsymbol{\beta}\boldsymbol{V}_{22}\right)^{-1} \tag{50}$$

We can identify regression x on y and y on x respectively when $\boldsymbol{\beta}$ equals zero and inverse equals $\boldsymbol{\beta}^{-1}$ zero. To avoid the problem with the zero determinant of the $\boldsymbol{U}_z$ matrix, we can insert small variance values respectively to achieve an extremally cases: regression y on x or x on y . From (48) we have

$$\boldsymbol{\Delta Y}_{vertex} = \boldsymbol{\beta}\boldsymbol{\Delta X}_{vertex} \quad \text{or} \quad \boldsymbol{\Delta X}_{vertex} = \boldsymbol{\beta}^{-1}\boldsymbol{\Delta Y}_{vertex} \tag{51a,b}$$

In this way regression x on y can be identified by $\boldsymbol{\beta} = \mathbf{0}$ because of $\boldsymbol{\Delta Y = \Delta Y_{vertex} = 0}$. In the limit at almost zero elements of the diagonal matrix $\boldsymbol{U_Y \to 0 (U_{XY} = V_3 = 0), V_{22} \to \infty}$ (diagonal elements) is obtained:

$$\boldsymbol{\beta = -(V_{11} + a V_3)(V_3^T + a V_{22})^{-1} \quad \to \quad 0} \tag{52}$$

Analogically regression y on x can be identified by $\boldsymbol{\beta^{-1}} = 0$ because of $\boldsymbol{\Delta X = \Delta X_{vertex} = 0}$. In the limit at almost zero elements of the diagonal matrix $\boldsymbol{U_X \to 0 (U_{XY} = V_3 = 0), V_{11} \to \infty}$ (diagonal elements) is obtained:

$$\boldsymbol{\beta^{-1} = -(V_{11} + a V_3)^{-1}(V_3^T + a V_{22}) \quad \to \quad 0} \tag{53}$$

In noncorrelated case when $\boldsymbol{U_{XY} = 0}$, $\boldsymbol{U_X}$ and $\boldsymbol{U_Y}$ are diagonal $[\boldsymbol{U_X}]_{ii} = u^2(X_i)$,$[\mathbf{U_y}]_{ii} = u^2(Y_i)$, i=1,..,n. If all matrixes contain only diagonal elements, then $\boldsymbol{\beta = \beta_{diag}}$ is also a diagonal matrix

$$\boldsymbol{\beta_{diag}} = \begin{bmatrix} \beta_{11} & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & \beta_{nn} \end{bmatrix} \text{ or } \boldsymbol{\beta_{diag}^{-1}} = \begin{bmatrix} \beta_{11}^{-1} & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & \beta_{nn}^{-1} \end{bmatrix} \tag{54a,b}$$

Then the crossing projection lines have slopes $\beta_{ii} = \beta_i = \dfrac{-1}{a} \dfrac{u^2(Y_i)}{u^2(X_i)}$ i=1,..n, and effective inverse covariance matrix is diagonal too with elements:

$$[\boldsymbol{U_{Yeff}^{-1}}]_{ii} = (a^2 u^2(X_i) + u^2(Y_i))^{-1} \tag{55}$$

As a results (55) well known method of effective variance can be applied to find solution for regression problem. The $\boldsymbol{\beta}$ matrix in noncorrelated case is then diagonal. Other elements of $\boldsymbol{\beta}$ matrix are equal zero and the diagonal elements are the slops of crossing lines see figure 5.

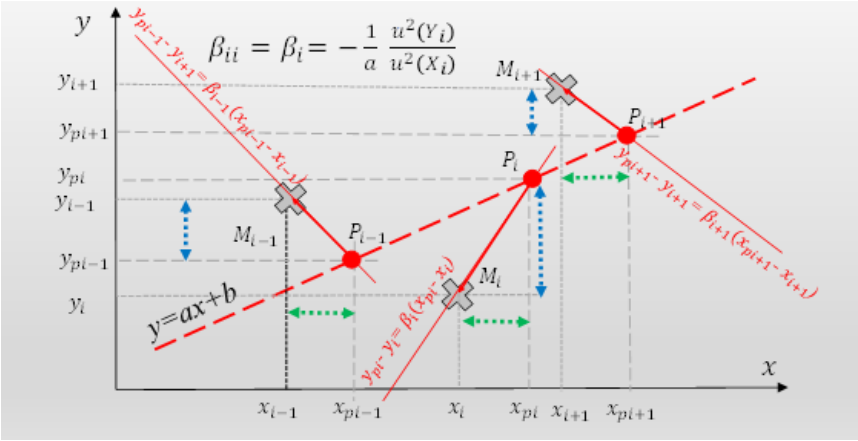


Figure 5: Interpretation of diagonal elements of matrix $\boldsymbol{\beta_{diag}}$ for straight line regression without correlation.

The constant ratio between variances leads to the parallel projections - at this case the analytical solution as roots of quadratic equation are available (Deming method) - When the variance are equals we have perpendicular projections it means the OLS case. In correlated case the expression for slope of crossing line are more complicated - all elements of matrix $\boldsymbol{\beta}$ are existing - its linear combination between error of x and y. And, when a matrix $\boldsymbol{\beta}$ is not exclusively diagonal, it means that the coordinates x and y are correlated e.g. $\boldsymbol{V}_{11}$or $\boldsymbol{V}_{22}$ or $\boldsymbol{V}_{3}$ are not diagonal . In this case, any errors selected toward y are a linear combination of all errors in the x direction. Also, any errors selected toward x are a linear combination of all errors in the y direction. Hence, the slopes for crossing lines in projections points from measurement points $\boldsymbol{X}$, $\boldsymbol{Y}$ on the fitting regression straight line define by mean points $\boldsymbol{X}_{p},\boldsymbol{Y}_{p}$ can be obtained from

$$\frac{\Delta Y_{vertexi}}{\Delta X_{vertexi}}=\frac{\sum_{j=1}^{n}\beta_{ij}\,\Delta X_{vertex\,j}}{\Delta X_{vertexi}} \tag{56}$$

and i=1,…,n. In the case when both covariances matrixes are equal without cross-correlations and have the same units we can define the condition for generalization of orthogonal regression. In the special case when $\boldsymbol{U}_{XY}=\boldsymbol{0}$, the formula for the slopes is reduced to the expression $\boldsymbol{\beta}=\frac{-1}{a}\boldsymbol{V}_{11}\boldsymbol{V}_{22}^{-1}=\frac{-1}{a}\boldsymbol{U}_{X}^{-1}\boldsymbol{U}_{Y}$. When both covariance matrixes are equal $\boldsymbol{U}_{X}=\boldsymbol{U}_{Y}$ then $\boldsymbol{\beta}$ is diagonal like in noncorrelated case and all slopes are equal $\frac{-1}{a}$ *(perpendicular projections).*

Thus, in the case *w*hen both coordinates have the same units as the above case with $\boldsymbol{U}_{X}=\boldsymbol{U}_{Y},\boldsymbol{U}_{XY}=0$ it can be defined as a generalization of an orthogonal regression.
Also when all matrixes $\boldsymbol{U}_{X},\boldsymbol{U}_{Y}$ and $\boldsymbol{U}_{XY}$ are diagonal the inverse of covariance matrix has the same structure and $\boldsymbol{\beta}$ is diagonal as well as $\boldsymbol{U}_{Yeff}^{-1}$ matrix. This is the second case for testing. In the special case when $\boldsymbol{U}_{XY},\boldsymbol{U}_{X},\boldsymbol{U}_{Y}$, are diagonal – correlations between every pairs x_i and y_i only, then are $\boldsymbol{V}_{11}$ and $\boldsymbol{V}_{22}$ and $\boldsymbol{V}_{3}$ diagonal and finally matrix of weight coefficients („slopes") β is diagonal too (case 2).

$$\boldsymbol{U}=\begin{bmatrix} w_{x11} & 0 & 0 & w_{xy11} & 0 & 0 \\ 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & 0 & w_{xnn} & 0 & 0 & w_{xynn} \\ w_{xy11} & 0 & 0 & w_{y11} & 0 & 0 \\ 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & 0 & u_{xynn} & 0 & 0 & w_{y2n2n} \end{bmatrix} \Rightarrow \boldsymbol{U}^{-1}=\begin{bmatrix} v_{x11} & 0 & 0 & v_{xy11} & 0 & 0 \\ 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & 0 & v_{xnn} & 0 & 0 & v_{xynn} \\ v_{xy11} & 0 & 0 & v_{y11} & 0 & 0 \\ 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & 0 & v_{xynn} & 0 & 0 & v_{y2n2n} \end{bmatrix}$$

$$\Rightarrow \boldsymbol{\beta}_{diag}=\begin{bmatrix} \beta_{11} & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & \beta_{nn} \end{bmatrix} \tag{57}$$

9. A New Algorithm For Numerical Calculation of Straight Line Regression Parameters

The algorithm (see figure 6) for sampling characteristic *G(a)*, which is a very short procedure, start from first step: the matrix $\boldsymbol{U_Z}$ is inverted and partitioned to the four elements. Next the values of characteristic *G(a)* is calculated in series points from left side to the right side of the minimum with Δa increment step: at any points the matrix $\boldsymbol{V}$ is determined and inverted – this is the critical moment of the method because this operation must be done with highest accuracy, next inverse effective of covariance matrix $\boldsymbol{U_{Yeff}^{-1}}$ is calculated, also parameters S, $S_x, S_y, S_{xy}, S_{xx}, S_{yy}$ and intercept b for local minimum. Block *G(a)* is repeated at any selected points of *a*. Finally value of function *G(a)* is determined which satisfy the following relations: $G(\boldsymbol{\Delta X}, a, b) \geq G(a,b) \geq G(a)$.

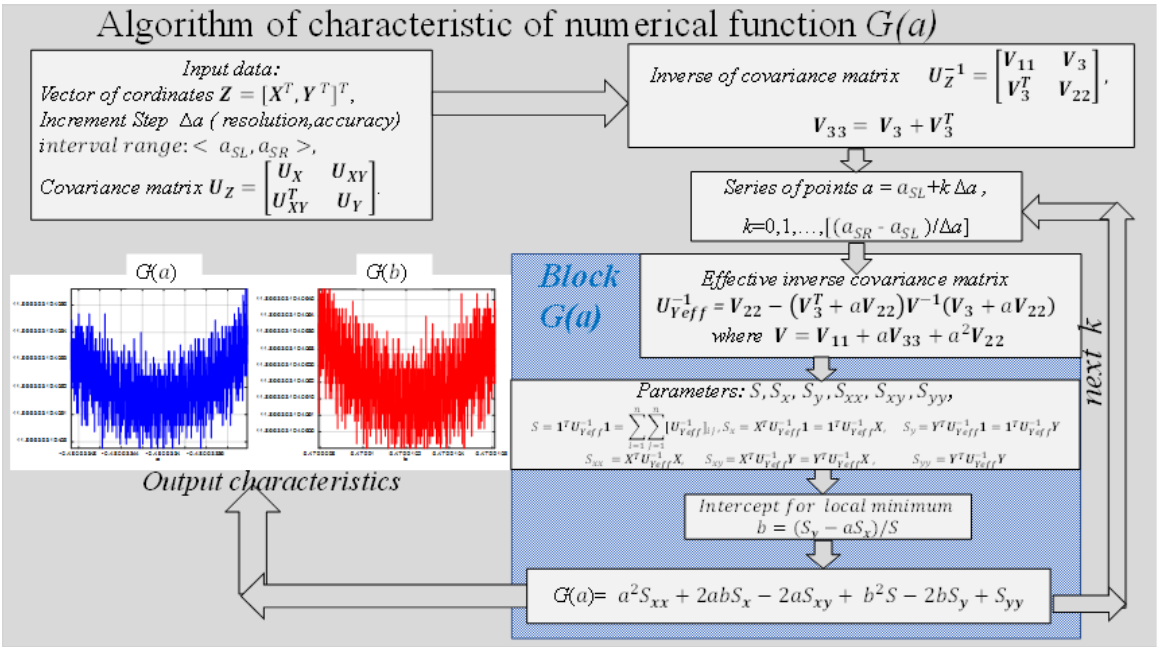


Figure 6: *Block diagram for determination numerical characteristic function G(a), G(b)- (see Appendix B).*

The input data are loaded in the EXCEL worksheet and includes formatted input parameters like: the number of measurement points, all both coordinates of measurement points e.g. $\boldsymbol{X,Y}$ vectors, elements of $\boldsymbol{U_X}$, **Uy** and **Uxy**$(\boldsymbol{U_{XY}^T})$ matrixes - it means the whole matrix U_Z and also increment step Δa and left a_{SL} and right a_{SR} values of interval range. A very short of MATLAB script named Plot_G.txt is written. In the above script it is used function G included in G.m file – see Appendix B. After running script, in a short time, depending on the number of steps M=integer[(a_{SR}-a_{SL})/Δa] the two characteristic *G(a)* and *G(b)* are plotted – see figure 6. We propose the method of determining the minimum with the use manually of zoom function in MATLAB environment - we zoom in to the minimum area and select two values of *a* and *b* where the minimum is inside in. On this basis we determine the average value and error for parameters *a* and *b*. The correct numerical value of slope is assumed as $a_N = \frac{1}{2}(a_L + a_R)$: with numerical error $\varepsilon_a = \frac{1}{2}|a_L - a_R|$. Simultaneously, the correct numerical value of intercept *b* is determined as $b_N = \frac{1}{2}(b_L + b_R)$ with numerical error $\varepsilon_b = \frac{1}{2}|b_L - b_R|$.

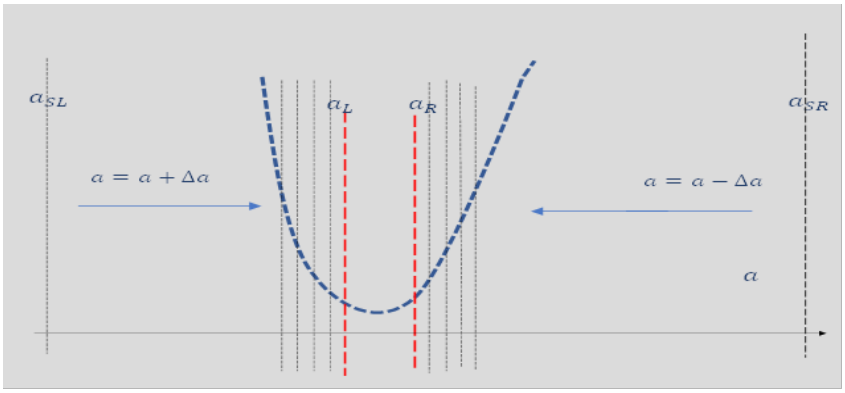


Figure 7: *Scheme of automatization of determining minimum by increasing/decreasing the values of interval range* a_{SL} / a_{RL} *within the increment step* Δa.

The algorithm for automatization for determining of *a*, *b*, and $\boldsymbol{U_{ab}}$ is applied– see figure 8.

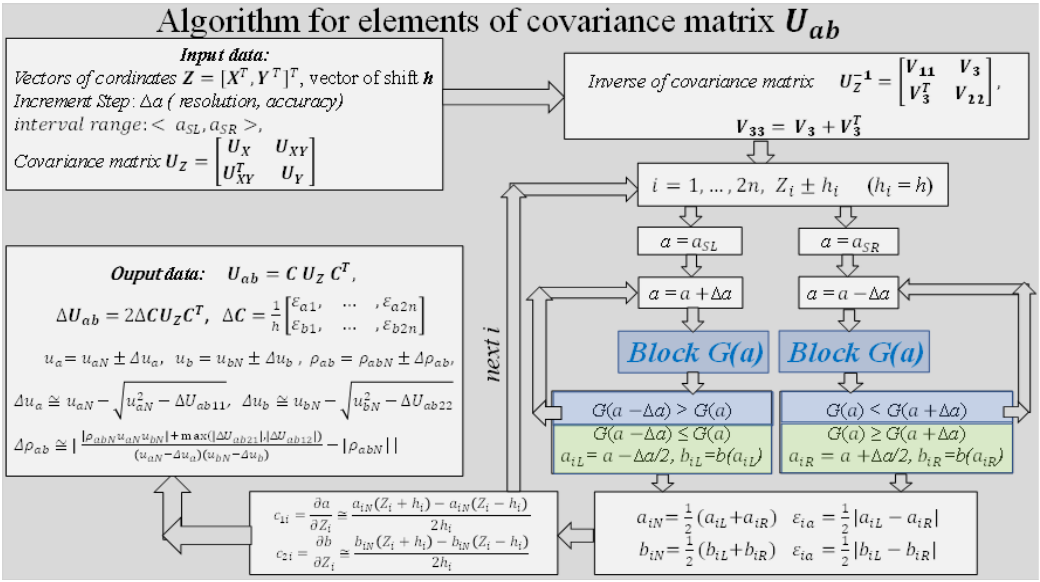


Figure 8: *Block diagram for numerical determination of* $\boldsymbol{U_{ab}}$ *matrix –(see Appendix C).*

We assume that the only one minimum in the given interval range $[a_{SL}; a_{SR}]$ is always existing for very small changing of every coordinates. The same method for average a_N, b_N and errors ε_a, ε_b can be used as for previous manually determine. If we have one minimum in the considered interval range, which is confirmed by determination of the characteristic of *G(a)* using script Plot_G.txt (see Appendix B). Then we can apply method of increasing and decreasing of *a* from both side of interval range to approach the points very close on the left and right side of minimum (see Appendix C). Two-way calculation of objective function values in two opposite directions are used with very small increment step .$\Delta a = 5 \cdot 10^{-8}$ To avoid the situation of pass-through, the real minimum of *G(a)* in increasing or decreasing values *a* the correct value of *a* in the last step should be decreased (increased) by $\Delta a/2$ during increasing (decreasing) process. In this way we assume that the curve of *G(a)* at very close to the minimum is almost symmetric. The method for finding parameters a_N, b_N can be repeated for numerical differentiation of parameters *a* and *b* due to the all coordinates to estimate sensitivity matrix $\boldsymbol{C}$ elements defined by partial derivatives:

$$\boldsymbol{C}=\begin{bmatrix}\frac{\partial a}{\partial Z_1} & \cdots & \frac{\partial a}{\partial Z_{2n}}\\ \frac{\partial b}{\partial Z_1} & \cdots & \frac{\partial b}{\partial Z_{2n}}\end{bmatrix},\boldsymbol{C}^{\boldsymbol{T}}=\begin{bmatrix}\frac{\partial a}{\partial Z_1} & \frac{\partial b}{\partial Z_1}\\ \cdots & \cdots\\ \frac{\partial a}{\partial Z_{2n}} & \frac{\partial b}{\partial Z_{2n}}\end{bmatrix} \tag{58a,b}$$

So, in order to apply the matrix law of propagation of uncertainty to obtain covariance matrix $\boldsymbol{U_{ab}}$

$$\boldsymbol{U_{ab}}=\boldsymbol{C}\,\boldsymbol{U_Z}\,\boldsymbol{C}^{\boldsymbol{T}} \tag{59}$$

It is necessary to calculate first the sensitivity coefficients by numerical differentiation. Thus the sensitivity coefficients can be estimated by:

$$\frac{\partial a}{\partial Z_i}\cong\frac{a_N\left(Z_i+h_i\right)-a_N\left(Z_i-h_i\right)}{2h_i},\frac{\partial b}{\partial Z_i}\cong\frac{b_N\left(Z_i+h_i\right)-b_N\left(Z_i-h_i\right)}{2h_i} \tag{60 a,b}$$

and i=1,…,2n .The expressions (60a,b) are closely to the results for Taylor series with rests of third derivatives. In most cases we can assume h_i=h=const i=1,…,2n. It is necessary to optimize the constant value of h to minimalize influence of the error due to third derivatives a''' and b'''. So the coefficients of $\boldsymbol{C}$ matrix can be determine by 4 x n for a and for b solutions for modified the input EXCEL data e.g. vectors $\boldsymbol{X,Y}$ in script U_ab.txt (see Appendix C). It is assumed that h is selected so the rests with third derivatives in interval range (Z_i-h, Z_i+h) expressed by $\left|a'''\right|\frac{h^3}{3!}$ and $\left|b'''\right|\frac{h^3}{3!}$ can be negligible in comparison of ε_a, ε_b. On the one hand, reducing the value of h will increase the error on the matrix coefficients **C**. On the other hand, increasing the h-value may result in an increase in the error associated with third derivatives. After several numerical simulations in our testing cases, the value $h=2\cdot10^{-2}$ is accepted, which is optimal, ensuring the determination of coefficients (60a,b) with a numerical error about 10^{-5}.

The numerical errors of estimation for elements $\boldsymbol{U_{ab}}$ matrix and u_a,u_b uncertainties and also correlation coefficient ρ_{ab} are given in the following way. From errors of slops and intercepts with modified input data the matrix $\boldsymbol{U_{ab}}$ can be estimated with matrix error $\boldsymbol{\Delta U_{ab}}$:

$$\boldsymbol{U_{ab}}\pm\boldsymbol{\Delta U_{ab}}=\boldsymbol{U_{ab}}\pm2\,\boldsymbol{\Delta C}\,\boldsymbol{U_Z}\,\boldsymbol{C}^{\boldsymbol{T}}, \tag{61}$$

where numerical errors of sensitivity matrix are given by: $\Delta\boldsymbol{C}=\frac{1}{2h}\begin{bmatrix}\varepsilon_{a1}, & \cdots & ,\varepsilon_{a2n}\\ \varepsilon_{b1}, & \cdots & ,\varepsilon_{b2n}\end{bmatrix}$

where $\varepsilon_{ai}=\left|\varepsilon_{+ai}\right|+\left|\varepsilon_{-ai}\right|$ and $\varepsilon_{bi}=\left|\varepsilon_{+bi}\right|+\left|\varepsilon_{-bi}\right|$ and i=1,…, 2n, and index (+) means for the approaching Z_i+h_i and index (-) means for the approaching Z_i-h_i to obtain minimum of *G(a).*

In the considering the worst case, because of this $\boldsymbol{U_Z}$ is the symmetric matrix and all absolute values of four elements of matrix $\boldsymbol{\Delta C\,U_Z\Delta C}^{\boldsymbol{T}}$ are always much smaller than corresponding absolute values of four elements of matrix $\boldsymbol{2\Delta C}\left|\boldsymbol{U_Z C}^{\boldsymbol{T}}\right|$, the positive values of errors of covariance matrix $\boldsymbol{\Delta U_{ab}}$ can be estimated as:

$$\boldsymbol{\Delta U_{ab}}=\begin{bmatrix}\Delta U_{ab\,11} & \Delta U_{ab\,12}\\ \Delta U_{ab\,21} & \Delta U_{ab\,22}\end{bmatrix}=2\Delta \boldsymbol{C}\left|\boldsymbol{U_Z C}^{T}\right| \tag{62}$$

Then the numerical results are: $u_{aN}=\sqrt{U_{ab\,11}}, u_{bN}=\sqrt{U_{ab\,22}}$ and $\rho_{abN}=U_{ab\,12}/(u_{aN}u_{bN})$ and have the maximum numerical errors estimated by:

$$\Delta u_a=\left|u_{aN}-\sqrt{u_{aN}^2-\Delta U_{ab\,11}}\right|>\left|\sqrt{u_{aN}^2+\Delta U_{ab\,11}}-u_{aN}\right|, \tag{63a}$$

$$\Delta u_b=\left|u_{bN}-\sqrt{u_{bN}^2-\Delta U_{ab\,22}}\right|>\left|\sqrt{u_{bN}^2+\Delta U_{ab\,11}}-u_{bN}\right|, \tag{63b}$$

$$\Delta\rho_{ab}=\left|\frac{\left|\rho_{abN}u_{aN}u_{bN}\right|+max\left(\left|\Delta U_{ab\,21}\right|,\left|\Delta U_{ab\,12}\right|\right)}{(u_{aN}-\Delta u_a)(u_{bN}-\Delta u_b)}-\left|\rho_{abN}\right|\right| >$$

$$> \left|\left|\rho_{abN}\right|-\frac{\left|\rho_{abN}u_{aN}u_{bN}\right|+max\left(\left|\Delta U_{ab\,21}\right|,\left|\Delta U_{ab\,12}\right|\right)}{(u_{aN}+\Delta u_a)(u_{bN}+\Delta u_b)}\right| \tag{63c}$$

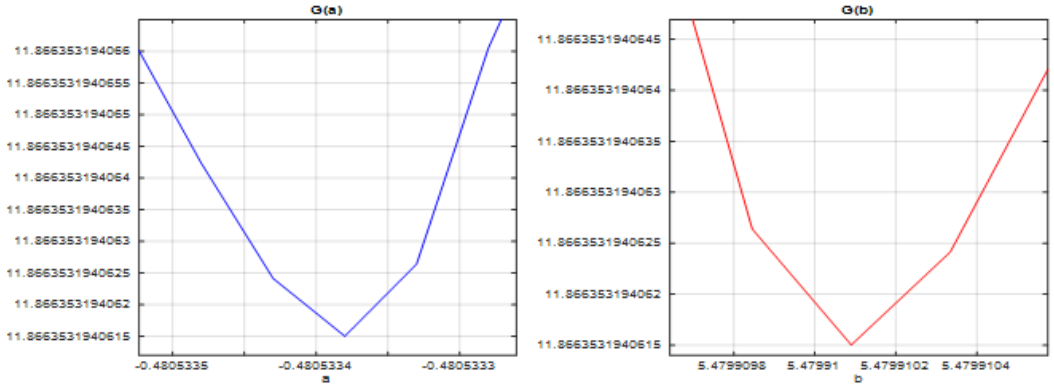
Of course it is assuming that $\rho_{ab}\Delta u_a\Delta u_b\approx 0$. The accuracy of each numerical method is limited by a finite decimal representation of the variables used and by the error of method caused by the use of approximate mathematical formulae. For each method that coincides with the numerically determined value, it is necessary to estimate numerical errors, since the numerical solution is not specified exactly. For the algorithm used, the truncating errors caused by the finite representation of the number seems to be omitted and negligible – the values of the numbers on which the calculations are performed in MATLAB have an accuracy above 10^{-10} and only the method errors estimated above remain. So the numerical results are burdened with errors: $a=a_N\pm\varepsilon_a$, $b=b_N\pm\varepsilon_b$, $u_a=u_{aN}\pm\Delta u_a, u_b=u_{bN}\pm\Delta u_b$ and $\rho_{ab}=\rho_{abN}\pm\Delta\rho_{ab}$.

The effectiveness of the method has been demonstrated in three examples used for testing in previous publications [9,10,12]. The implementation is prepared in MATLAB enviroment-see Appendix B and C.

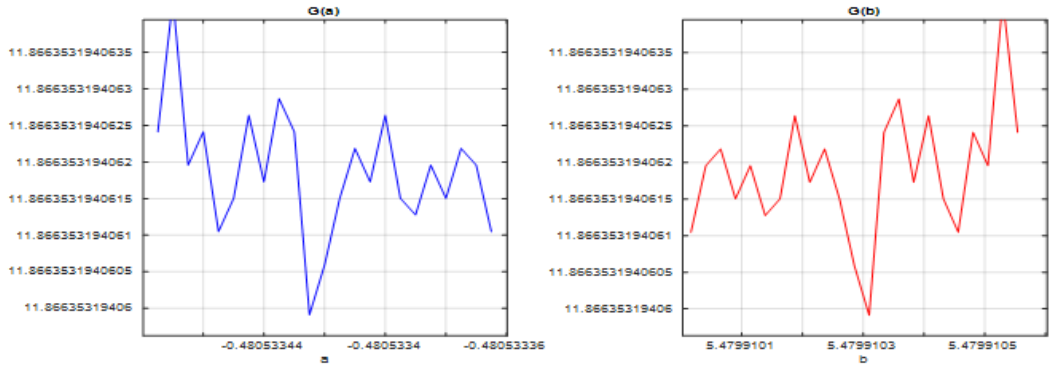
10. Testing Cases

Three testing cases of input data analyzed before [14,7,5] are considered.

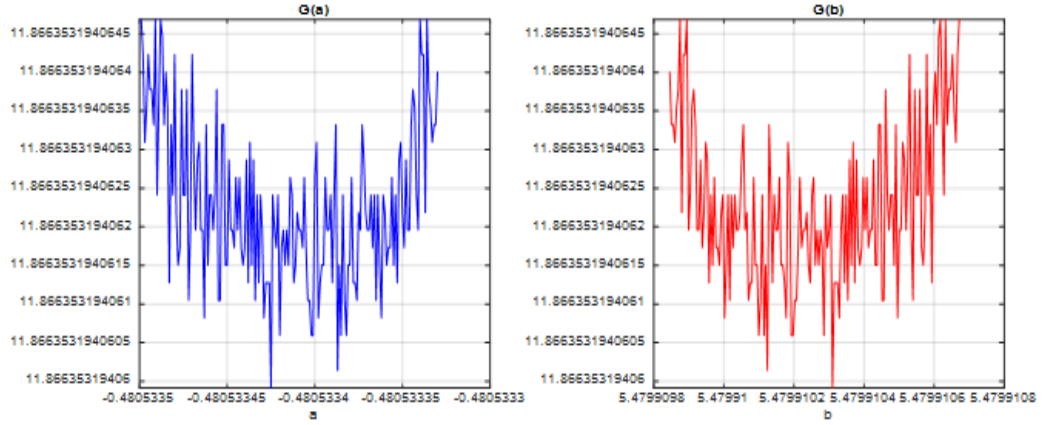
First Pearson's data with York's weights as noncorrelated case which represents a case of a highly varying uncertainty - strong heteroscedasticity in both variables is analyzed. Input data are stored in the Table 1. This situation arises when the variances of the observed values are unequal, but where no correlations exist among the observed variances. So the covariances matrixes are diagonal and **Uxy=0** In the four figures below the four characteristics of numerical function *G(a)* and *G(b)*, obtained from script Plot_G.txt are demonstrated see figure 9 for different increment steps from 5.10^{-8} to 10^{-10}.



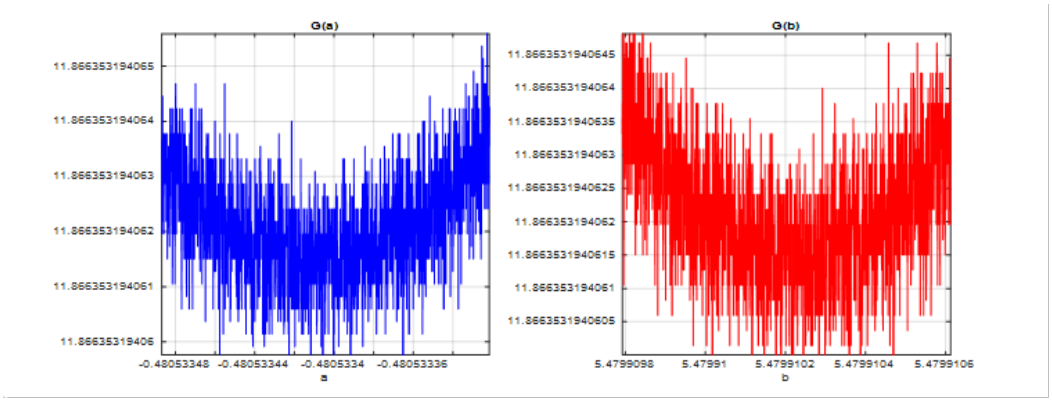
a) $\Delta a = 5.10^{-8}$



b) $\Delta a = 5.10^{-9}$



c) $\Delta a = 10^{-9}$



d) $\Delta a = 10^{-10}$

Figure 9: *Characteristics of G(a) and G(b) for various increment step: a)* $\Delta a = 5 \cdot 10^{-8}$ *, b)* $\Delta a = 5 \cdot 10^{-9}$ *c)* $\Delta a = 10^{-9}$ *d)* $\Delta a = 10^{-10}$.

As we see from figure 9 a) $\Delta a = 5 \cdot 10^{-8}$ the characteristic is very smooth, regular and the proposed algorithm from fig.8 can be used for determination of a, b parameters and matrix $\mathbf{U_{ab}}$ while for very small value increment step 10^{-10} the accuracy of parameters of straight regression line will be worst due to not regular characteristic which is required a special filtering algorithm to find trend line - see figure 9 d). It easy to notice that the main reason for this chaotic numerically determined function G is the library function designating the inverse matrix $\boldsymbol{V}$ with very small step Δa . This chaotic course increases with decreasing increment step -see figure 9 b), c) and d). The very critical moment which limits the accuracy of calculations is the library MATLAB function for inversion of matrix $\boldsymbol{V}$. So to obtain better accuracy than 10^{-8} for slope of a (maximum accuracy for G(a) is eleven digit) is required to prepare own function for inversion of matrix $\boldsymbol{V}$, based on much more representative digits because of domination of truncation error. That why we used in our tests increment step equal $\Delta a = 5 \cdot 10^{-8}$ from figure 9 a) and we have reduced the maximum accuracy.

The most accurate values can be read manually for the smallest increment step equal 10^{-10} using Plot_G.txt script from figure 9 d. The maximum accuracy of slope is almost eight digits after point. The plotting of this characteristic in a very tin interval range takes few second of calculation on the platform Intel(R) Core(TM) i5-1035G4 CPU @ 1.10GHz 1.50 GHz RAM 12,0 GB Flash SSD 512 GB , but the use of this step value for automation requires method of a filtering algorithm, determining the trend of lines.

The very good agreement between proposed and previous methods of accuracy of *a* and *b* parameters are obtained, but in the case of uncertainties only almost four digits after point are identical. Therefore according to table 1 the best accuracy for uncertainties and correlation coefficient is obtained for proposed method.

Table 1: *Data, the results and the errors obtained for numerical method- U_ab.txt script* a_{SL}*=-0,483;* a_{SR}*-0,476; h=0,02;* $\Delta a = 5 \cdot 10^{-8}$ *. Output data is saved to the result.txt file.*

Point no.	x_i	$u^{-2}(X_i)$	Y_i	$u^{-2}(Y_i)$
1	0	1000	5,9	1
2	0,9	1000	5,4	1.8
3	1,8	500	4,4	4
4	2,6	800	4,6	8
5	3,3	200	3,5	20
6	4,4	80	3,7	20
7	5,2	60	2,8	70
8	6,1	20	2,8	70
9	6,5	1.8	2,4	100
10	7,4	1	1,5	500

Input data

Parameter	Proposed WTLS numerical solution	Maximum numerical errors ε_a $\varepsilon_b, \Delta u_a,$ $\Delta u_b \Delta \rho_{ab}$	Method by Ref.[10]	Method by Ref.[12]	Exact Solution
a	−0,48053337	5.10^{-8}	−0,48053341	−0,48053341	−0,48053341
b	5,47991007	$2{,}4.10^{-7}$	5,47991022	5,47991022	5,47991022
ua	0,05761755	10^{-7}	0,05798501	0,05757171	-
ub	0,29193582	$2{,}9 \cdot 10^{-6}$	0,29497073	0,29237148	-
ϱab	−0,96230411	$9{,}3 \cdot 10^{-6}$	−0,96309914	−0,96241604	-

Results

Based on the a- slope parameter matrix β is also determined and straight line regression with crossing lines and measurement points are plotted – see figure.10.

$\beta =$

2081,02	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
0,00	1156,12	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
0,00	0,00	260,13	0,00	0,00	0,00	0,00	0,00	0,00	0,00
0,00	0,00	0,00	208,10	0,00	0,00	0,00	0,00	0,00	0,00
0,00	0,00	0,00	0,00	20,81	0,00	0,00	0,00	0,00	0,00
0,00	0,00	0,00	0,00	0,00	8,32	0,00	0,00	0,00	0,00
0,00	0,00	0,00	0,00	0,00	0,00	1,78	0,00	0,00	0,00
0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,59	0,00	0,00
0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,04	0,00
0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,004

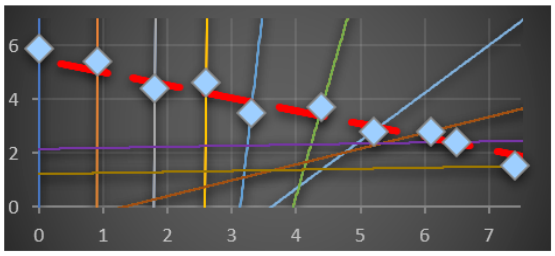


Figure 10: *Matrix β and the crossing lines with measurement points for first case.*

In the case 2 the input data is given in table with cross-correlations coefficients, with assumption of diagonal matrix **Ux**,**Uy** and **Uxy**. Hence the cross-correlations is taken only into account. The results and numerical errors of the proposed method, and also results of previous method are given in table 2 Result I.

Table 2: *Data, the results and the errors obtained for numerical method- U_ab.txt script (a_{SL}=1.98; a_{SR}=2,03, h=0,02, $\Delta a=5.10^{-8}$). Output data is saved to the result.txt file.*

Point no.	xi	u(xi)	yi	u(yi)	ρxiyi
1	0,9995	0,005	3,0073	0,009	0,5
2	1,9968	0,002	5,0105	0,009	0,55
3	3,0009	0,005	7,0061	0,007	0,6
4	3,9969	0,004	8,9939	0,008	0,65
5	4,9998	0,002	11,0034	0,014	0,7
6	6,0025	0,007	12,9995	0,001	0,75
7	6,9875	0,014	15,0008	0,002	0,8
8	7,9962	0,013	17,0012	0,005	0,85
9	9,0045	0,013	19,004	0,006	0,9
10	9,9891	0,006	20,9959	0,002	0,95

Input data

Parameter	Proposed WTLS numerical solution	Maximum numerical errors $\varepsilon_a \quad \varepsilon_b, \Delta u_a$ $\Delta u_b \Delta \rho_{ab}$	Method by Ref.[10]	Method by Ref.[12]
a	2,00010587	5.10^{-8}	2,00010589	2,00010590
b	1,00659374	$2,1.10^{-7}$	1,00659367	1,00659365
ua	0,00122460	5.10^{-8}	0,00122506	0,00122460
ub	0,00607293	$1,5.10^{-7}$	0,00607500	0,00607294
ϱab	−0.84511293	$1,1.10^{-5}$	−0,84522792	−0.84511327

Results I

Parameter	Proposed WTLS numerical solution	Maximum numerical errors $\varepsilon_a \varepsilon_b$,	Analytical solution (Appendix A)	Correlation coefficient ρ
a	2,00013000	7,5.10-8	2,00013003	0,5
b	1,006805234	4.12.10-7	1,00680519	
a	2,00013427	5.10-8	2,00013433	0,9
b	1,00678184	$2.75.10^{-7}$	1,00678155	

Results II Ux=0,006, Uy=0,009, coordinates are used from Input data

β=

-1,3	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
0,00	32,22	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
0,00	0,00	-0,24	0,00	0,00	0,00	0,00	0,00	0,00	0,00
0,00	0,00	0,00	-2,00	0,00	0,00	0,00	0,00	0,00	0,00
0,00	0,00	0,00	0,00	13,52	0,00	0,00	0,00	0,00	0,00
0,00	0,00	0,00	0,00	0,00	0,10	0,00	0,00	0,00	0,00
0,00	0,00	0,00	0,00	0,00	0,00	0,11	0,00	0,00	0,00
0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,30	0,00	0,00
0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,39	0,00
0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,31

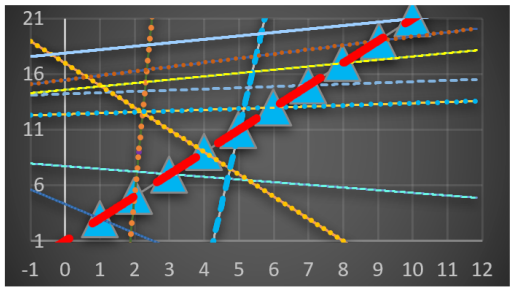


Figure 11: *Matrix* $\boldsymbol{\beta}$ *and the crossing lines with measurement points for second case.*

As it is shown in table 2 (Results I) the agreement in *a* and *b* parameters is no less than seven digits after point while in uncertainties we have almost six digits identical and in correlation coefficient we have almost four digits identical. From columns of errors the proposed method is able to be rather more accurate than previous. Additionally the case (Results II) of the same correlations between measured X and Y coordinates with constant uncertainties at the measurement points according to the analytical solutions included in Appendix C gives almost seven digits of accuracy. The matrix $\boldsymbol{\beta}$ and regression line with crossing lines you can find on figure 11.

The third example case uses input including correlations within *x* and *y* and cross-correlations *x* between *y* [1].The covariance symmetric matrices **Ux** and **Uy** and **Uxy** and also asymmetric $\mathbf{U}_{XYA}$ are defined by:

$$\mathbf{Ux=Uy}=(0,01)^2 \begin{vmatrix} 1 & 0,2 & 0,2 & 0,2 & 0,2 \\ 0,2 & 1 & 0,2 & 0,2 & 0,2 \\ 0,2 & 0,2 & 1 & 0,2 & 0,2 \\ 0,2 & 0,2 & 0,2 & 1 & 0,2 \\ 0,2 & 0,2 & 0,2 & 0,2 & 1 \end{vmatrix} \qquad \mathbf{Uxy}=(0,01)^2 \begin{vmatrix} 0,2 & 0,1 & 0,1 & 0,1 & 0,1 \\ 0,1 & 0,2 & 0,1 & 0,1 & 0,1 \\ 0,1 & 0,1 & 0,2 & 0,1 & 0,1 \\ 0,1 & 0,1 & 0,1 & 0,2 & 0,1 \\ 0,1 & 0,1 & 0,1 & 0,1 & 0,2 \end{vmatrix} \tag{64a,b}$$

$$\boldsymbol{U}_{XYA}=(0{,}01)^2\begin{vmatrix} 0{,}2 & 0 & 0 & 0 & 0 \\ 0{,}1 & 0{,}2 & 0 & 0 & 0 \\ 0{,}1 & 0{,}1 & 0{,}2 & 0 & 0 \\ 0{,}1 & 0{,}1 & 0{,}1 & 0{,}2 & 0 \\ 0{,}1 & 0{,}1 & 0{,}1 & 0{,}1 & 0{,}2 \end{vmatrix} \quad (64a,b,c)$$

Table 3: *Data for analytical solutions and results and errors obtained for numerical method -U_ab.txt script (a_{SL}=1,98; a_{SR}=2,04; h=0,02;) for above covariances matrixes $\boldsymbol{U}_X$ and $\boldsymbol{U}_Y$ and $\boldsymbol{U}_{XY}$($\boldsymbol{U}_{XYA}$). Output data is saved to the result.txt file.*

Point No	x_i	y_i
1	1,0089	3,013
2	1,9905	5,0022
3	2,9896	6,9923
4	3,9907	9,0116
5	4,9695	10,9815

Input data

Parameter	Proposed WTLS numerical solution	Numerical errors $\varepsilon_a, \varepsilon_b, \Delta u_a$ $\Delta u_b \Delta \rho_{ab}$	Method by Ref.[6]
a	2,01043975	2.10^{-8}	2,01043979
b	0,98922682	7.10^{-8}	0,98922669
u_a	0,00607387	10^{-8}	0,00607382
u_b	0,02151838	$1{,}5.10^{-7}$	0,02151819
ρ_{ab}	−0,84392639	$8{,}5\cdot10^{-6}$	−0,84392476

Results I

Parameter	Domination of U_y U_z=U_y Analytical solution $\beta^{-1}=0$	WTLS numerical solution $U_Z \to U_{Yeff}^{-1}$ $U_X \to 0$ $u^2(X_i)=10^{-10}$ $\beta^{-1} \to 0$	Domination of U_y U_z=U_y Analytical solution $\beta^{1}=0$	WTLS numerical solution $U_Z \to U_{Yeff}^{-1}$ $U_Y \to 0$ $u^2(Y_i)=10^{-10}$ $\beta \to 0$
a	2,01043126	2,01043125	2,01044147	2,01044150
b	0,98925221	0,98925223	0,98922166	0,98922159
u_a	0,00285081	0,00285081	0,00573149	0,00573149
u_b	0,01042351	0,01042348	0,02095614	0,02095619
ρ_{ab}	−0,81771599	−0,81771431	−0,81771817	−0,81771921

Results II

Parameter	Proposed WTLS numerical solution for asymmetric matrix $\boldsymbol{U}_{XYA}$	Numerical errors ε_a , $\varepsilon_b, \Delta u_a$ $\Delta u_b \Delta \rho_{ab}$
a	2,01043995	7.10^{-8}
b	0,98922622	$2{,}2.10^{-7}$
U_a	0,00590329	5.10^{-8}
U_b	0,02146788	$6{,}5.10^{-7}$
ρ_{ab}	−0,82216794	$4{,}3\cdot10^{-5}$

Results III

For fully correlated case (Results I) we have almost seven digits identical for *a, b* $\mathbf{U_{ab}}$ parameters and almost five digits identical for correlation coefficient. The results presented in Table 3 Ref. [6]

in the last columns confirm the conformity of the numerical values obtained with those previously published taking into account the errors. We obtain additional symmetric matrix β and parallel projections – see figure 12. In comparison to the noncorrelated case we have 4-16% percent of widening of coverage corridor.

Simulations have been also made (Results II) using the WTLS for covariances matrix **Uz** where it has been assumed **Uxy=0** confirming its convergence with analytical solutions for regression y on x (30,34,35) where matrix **Ux**→0 has diagonal elements $(0{,}0001)^2$ and solution for regression x on y (42,45,47) where matrix **Uy**→0 has diagonal elements $(0{,}0001)^2$. Results have been obtained in accordance with the analytical solutions in table3 ResultsII with an accuracy of for 7.10^{-8} uncertainties and correlation coefficient 10^{-6}.

Table 3 of Results III contains the results for the symmetric convariance matrix set $\mathbf{U}_x$ and $\mathbf{U}_y$ and an asymmetric matrix representing cross correlation $\mathbf{U}_{XYA}$.

$$\boldsymbol{\beta} = \begin{bmatrix} -0{,}35701 & 0{,}040083 & 0{,}040083 & 0{,}040083 & 0{,}040083 \\ 0{,}040083 & -0{,}35701 & 0{,}040083 & 0{,}040083 & 0{,}040083 \\ 0{,}040083 & 0{,}040083 & -0{,}35701 & 0{,}040083 & 0{,}040083 \\ 0{,}040083 & 0{,}040083 & 0{,}040083 & -0{,}35701 & 0{,}040083 \\ 0{,}040083 & 0{,}040083 & 0{,}040083 & 0{,}040083 & -0{,}35701 \end{bmatrix}$$

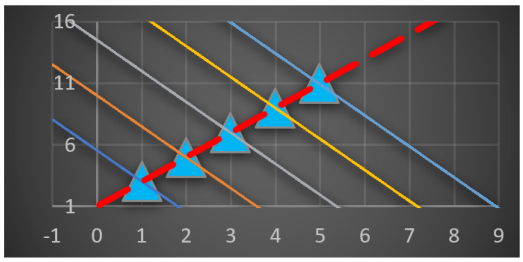


Figure 12: Matrix $\boldsymbol{\beta}$ and the crossing lines with measurement points for third case.

In the final phase – third case for different representation of matrix ***Uz*** for fully correlated random variables), the expanded two uncertainties with extended coefficient $t_{0,95;5-2} \cong$ 2,35 and the correlation coefficient $\rho_{y1,2}$ are determined from the two chosen points from straight regression line with maximum numerical errors less than 10^{-5} for y and correlation coefficient – see table 4.

In table 4 we have five different cases for two point of straight regression line: the widest confident interval is for autocorrelation **Ux**,**Uy**, a little smaller is for fully correlated matrix (case 3), and smallest for noncorrelated case when we have the smallest correlation coefficient excluding two extreme cases with only **Ux** or **Uy** matrixes. For asymmetric $\mathbf{U}_{XYA}$ case the confident interval is smaller than in the case of lack of positive cross correlation but it widest when the matrix $\mathbf{U}_{XY}$ is symmetric with positive elements.

Table 4: Confident interval and correlation coefficient for two selected points of straight line regression in third case with different configuration of matrixes **Ux,Uy**,**Uxy**.

Representation of matrix Uz	Coordinates y with expanded uncertainty		Correlation coefficient $\rho_{y1,2}$
	for the first point $x_1=2{,}0000$	for the second point $x_2=2{,}9889$	
Ux, **Uy**-diagonal, **Uxy=0** Noncorrelated case	$y_1=5{,}0101 \pm 0{,}0289$	$y_2 = 6{,}9982 \pm 0{,}0236$	0,8175
Ux, **Uy**=0	$y_1=5{,}0101 \pm 0{,}0314$	$y_2 = 6{,}9982 \pm 0{,}0284$	0,9051
Uy, **Ux**=0	$y_1=5{,}0101 \pm 0{,}0156$	$y_2 = 6{,}9982 \pm 0{,}0141$	0,9051
Ux,**Uy**, **Uxy**=0	$y_1=5{,}0101 \pm 0{,}0350$	$y_2 = 6{,}9982 \pm 0{,}0317$	0,9051
Ux,**Uy**,**Uxy**,**U^{T}xy**	$y_1=5{,}0101 \pm 0{,}0306$	$y_2 = 6{,}9982 \pm 0{,}0272$	0,8871
Ux,**Uy**,**UxyA**,**U^{T}xyA**	$y_1=5{,}0101 \pm 0{,}0318$	$y_2 = 6{,}9982 \pm 0{,}0287$	0,9024

11. Summary and Conclusion

A simple and fast algorithm for directly minimizing objective function to solve straight line regression problem is presented. The algorithm can be used in any lab to plot numerical characteristic of objective function and answer the question, "is it possible to minimize objective function at given measurement data with given covariance matrix to estimate the confidence region of straight line regression? The work demonstrates the linear regression method for correlated variables – fully correlated covariance matrix. The proposed numerical algorithm, which bypasses numerical minimization objective function due to the location of the projection points because of analytical derivation, is extremely fast and precise at determining the characteristic of the objective function as one-dimensional input parameters. In the case of noncorrelated data none of additional condition is required. In correlated case matrix $\boldsymbol{V}$ must be positive definite – at minimum of $G(a)$ and in considered interval range and the matrix $\boldsymbol{U}_{Yeff}^{-1}$ should have sum of all elements greater than zero or matrix $\boldsymbol{U}_{Yeff}^{-1}$ should be positive definite to avoid singularity. The analyzed interval range of slope should be chosen from selected extreme points, scattered on the XOY plane. Confirmation of the possibility of minimizing function G(a) is the receipt within the considered range of minimum. When V is not positively definite the proposed method can not be applied - when all eigenvalues of matrix V are negative the G(a) will have maximum - no possibility to minimalizing G(a) function. The short algorithm, has been implemented in in MATLAB scripts Plot_G.txt and U_ab.txt tested in three analyzed cases, published in previous articles. The numerical method is convergent to the classical cases with analytical solutions for the a and b parameters and their covariance matrix $\boldsymbol{U}_{ab}$**.** The effectiveness and reload of presented method is confirmed.

Conflict of interests: The authors declare that there is no conflict of interest.

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Appendix A

In order to illustrate accuracy of numerical method implemented in U_{ab} .txt script we compare the numerical results with analytical solution of least square method given in this section. We analyzed case with the effect of correlation between measured coordinates x_i and y_i with the same coefficient ρ and identical uncertainty constants, $u(x_i)=u_x$ and $u(y_i)=u_y$

Where i=1,...,n In this case the covariance matrix are described by

$$\boldsymbol{U}_Z=\begin{bmatrix}\boldsymbol{U}_X & \boldsymbol{U}_{XY}\\ \boldsymbol{U}_{XY}^T & \boldsymbol{U}_Y\end{bmatrix}$$

where the covariance matrixes $\boldsymbol{U}_x, \boldsymbol{U}_y$ are diagonal with constant variances

$$\boldsymbol{U}_X=\begin{bmatrix}u_x^2 & \dots & 0\\ \dots & \dots & \dots\\ 0 & \dots & u_x^2\end{bmatrix}, \boldsymbol{U}_y=\begin{bmatrix}u_y^2 & \dots & 0\\ \dots & \dots & \dots\\ 0 & \dots & u_y^2\end{bmatrix}$$

and covariance matrix $\boldsymbol{U}_{xy}$ has constant elements on diagonal i.e. elements with the same correlation coefficient ρ :

$$\boldsymbol{U}_{XY}=\begin{bmatrix}\rho u_x u_y & \dots & 0\\ \dots & \dots & \dots\\ 0 & \dots & \rho u_x u_y\end{bmatrix}$$

In this case effective inverse covariance matrix $\boldsymbol{U}_{Yeff}^{-1}$ is diagonal too with the same values on diagonal.The analytical solution in this particular case is existed and it seems like in the case of analytical solution as the root of the corresponding quadratic equation i.e. like in Deming method. Our objective function in this case is defined as:

$$G(a,b)=\sum_{i=1}^{n}\frac{(y_i-a x_i-b)^2}{u_{eff}^2}$$

where the effective uncertainty is equal to $u_{eff}^2=u_y^2-2\rho a u_x u_y+a^2 u_x^2$

The objective function takes the minimum if two conditions for zero derived values a and b are met the conditions:

$$1) \quad \frac{\partial G(a,b)}{\partial a}=0 \qquad \text{and} \qquad 2) \quad \frac{\partial G(a,b)}{\partial b}=0$$

From the second condition follows the dependence:

$$\sum_{i=1}^{n} -2(y_i - a x_i - b)=0$$

And $\sum_{i=1}^{n}(y_i - a x_i)=nb$ leads to the equation

$$b=\overline{y}-a\overline{x}$$

Inserting above relations into the first condition we obtain:

$$\sum_{i=1}^{n} \frac{(y_i - a x_i - \overline{y}+a\overline{x})(\overline{x}-x_i)u_{eff}^2 - (a u_x^2 - \rho u_x u_y)(y_i - a x_i - \overline{y}+a\overline{x})^2}{u_{eff}^4}=0$$

Simplifying the expression we get a quadratic equation:

$$Aa^2+Ba+C=0$$

where coefficients *A,B,C* are determined by:

$$A=-u_x\sum_{i=1}^{n}(\overline{x}-x_i)(\rho u_y(\overline{x}-x_i)+u_x(y_i-\overline{y})) \;\; ;$$

$$B=\sum_{i=1}^{n}(\overline{x}-x_i)^2 u_y^2 - u_x^2(y_i-\overline{y})^2;$$

$$C=u_y\sum_{i=1}^{n}(y_i-\overline{y})(u_y(\overline{x}-x_i)+\rho u_x(y_i-\overline{y})).$$

So, the solution is given by the root of quadratic equation for the minimum of G(a,b), i.e. when there is a change in the sign of the quadratic function from minus to plus. We always choose the sign (+).

$$a=\frac{-B+\sqrt{B^2-4AC}}{2A} \quad \text{and} \quad b=\overline{y}-a\overline{x}$$

Appendix B

Below the script for determination of characteristic G(*a*) and G(*b*) - the file Plot_G.txt with G function - the file G.m

file Plot_G.txt

```
% script for determination of the numerical characteristic of G(a) and G(b)
clear all
close all
```

```
clc
% reading EXCEL data file name Case  -  changing input data by changing name of file
INPUT = xlsread('Case_333');
% reading number of points from EXCEL data
N=INPUT(3,1);
% reading coordinates from EXCEL data
for i=1:N
      x(i)=INPUT(i,5);
      y(i)=INPUT(i,6);
% reading covariance matrix from EXCEL data
 for j=1:2*N
      U(i,j)=INPUT(i,j+6);
      U(i+N,j)=INPUT(i+N,j+6);
 end;
end;
% reading the step size from EXCEL data
del_a=INPUT(3,2);
% reading aL the  left limit of interval from EXCEL data
a_L=INPUT(3,3);
% reading aR the  right limit of interval from EXCEL data
a_R=INPUT(3,4);
% number of steps
M=fix((a_R-a_L)/del_a);
x=x(:);
y=y(:);
V=inv(U);
H=ones(1,N);
H=H(:);
%the  parts of inverse of covariance matrix
for i=1:N
 for j=1:N
        V_11(i,j)=V(i,j);
        V_22(i,j)=V(i+N,j+N);
        V_3(i,j)=V(i,j+N);
 end;
end;
V_33=transpose(V_3)+V_3;
% loops generating points for numerical characteristic
for k=1:M
      a_plot(k)=a_L+k*del_a;
      [G_ak(k), b_plot(k)]=G(a_plot(k),V_11,V_33,V_22,V_3,x,y,H);
end
% ploting G(a)
subplot(1,2,1);plot(a_plot,G_ak,'b-')
title('G(a)');xlabel('a')
grid on
```

```
% ploting G(b)
subplot(1,2,2);plot(b_plot,G_ak,'r-')
title('G(b)');xlabel('b')
grid on
```

file G.m

```
function [G_a,b]=G(a,V_11,V_33,V_22,V_3,x,y,H)
% numerical determination of value G(a)  and b(a)
U=inv(V_11+a*V_33+a^2*V_22);
V=V_22-(transpose(V_3)+a*V_22)*U*(V_3+a*V_22);
S_XX=transpose(x)*(V*x);
S_X=transpose(x)*( V*H);
S_XY=transpose(x)*( V*y);
S=transpose(H)*(V*H);
S_Y=transpose(y)*( V*H);
S_YY=transpose(y)*( V*y);
b=(S_Y-S_X*a)/S;
G_a=a^2*S_XX+2*a*b*S_X-2*a*S_XY+b^2*S-2*b*S_Y+S_YY;
end
```

Appendix C

Below the scripts for determination of *a, b* parameters and the covariance matrix U_{ab} - the file U-_ab.txt with G_ab function- the file G_ab.m (G.m is also needed).All output data are saved to the d:\results.txt - default output text file.

file U_ab.txt

```
%approaching the right corner of the minimum
      [aR, bR]=G_ab(asR,-dela,V_11,V_33,V_22,V_3,xw,yw,H);
%the numerical results of slope, intercept and their numerical  errors
      a_pm(j)=(aL+aR)/2;
      deltaa_pm(j)=abs(aR-aL)/2;
      b_pm(j)=(bL+bR)/2;
      deltab_pm(j)=abs(bR-bL)/2;
 end;
%elements of martix delC
 delaa(i)=(abs(deltaa_pm(1))+abs(deltaa_pm(2)))/(2*h);
 delbb(i)=(abs(deltab_pm(1))+abs(deltab_pm(2)))/(2*h);
%numerical differentiation of slope and intercept due to the coordinates- elements of matrix C
 AA(i)=(a_pm(1)-a_pm(2))/(2*h);
 BB(i)=(b_pm(1)-b_pm(2))/(2*h);
end;
delaa=delaa(:);
delbb=delbb(:);
AA=AA(:);
BB=BB(:);
%matrix C
```

```
AB=[AA,BB];
%matrix Uab
UAB=transpose(AB)*(U*AB);
%matrix delC
delC=[delaa,delbb];
%matrix delUab
delUAB=2*transpose(delC)*(U*AB);
%output data of matrix Uab
ua=sqrt(UAB(1,1))
ub=sqrt(UAB(2,2))
delua=abs(sqrt(UAB(1,1))-sqrt(UAB(1,1)-delUAB(1,1)))
delub=abs(sqrt(UAB(2,2))-sqrt(UAB(2,2)-delUAB(2,2)))
ro=UAB(1,2)/(ua*ub)
delro=abs((ro*ua*ub+max(abs(delUAB(2,1)),abs(delUAB(1,2))))/((ua-delua)*(ub-delub))-ro)
%matrix BETA
BETA=-(V_11+aN*V_3)*inv(transpose(V_3)+aN*V_22);
%error vector of X
D_V_X=-(transpose(V_3)+aN*V_22)*inv(V_11+aN*V_33+aN^2*V_22)*(y-aN*x-bN*H);
%error vector of Y
D_V_Y=(V_11+aN*V_3)*inv(V_11+aN*V_33+aN^2*V_22)*(y-aN*x-bN*H);
slopes=D_V_Y./D_V_X;
%writting output data to the results.txt file
fileID = fopen('d:\results.txt', 'w');
fprintf(fileID,'a=%12.8f\n dela=%12.8f\n b=%12.8f\n delb=%12.8f\n',aN,deltaaN,bN,deltabN);
fprintf(fileID, 'ua= %12.8f \n delua=%12.8f \n ub=%12.8f \n delub=%12.8f \n ro=%12.8f \n delro=
%12.8f \n',ua,delua,ub,delub,ro,delro);
fprintf(fileID, 'MATRIX BETA= \n');
for i=1:N
  for j=1:N
        fprintf(fileID, '%12.8f',BETA(j,i));
  end;
fprintf(fileID, ' \n');
end
fprintf(fileID, 'SLOPES OF CROSSING LINES= \n');
for i=1:N
        fprintf(fileID, '%12.8f',slopes(i));
end;
fclose(fileID);
display('Output data are saved in d:\results.txt file')
```

file G_ab.m

```
function [a_previous, b_previous]=G_ab(a,dela,V_11,V_33,V_22,V_3,x,y,H)
%function for the numerical determination of parameters a, b  situated very close to  the left or right of side
of the minimum
[G_next, b]=G(a,V_11,V_33,V_22,V_3,x,y,H);
G_previous=G_next+0.1;
while G_previous > G_next
```

```
a_previous=a;
G_previous=G_next;
a=a+dela;
[G_next, b]=G(a,V_11,V_33,V_22,V_3,x,y,H);
end
% special case for the widening numerical errors because of pass through the minimum
a_previous=a_previous-dela/2;
[G_next, b_previous]=G(a_previous,V_11,V_33,V_22,V_3,x,y,H);
```