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RESEARCH ARTICLE

Nonlinear Curve Fitting to Measurement Points with WTLS Method Using Approximation of Linear Model

Jacek Grzegorz Puchalski*

International Cooperation and Analyses Department, Central Office of Measures, Glowny Urząd Miar.

Abstract

The paper presents an approximate method of fitting measurement points to parameterized arbitrary nonlinear curves described by complex equations, even implicit ones, the most commonly used method of least squares in general WTLS. An approximation of a linear model is used here, in which the laws of propagation of error and propagation of uncertainty are true, so that only the first derivative of the transforming function is relevant. The effectiveness of the method has been demonstrated in several numerical examples. The method was verified on several nonlinear functions using the iterative algorithm by Monte Carlo propagation of distribution and the classical method based on the Levenberg-Marquardt algorithm for nonlinear optimization.

Key Words: *Weighted Total Least Squares (WTLS); Numerical methods; Optimalization problem*

1. Introduction

The most commonly used in many technical sciences, in geodesy, physics, chemistry, in general in metrology or measurement science is the determination of linear characteristics on the basis of coordinates of measurement points derived from a series of measurements in the XOY Cartesian system. The uncertainties – standard deviations of the coordinates – are not important, and it is assumed that they are the same and do not affect the adjustment method, which is usually the minimization of the sum of squares of errors determined in the direction of the Y axis – the so-called OLS method. In addition, the Best Linear Unbiased Estimator is used to estimate the corridor around a line, resulting from the Gauss-Markov theorem as an estimator among the linear, unbiased estimators of the linear regression model. Such a solution exists in an analytical form, requiring the use of basic mathematical operations [1]. Taking into account the uncertainty of measurements and mutual correlations for the least squares method will result in the equation of the line being similar to the OLS model, but slightly different.

***Corresponding Author**: Puchalski JG, Chief Specialist, International cooperation and Analyses Department, Center Office of Measures, Elektoralna Street2, Glowny Urzad Milar, E-mail: jacek.puchalski@gum.gov.pl*

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Similarly, the corridor of uncertainty around the straight line will change, i.e. narrow or widen. As a result, the arrangement of the line will depend not only on the coordinates of the measurement points, but also on the covariance matrix of the input quantities. Finding the parameters of a line in such a case is much more difficult and requires the use of various numerical methods, including iterative ones, requiring much more computing power and calculation time for a program/application running on a PC. The situation is similar for nonlinear curves, but the calculations become more and more complicated.

In general, it can be seen that the use of different methods minimizing the sum of squares errors determined in different directions–the positions of the points on the curve corresponding to the measurement points with respect to which the errors are determined, are located in different configurations, taking into account the weights of individual errors, in the case of decreasing adjustment errors. It will lead to the convergence of different solutions to a single idealized curve. Therefore, the obtained parameters of the curves for different methods should be similar.

In metrology, we most often make measurements that are almost always subject to uncertainties. Uncertainties are most often associated with standard deviations, which are the standard deviations of probability density distributions. Most often these are the dominant type A uncertainties derived from statistical measurements, but in general they are the geometric sum (resulting from convolutions) of type A uncertainty and type B uncertainty, which results from the dispersion of measurements resulting from non-statistical reasons. Determination of the uncertainty at a given measurement point, as well as and above all the expected value of the measurements, may involve measurements of other quantities. In this case, we are dealing with intermediate measurements, which in many cases leads to an approximate determination of the uncertainty of the initial quantity. A linear model is used that linearizes the total measurement function, and the output errors and uncertainties are appropriately transferred according to the law of propagation of error the complete differential method and the law of propagation of uncertainty/variance using the first partial derivatives of the measurement functions. Note that the law of propagation of uncertainty even for uncorrelated input variables usually leads to output variables that are already correlated.

Thus, in intermediate measurements, it is practically impossible to avoid correlations between the output variables, which should be included in the covariance matrix. If U_{in} is a matrix of covariance of input variables that can also be correlated or not, then the covariance matrix of the output quantities U_{out} according to the law of propagation of uncertainty (standard deviations, variances) is expressed by $U_{out} = C^T U_{in} C$, where C is the sensitivity matrix characterized by the first partial derivatives. As a result, on the basis of a multivariate Gaussian distribution with a covariance matrix, which contains the standard deviations of all coordinates of measurement points and mutual correlations between each two coordinates [2], the output covariance matrix is determined – for a simple straight line, it is the covariance matrix of the slope coefficient and the intercept. On this basis, the width of the uncertainty corridor around the line is determined for each coordinate value, half of which is the sought uncertainty for the fitted curve. Of course, the most accurate way of fitting is to use the generally correlated probability distributions for each coordinate of the measurement points and to determine the U_{in} probability density distributions of the parameters of the curve/function to be fitted by the analytical method or the Monte Carlo method, i.e. by numerically generating the distributions and determining the density distribution for each estimated parameter of the fitted function. If the input density distributions are correlated, the covariance matrix must be decomposed U_{in} Cholesky method and on samples from the normal Gaussian distribution determine the samples of input distributions. By determining

the parameter distributions of the fitting function, it is easy to estimate the expanded uncertainty for any value of the x coordinate in the form of an interval for the coverage of 0.95, which is a single element of the uncertainty corridor.

The Monte Carlo method can be easily implemented to fit a polynomial function (polynomial of any degree) for regression y on x-only y coordinates are associated with uncertainties, at the same time a precise measurement of the x coordinate is performed, which is not associated with errors and has no associated uncertainty. Using the method of determinants, i.e. operations consisting of basic mathematical operations, it is possible to determine the probability density distributions of the parameters that make up a polynomial function [3-5]. Figure 1 compares the method of distribution propagation to determine the expansion interval at a single measurement point with n input variables x and the method of fitting the curve at n measurement points with coordinates in XOY Cartesian system (x_i,y_i) containing a vector of m - parameters p =$[p_1,\ldots, p_m]^T$ of the considered functions $f(x)$. In both cases, probability density distributions g_{xi} (i from 1 to n) are generated for each single vectors of the random variables in the first for coordinates $X = [x_1,\ldots, x_n]$ and in the second $2n$ random variables defined by vector $Z=[z_1,\ldots, z_{2n}]^T = [x_1,\ldots, x_n, y_1,\ldots, y_n]^T$ and distribution g_{zi} (i from 1 to n). On this basis, from the relevant measurement equations for the first case, the density distribution of the output variable of defined function with known parameters is generated, and hence the expected value and coverage interval for 0.95 probability in the first case described in the document JCGM 101:2008 Evaluation of measurement data—Supplement 1 to the "Guide to the expression of uncertainty in measurement"—Propagation of distributions using a Monte Carlo method.

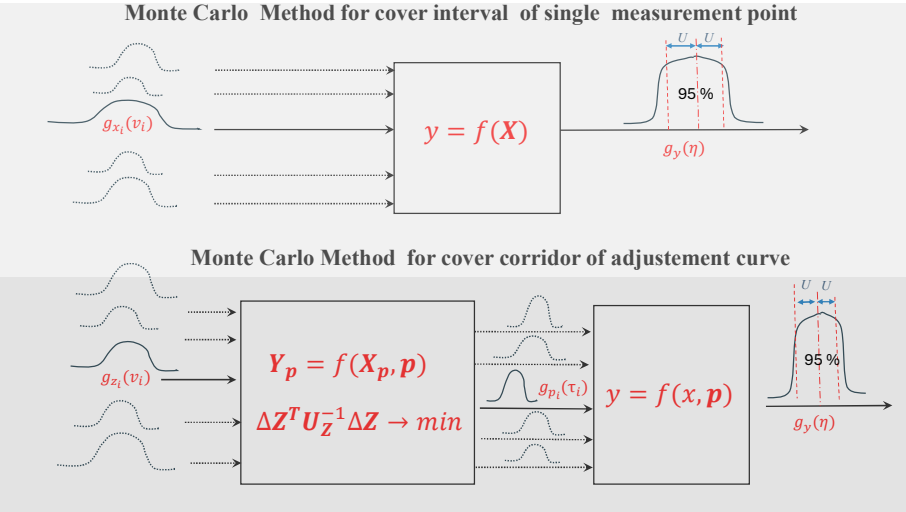

Figure 1: *Comparison of monte carlo method for cover interval estimation and cover corridor of adjustment curve.*

In the second case of fitting the nonlinear curve to the measurement points the corresponding function is composed only by type of standard library mathematical function but with unknown parameters, so it is necessary to determine the probability density distributions g_{pi} of all parameters described by vector $\boldsymbol{p}$ of the function using the minimization of the dimensionless criterion function described by the equation for WTLS least squares method:

$$\phi(\Delta Z, p) = \Delta Z^T U_Z^{-1} \Delta Z \rightarrow min \quad (1)$$

where the adjustment error vector $\Delta Z = Z - Z_p$, and the vector $Z_p = [z_{p1},\ldots, z_{p2n}]^{\mathrm{T}} = [x_{p1},\ldots, x_{pn}, y_{p1},\ldots, y_{pn}]^{\mathrm{T}}$ contains the coordinates of the points lying on the fitted curve - for the explicit function *f*: $Y_p = f(X_p, p)$ where $X_p = [x_{p1},\ldots, x_{pn}]^T$, $Y_p = [y_{p1},\ldots, y_{pn}]^T$ and in general a full covariance symmetric matrix U_Z taking into account autocorrelations within *X* and *Y* and cross-correlations of *X* and *Y*. The covariance matrix U_Z and its inverse are denoted by covariance matrixes U_X, U_Y, U_{XY} size *n* x *n* form**:**

$$U_Z = \begin{bmatrix} U_X & U_{XY} \\ U_{XY}^T & U_Y \end{bmatrix}, \quad U_Z^{-1} = \begin{bmatrix} V_1 & V_3 \\ V_3^T & V_2 \end{bmatrix} \tag{2}$$

where, in order to simplify mathematical operations, the designations of the matrix V_1, V_2, and V_3 sizes *n* x *n* were introduced, forming an inverse matrix to the one U_Z denoted by U_Z^{-1}.

Finally, the uncertainty corridor defined by the coverage intervals for any *x* is determined from the probability density distribution of the output variable *y* for this *x* and the determined probability density distributions g_{pi} for all parameters of the vector *p*.

Unfortunately, in most cases this type of solution cannot be implemented directly using basic mathematical operators, because each output sample of function parameters is determined from more complicated formulas, sometimes numerical algorithms solving complex nonlinear equations or even implicit equations [6-11]. Therefore, an approximate method that does not require such complex algorithms is proposed below. A allows you to adjust the parameters of the curve and its corridor and uncertainties based on the solution for a straight line.

The task of calculations of parameters of the fitted curve is to minimize the defined criterion function (1) and in general to determine *the m*-element vector of the parameters ***p-*** and *n*-element vector of coordinates of the points lying on the fitted curve, therefore it is enough to determine the vector. X_p, this gives in total n+*m* independent variables. This task, taking into account the computing capabilities of modern computers with a large number of measurement points, cannot still be solved by free search of all independent variables. Therefore, an appropriate algorithm of classical methods based on numerical determination of the gradient of a multidimensional function should be used [6-9].

In the following paper, we will present an approximate method of reducing the number of *n*+*m* variables affecting the criterion function by determining its local minimum for the vector X_p , to the number of *m* parameters, two of which are dependent on each other. This greatly simplifies the calculation, because with a small number of parameters of the matched nonlinear function, it can be minimized by freely searching the *m*-1 value, monitoring the area of the local minimum of criterial function. In the examples given, the number *m*=3 (*m*-1=2) for fitting catenoid curve, *m*=5 (*m*-1=4) for fitting ellipse and *m*=3 (*m*-1=2) for parabolic curve and *m*=4 (*m*-1=3) for sum of exponent and sine functions.

To compare the results of calculations performed for the same input data e.g. coordinates of measurement points associated with uncertainties, for proposed approximate method, the classical gradient method was used, based on the Levenberg-Marquardt iterative algorithms used to solve non-linear least squares problems which interpolates between the Gauss–Newton algorithm and the method of gradient descent, starting with a vector of size *n*+*m* of initial input data, performing numerical calculation of the gradient of a multivariate function using the numerically determined Hessian matrix [8,9]. The algorithm is implemented in the

environment *R* using standard library function. The calculation for Levenberg-Marguardt method was made using the method implemented on the website [12] after installing the Pracma and Matlib packages.

2. Approximate Method Using Straight Line Fitting

As we know, in the case of fitting a straight line $y = ax + b$, the condition of minimization of the criterion function due to the positions of the selected points on the fitted line with respect to which the misfit errors are calculated, leads to the use of the effective covariance symmetric matrix for regression y on x, and finally to make the criterion function quasi-quadratic dependent only on the slope coefficient a or depend only on intercept b. As a result, we obtain quasi-parabolic characteristics of the criterion function depending on one of the variables, i.e. the slope coefficient or the intercept b. In order to find the global minimum or one, one of the functions should be numerically examined by calculating for example in the assumed series of values of the slope coefficient [13].

For a straight-line fit, the local minimum for the effective covariance matrix is related to the matrix β [13,14] in general nonsymmetric.

$$\boldsymbol{\beta} = -(\boldsymbol{V}_1 + a\boldsymbol{V}_3^{\mathrm{T}})(\boldsymbol{V}_3 + a\boldsymbol{V}_2)^{-1} \text{ or } \boldsymbol{\beta}^{-1} = -(\boldsymbol{V}_1 + a\boldsymbol{V}_3^{\mathrm{T}})^{-1}(\boldsymbol{V}_3 + a\boldsymbol{V}_2) \tag{3}$$

Then the dependencies are true, and the errors propagate in the following way $\Delta Y = \beta \Delta X$ and $\Delta X = \beta^{-1}\Delta Y$. The equations are true for any and for the minimizing criterion function. Hence, for example, for the diagonal elements of the matrix U_X when all uncertainties $u(x_i)$ are close to zero the errors in their entirety are determined in the y direction, because $u(x_i) \to 0$ then $V_1 \to \infty$ and then $\beta^{-1} \to 0$ and $\Delta X \to 0$ .This applies not only to a straight line, but to any kind of nonlinear curve that is fitted. If the uncertainties for the x-coordinate measurements are negligible, the adjustment errors are determined only in the y-direction. This fact can be used when testing the accuracy of our fit, because by setting very small uncertainties for the x coordinate for curves described by polynomials, we can check whether they are consistent with analytical solutions. In this case for fitting any nonlinear functions the Levenberg-Marquardt iterative algorithm solves only m nonlinear equations for parameters p.

2.1. The least squares method optimalization equation

The covariance matrix $\boldsymbol{U_Z}$ of size 2 n x 2 n is given by:

$$U_Z = \begin{bmatrix} u_{z_1}^2 & \dots & \rho_{z_1 z_{2n}} u_{z1} u_{z_{2n}} \\ \dots & \dots & \dots \\ \rho_{z_1 z_{2n}} u_{z_1} u_{z_{2n}} & \dots & u_{z_{2n}}^2 \end{bmatrix} = \begin{bmatrix} u_{z_1} & \dots & 0 \\ \dots & \dots & \dots \\ 0 & .. & u_{z_{2n}} \end{bmatrix} R \begin{bmatrix} u_{z_1} & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & u_{z_{2n}} \end{bmatrix} \tag{4}$$

where correlator matrix $R = \begin{bmatrix} 1 & \dots & \rho_{z_1 z_{2n}} \\ \dots & \dots & \dots \\ \rho_{z_1 z_{2n}} & \dots & 1 \end{bmatrix}$ and $\rho_{z_i z_j}$ is the correlation coefficients between the coordinates of the z_i and z_j, and i and $j = 1, \dots, 2n$.

From (1) and (4) and if we assume $[R^{-1}]_{ij} = [Q]_{ij}$, then the criterial function is given by:

$$\phi(\Delta \boldsymbol{Z}, \boldsymbol{p}) = \begin{bmatrix} \Delta z_1 \\ \dots \\ \Delta z_{2n} \end{bmatrix}^T \boldsymbol{U_Z^{-1}} \begin{bmatrix} \Delta z_1 \\ \dots \\ \Delta z_{2n} \end{bmatrix} = \begin{bmatrix} \frac{\Delta z_1}{u_{z1}} & \dots & 0 \\ \dots & \dots & \dots \\ 0 & .. & \frac{\Delta z_{2n}}{u_{z2n}} \end{bmatrix} \boldsymbol{R^{-1}} \begin{bmatrix} \frac{\Delta z_1}{u_{z1}} & \dots & 0 \\ \dots & \dots & \dots \\ 0 & .. & \frac{\Delta z_{2n}}{u_{z2n}} \end{bmatrix} = \sum_{i=1}^{i=2n} \sum_{j=1}^{j=2n} Q_{ij} \frac{\Delta z_i}{u_{zi}} \frac{\Delta z_j}{u_{zj}} \tag{5}$$

Multiplying and dividing each of the elements $\frac{\Delta z_i}{u_{zi}}$ by the same nonzero values does not change the value. If these values are the values of the first derivatives of the transforming functions at the measured points, then the criterion function is given a new interpretation $\phi(\Delta Z, p)$. See Appendix A to find the types of the least squares methods dependent on co-factors Q_{ij}.

3. The Proposed Approximation Method

By fitting a nonlinear function with separable variables x and y, which can be written as:

$$\psi(y,p) = A\xi(x,p) + B \tag{6}$$

where A-multiplication coefficient (slope of straight line in new coordinates ξ and ψ), B-additive coefficient (intercept of straight line in new coordinates ξ and ψ) then the criterial function can be transformed using function ψ and ξ and also based on the:

The law of propagation of error

$$\Delta\psi \approx \psi'(y,\boldsymbol{p})\Delta y \text{ and } \Delta\xi \approx \xi'(x,\boldsymbol{p})\Delta x \tag{7}$$

The law of propagation of uncertainty (LPU)

$$u(\psi) \approx |\psi'(y,p)|u(y) \text{ and } u(\xi) \approx |\xi'(x,p)|u(x) \tag{8}$$

can be transformed to the form

$$(\Delta Z, p) = \Delta Z^T U_z^{-1} \Delta Z \approx [\Delta\xi\ , \Delta\Psi] \begin{bmatrix} U_\xi & U_{\xi\,\psi} \\ U_{\xi\,\psi}^T & U_\psi \end{bmatrix}^{-1} \begin{bmatrix} \Delta\xi \\ \Delta\Psi \end{bmatrix} \to \min \tag{9}$$

where covariance matrix after transforming to the new coordinates became:

$$\begin{bmatrix} U_\xi & U_{\xi\,\psi} \\ U_{\xi\,\psi}^T & U_\psi \end{bmatrix} = \begin{bmatrix} \xi'(x_1,p) & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & \psi'(y_n,p) \end{bmatrix} \begin{bmatrix} U_X & U_{XY} \\ U_{XY}^T & U_Y \end{bmatrix} \begin{bmatrix} \xi'(x_1,p) & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & \psi'(y_n,p) \end{bmatrix} \tag{9a}$$

The covariances matrixes U_ξ , U_ψ and $U_{\xi\,\psi}$ size n x n after the coordinate's transformation correspond to the covariance matrixes before the transformation U_X, U_Y, U_{XY}.

If we are dealing with negative values of the first derivatives, then on non-diagonal elements of covariance matrix in new coordinates system there may be a change in the sign of correlation coefficients because uncertainties are always positive.

Mathematically, the search for the minimum means that below conditions are satisfied:

$$\nabla_{\xi_p}\phi = \frac{\partial\phi}{\partial\xi_p} = 0\ , \quad \frac{\partial\phi}{\partial A} = 0, \text{and } \frac{\partial\phi}{\partial B} = 0 \tag{10a, b, c}$$

The first condition is analytically solvable and leads to obtaining a local minimum for the inverse effective covariance matrix – see Appendix B to find the proper formulas of the matrix:

$$U_{Yeff}^{-1} = V_{22} - (V_{13}^T + AV_{22})U^{-1}(V_{13} + AV_{22}) \tag{11}$$

where symmetric matrix $U = V_{11} + A(V_{13}^T + V_{13}) + A^2 V_{22}$ and inverse covariance matrix after transformation to the new coordinates is $\begin{bmatrix} U_\xi & U_{\xi\,\Psi} \\ U_{\xi\,\Psi}^T & U_\Psi \end{bmatrix}^{-1} = \begin{bmatrix} V_{11} & V_{13} \\ V_{13}^T & V_{22} \end{bmatrix}$. Denoted by V_{11}, V_{13} and V_{22} covariance matrixes size n x will create the inverse matrix to the covariance matrix obtained after the coordinates transformation.

The value of the criterion function is determined using the formula:

$$\phi_{\psi\xi}(A,p) = A^2\left(S_{\xi\xi} - \frac{S_\xi^2}{S}\right) + 2\left(\frac{S_\xi S_\psi}{S} - S_{\xi\psi}\right)A + S_{\psi\psi} - \frac{S_\psi^2}{S} \quad (12)$$

where axillary parameters which depend on slope coefficient A are: $S = 1^T\, U_{eff}^{-1} 1 = \sum_{i=1}^{n}\sum_{j=1}^{n}[\,u_{yeff}^{-1}]_{ij} > 0$, $S_\xi = \xi^T U_{Yeff}^{-1} 1 = 1^T U_{Yeff}^{-1}\xi$, $S_{\xi\xi} = \xi^T U_{Yeff}^{-1}\xi, S_\psi = \Psi^T U_{Yeff}^{-1} 1 = 1^T U_{Yeff}^{-1}\Psi$, $S_{\psi\psi} = \Psi^T U_{Yeff}^{-1}\,\xi$, $S_{\xi\psi} = \xi^T U_{Yeff}^{-1}\Psi = \Psi^T U_{Yeff}^{-1}\xi$ and $B = (\,S_\psi - A\,S_\xi)/S$.

On the basis of the relation (12) we can conclude that the dependence of the criterion function on the slope coefficient A (also of the free term B) is quasi-quadratic and this relation for each vector p has a quasi-vertex constituting the local minimum. Therefore, by increasing/decrementing the parameter vector p with the step Δp, we search the criteria function so that the local minimum reaches the value of the global one.

The standard/expanded uncertainty are defined for the uncertainty corridor around the straight line described by (6) follows from the law of propagation of uncertainty and the using of relationships $u_y = u_\psi/|\psi'|$ are:

$$u_y \approx \sqrt{u^2(A)\xi^2 + 2\xi u(A)u(B)\rho_{AB} + u^2(B)}/|\psi'| \quad \text{and} \quad U_y = t_{1-\frac{\alpha}{2},n-2}u_y \quad (13a,b)$$

where u(A) and u(B) are uncertainties of slope and intercept and ρ_{AB} is correlation coefficient between A and B, u_y is standard uncertainty and U_y is expanded uncertainty after adjustment and $t_{1-\frac{\alpha}{2},n-2}$ is the coefficient (inverse of distribution) from t-Student distribution for n-2 degree of freedom and $\alpha = 0.05$ for coverage 95 %.

In this way we assume that the uncertainty of parameter vector is close to zero $u(\boldsymbol{p}) \approx 0$ at the beginning except of after adjustment curve the uncertainties u(A) and u(B) for two parameters A and B and the correlation coefficient between them ρ_{AB} , on which the width of the interval depends coverage corridor. However, these two parameters acquire uncertainties from the coordinates of the measurement points only after fitting a nonlinear curve using the law of propagation of uncertainty for the determined covariance matrix after the coordinate transformation. The problem can be solved for example in EXCEL workbook, R or Matlab environment. We have only area for A and p vector for minimalization. It means we have m-1 dimensional space for optimalization – A and B are functionally related and are part of p. Matching consists in taking a series of parameter values, A for example with a step Δ e.g.. $A_j = A_0 + (j-1)\Delta$ and j =1, …, m, whereby A_0 is the initial value assumed in such a way that the determined values of the criterion function $\phi_{\xi z}(A_j)$ make visible the local minimum. At any step we obligatorily determine the matrix U_{Yeff}^{-1} which depends on the A_j. Parameter p must be accepted in advance. Then, by changing its value from p_{min} to p_{max} while respecting the local minimum $\phi_{\xi z local\,min}(A_j)$ the criterion function shall be minimized in such a way as to obtain a global minimum $\phi_{\xi z global\,min}(A_j)$. During this process, we can change both the value

of A_0 as well as the step Δ, so that on the chart $\phi_{\xi z}(A)$ a local minimum has appeared. In each step leading to minimization, there is a relationship $B = (S_\psi - A\,S_\xi)/S$.

Compared to gradient methods, e.g. the Levenberg-Marquardt (L-M) where we do not perform coordinate transformations, the criterion function is numerically differentiable by m – parameters and by n coordinates of the vector Xp , which exhaust the domain of the function. The criterion function for the gradient method in general form is always greater than the criterion function after the transformation of coordinates into a linear relationship due to the selection of the effective covariance matrix: $\phi_z(\Delta Z, p) \geq \phi_z(p) \approx \phi_{\psi\xi}(A, p)$.

4. Examples of Fitting a Curve to Measurement Points

Three examples of fitting a nonlinear curve to measurement points are presented below. The first concerns the shape of the high-voltage overhead line. The second is to determine the semi-axis of the ellipse, and the third is to determine the electronic system consisting of a diode and a resistor.

4.1 Fitting catenoid curve

Measurements of high voltage catenoid lines [15] were performed in 10 measurement points, the data of which are presented in Table 1 by Laser Rangefinder with standard uncertainty 0.01 m.

Tabel 1a: *Coordinates of measurement points for measurements of high voltage catenoid lines.*

x [m]	0	50	60	80	100	110	140	160	180	220
y [m]	177.29	173.94	173.63	173.36	173.49	173.94	175	177.2	179.53	185.64

Looking for parameters $A=H/w$, $p=L$, and B= h_{min} determined for the equation of the high-level overhead line voltage described by the catenoid curve:

$$y = \frac{H}{w}\left[cosh\frac{w}{H}(x - L) - 1\right] + h_{min} \tag{14}$$

where: H−tension of the conductor at the lowest point of the conduit, w−dead weight of the cable, x, y−wire coordinates, L-distance of the first column from the x coordinate corresponding to the lowest overhang, i.e. the height h_{min}.

In order to use the least squares method for uncorrelated variables, we minimize the criterion function given by:

$$\phi_{xy}(\Delta x, \Delta y, p) = \sum_{i=1}^{n} \frac{\Delta x_i^{\,2}}{u^2(x_i)} + \frac{\Delta y_i^{\,2}}{u^2(y_i)} \rightarrow \min \tag{15}$$

That $\phi_{xy}(\Delta x, \Delta y, p)$ can be estimated by $\phi_{\xi y}(\Delta\xi, \Delta y, p)$.

$$\phi_{\xi y}(\Delta\xi, \Delta y, p) = \sum_{i=1}^{n} \frac{\Delta\xi_i^{\,2}}{u^2(\xi_i)} + \frac{\Delta y_i^{\,2}}{u^2(y_i)} \rightarrow \min \tag{16}$$

Where $\xi(x_i) = cosh\big((x_i - p)/A\big)$ and uncertainty of new coordinates are: $u(\xi_i) = \left|sinh\left(\frac{(x_i - p)}{A}\right)\right| u(x_i)/A$. In such a representation of coefficients A, B and parameter p, the

coordinates of the measurement points change with the change of *A*, but the condition (10a) is satisfied by the inverted effective covariance matrix and equation (6) also is satisfied.

As a result, the following characteristics of the criterion function are obtained with visible global minima- Figure 2a in dependence on *A* and 2b in dependence on *B*.

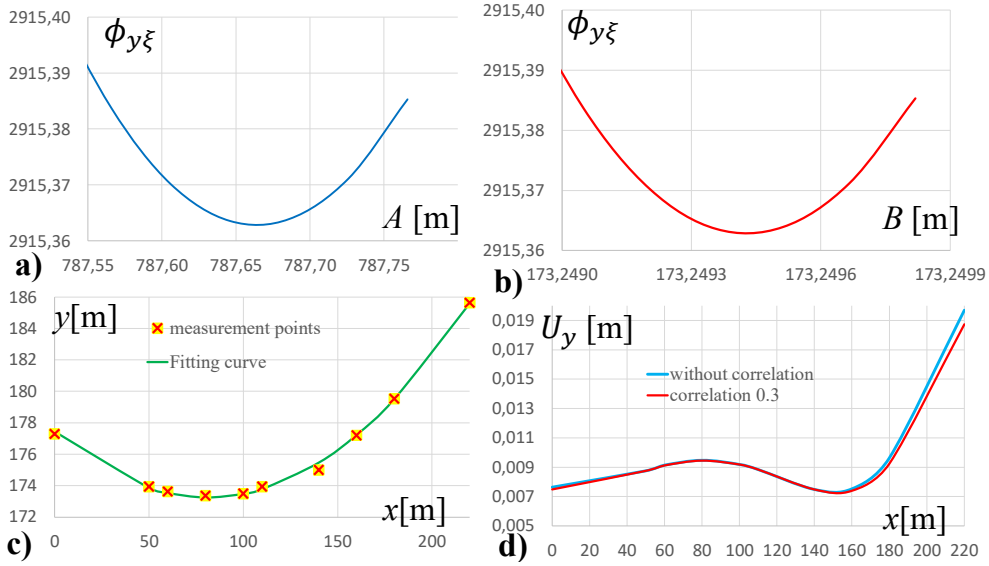

Figure 2: *Characteristics of the criterial function for non-correlated coordinates: a) depend on A and b) depend on B.*
c) Measurement points and fitting curve in XOY cartesian system, d) Expanded uncertainty for correlated and noncorrelated coordinates.

The minimization for the L-M method concerned n+m=13 parameters. The results of fitting parameters for both methods are presented in Table 1b) below.

Table 1b: *The results of numerical calculations for fitting catenoid curve.*

	A		*L=p*		*H*		$\phi_{\xi ymin\_global}$	
Type of method	**without correlation**	**with correlation 0.3**	**without correlation**	**with correlation 0.3**	**without correlation**	**with correlation 0.3**	**without correlation**	**with correlation 0.3**
Proposed approximate method	787.66 ± (0,7)	787.12 ± (0,7)	81	81	173.25 ± (0,1)	173.25 ± (0,1)	2915.38	3037.94
Levenberg - Marguardt method	787.58	787.1	81.01	80.96	173.25	173.25	2913.73	3038.83

The fitted curve with 10 input points is presented in figure 1c). The expanded uncertainty is estimated from the parameters of standard uncertainties u(*A*) and *u(B)* and correlation coefficient ρ_{AB} which are determined by numerically differentiation of solutions for A and *B* as a linear dependence of all coordinates and using matrix law of propagation of uncertainty.

For the Levenberg-Marguardt method, correlations were obtained by modifying the criterion function, i.e. the coefficient on the diagonal of the matrix inverse to the correlator matrix–a coefficient of about 1.099 and adding 10 mixed elements with a coefficient of about 0.66.

The results of adjustment parameters indicate differences at a level not exceeding 0.01% for the values of parameters–there is a maximum difference of 0.06% in the criterion function for uncorrelated coordinates.

The characteristic of expanded uncertainty is presented in figure 1d). The expanded uncertainty is greater than 0.007 m and less than 0.019 m in whole range. For the uncorrelated coordinates x_i and y_i is slightly higher than for the correlated in the entire studied range. This difference does not exceed 0.001 m for x=220 m.

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4.2 Fitting the ellipse to the measuring points

A cylinder with an elliptical cross-section was measured with a coordinate-measuring machine (CMM). The following coordinates were obtained: 10 points of the boundary surface in the cross-section plane. The measurements coordinates are included in table 2.

Table 2: *Measured coordinates of the elliptical cross-section object under study.*

x′[mm]	29.19	34.55	35.75	36.56	31.21	26.18	24.53	19.54	23.96	27.15
y′[mm]	12.91	15.33	15.46	14.11	9.71	11.36	10.39	5.16	5.78	7.26

In the coordinate system related to the center of the ellipse justified with respect to the semi-axis λ_x, λ_y the equation of the ellipse is as follows:

$$\frac{x^2}{\lambda_x^2} + \frac{y^2}{\lambda_y^2} = 1 \quad (17)$$

The nonlinear elliptic curve was measured in n=10 measurement points–generated from the nominal curve with absolute errors of coordinates not exceeding +/-0.1. The standard uncertainty of the measuring points is 0.01 mm for both coordinates.

The nominal half-axis is: λ_x=2, λ_y=10 and ellipse is rotated by an angle α=60 ° and offset r=30 mm for angle φ=20°. By performing successive rotations and translations of measurement points, equations for coordinates are obtained:

$$x' = x\cos\alpha - y\sin\alpha + r\cos\varphi \quad y' = x\sin\alpha + y\cos\alpha + r\sin\varphi \quad (18)$$

In order to obtain the coordinates satisfying the ellipse equation, the following operations should be performed:

$$x' - r\cos\varphi = x\cos\alpha - y\sin\alpha\,, \quad y' - r\sin\varphi = x\sin\alpha + y\cos\alpha \quad (19a,b)$$

And from here

$$\begin{cases} x = (x' - r\cos\varphi)\cos\alpha + (y' - r\sin\varphi)\sin\alpha \\ y = -(x' - r\cos\varphi)\sin\alpha + (y' - r\sin\varphi)\cos\alpha \end{cases} \quad (20a,b)$$

It is for these coordinates that we swap variables: $\psi(y,p) = y^2$, $\xi(x,p) = x^2$ whereas p is a three-dimensional vector $p = [r, \alpha, \varphi]$ which components will need to be matched.

The ellipse equation can be replaced by a linear equation

$$\psi(y,p) = A\xi(x,p) + B \tag{21}$$

where $A = -\frac{\lambda_y^2}{\lambda_x^2}$ oraz $B = \lambda_y^2$ and the square of uncertainties of new coordinates for noncorrelated measurements of coordinates x_i' and y_i' are given:

$$u^2(\xi_i) = 4((x_i\,' - rcos\varphi)cos\alpha + (y_i' - rsin\varphi)sin\alpha)^2(u^2(x_i')\cos^2\alpha + u^2(y_i')\sin^2\alpha), u^2(\psi_i) = 4((x_i\,' - rcos\varphi)cos\alpha + (y_i' - rsin\varphi)sin\alpha)^2(u^2(x_i')\sin^2\alpha + u^2(y_i')\cos^2\alpha) \tag{22a, b}$$

with correlation coefficients $\rho_{\xi_i\psi_i}$ for every pair ξ_i and ψ_i :

$$\rho_{\xi_i\psi_i} = 2sin2\alpha((x_i\,' - rcos\varphi)cos\alpha + (y_i' - rsin\varphi)sin\alpha)(-(x_i\,' - rcos\varphi)\sin\alpha + (y_i' - rsin\varphi)cos\alpha)/\,(u(\xi_i)\,u(\psi_i)) \tag{22c}$$

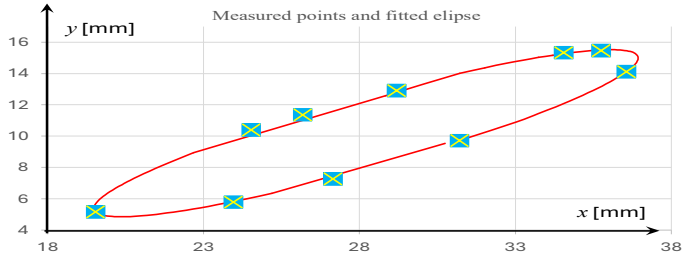

Figure 3: *Measured points and fitted ellipse.*

The result of the match is the following estimated values $A_{global\,min}$ = -24.4, $B_{global\,min}$ = 100,32, $p_{min} = [r_{min,}.\alpha_{min}, \varphi_{min}.] = [29.99\text{ mm}, 59.81°\text{ , }19.845°,]$. Values of fitted semi-axes with standard uncertainties of the ellipse are: λ_x = 2.02 mm ± (0.1 mm) and λ_y= 10.03 mm ± (0.2 mm) at global minimum of criterial function $\phi_{\xi\psi\,global\,min} \approx 321.81$. Figure 3 shows the measured points and the fitted ellipse in the XOY coordinate system.

In the case of the Levenberg-Marguardt method with numerical determination of the gradient, it failed to start. Many tests were made, even for an ellipse positioned in the center of the coordinate system. Unfortunately, the iterations ended in failure. This is a kind of flaw of the method, the initial vector of all variables involved in the minimization was not selected automatically. Therefore, it was not possible to compare the results.

4.3 Example of implicit function fitting

Nonlinear curve fitting to the measurement points, a series circuit of the connection of the semiconductor silicon diode with the internal resistance R powered by a constant voltage power supply is considered. In the arrangement according to figure 4 current is measured I ammeter with relative uncertainty $\delta(I) = 1\%$ and voltage U with relative uncertainty $\delta(U) = 1\%$.

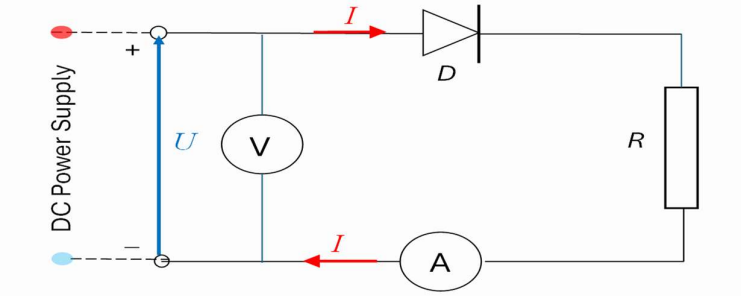

Figure 4: *The measuring system for the determination of non-linear matched characteristics U(I) to the measuring points.*

The diode is characterized by the following exponential dependence of current on the voltage measured at its terminals – the Shockley equation:

$$I = I_0 \left(\exp\left(\frac{U_d}{\varepsilon}\right) - 1 \right) \tag{23}$$

where I_0 – saturation current, ε – constant characteristic of a particular diode and operating temperature, diode voltage: $U_d = \varepsilon \ln(\frac{I}{I_0} + 1)$.

From Kirchoff's second equation it follows that the measured voltage on the circuit of the series connection of the internal resistance of the diode and the voltage across the diode and the current flowing through the circuit is:

$$IR + \varepsilon \ln\left(\frac{I}{I_0} + 1\right) = U \tag{24}$$

Equation (24) is an implicit function $h(I, U) = IR + \ln\left(\frac{I}{I_0} + 1\right) - U = 0$ because it is not possible to find analytically the relationship of current I as a function of voltage U.

The values of the measured voltage and current at ten measuring points n=10 of the system from figure 4 are given in table 3. Nominally parameters of such circuits are: ε = 26 mV, R=1 k Ω, I_0 = 1.5 pA.

Table 3: *The coordinates of the measured points for nonlinear curve given by measurement site–figure 4.*

I (μA)	3.01	6.32	14.48	34.76	48.06	64.97	89.01	123.21	165.1	225.9
U(mV)	378.01	406.32	438.48	484.76	508.06	534.97	569.01	613.21	665.1	735.9

From the current and voltage measurements, we determine the resistance R, parameter ε and saturation current I_0 by adjusting the nonlinear characteristic described by (24) using the method of weighted total least squares WTLS assuming no correlation between the measured quantities. For this purpose, we use the following substitution, which will allow us to fit both measured quantities into a straight line:

$$\psi = h(I, U) = \frac{U}{I} \text{ and } \psi = A\xi + B \tag{25a, b}$$

where: $A = \varepsilon$, $B = R$ and $p = I_0$, $\xi = \frac{1}{I}\ln\left(\frac{I}{p}+1\right)$. Thus, the measured values are transformed into new coordinates in the system $\psi = U/I$ and $\xi(I) = ln(I/p+1)/I$. After such a transformation, the least squares method will be used de facto as a match of the resistance of the system described by ψ, and not as a match of voltages as a function of the flowing current in the system under consideration.

Both new coordinates of (ξ_i, ψ_i) each point, due to their dependence on the measured current , *I*, are correlated with a positive non-zero correlation coefficient resulting from equal relative uncertainties $\rho_{z_i\xi_i} = \frac{1}{\sqrt{2}}$ because $\delta(I)$=$\delta(U)$=1 %. The uncertainty of the new coordinate can be estimated from the law of propagation of uncertainty, using its first derivative $\xi'(I)$. So, $u\left(\xi(I)\right) = |\frac{1}{I+p} - \frac{1}{I}\ln\left(\frac{I}{p}+1\right)|\delta(I)$ and uncertainty of variable ψ follows from this law and is equal:

$$u(\psi_i) = \frac{U_i}{I_i}\sqrt{\left(\delta(U_i)\right)^2 + \left(\delta(I_i)\right)^2} \quad (26)$$

Vectors $\boldsymbol{\xi} = [\xi_1, \dots, \xi_n]^T$ and $\psi = [\psi_1, \dots, \psi_n]^T$contain the coordinates of the survey points after the transformation. When coordinates are correlated, the diagonal inverse matrix is given by (B.4)– after transformation the correlation coefficient became positive because of $\xi'(I) < 0$. The fitted diode and resistor parameters are: $A_{global\ min} = \varepsilon = 26.45$ mV $\pm$ (0,27 mV), $B_{global\ min}$ =*R*=1.089 kΩ ±(0,057 kΩ), $p = I_0 = 1.73$ pA at $\phi_{\xi\psi mingloba} \approx 3.24$. As you can see, they are close to nominal values.

In this case, it was also not possible to initiate numerical iterations with the determination of a multidimensional gradient for the Levenberg-Marquardt method. Here it was probably a problem of one of the parameters I_0, which was below the value 10^{-5} in comparison to the other parametrs, which caused problems with numerical differentiation.

5. Verification of the Method

The verification of the approximate method was performed for two nonlinear functions: the quadratic function for which the parameter fit was performed, and the expanded uncertainty interval was determined, and the nonlinear function three described in the position [16] in which only the parameters fit was performed.

5.1 Example of adjustment to the quadratic function

The approximate method of fitting the nonlinear function to the measurement points was verified on the quadratic function described by the equation (2):

$$f(x) = a_2x^2 + a_1x + a_0 \quad (27)$$

where the nominal values are: a_2 =0,133 a_1=0,04 and a_0=1. The coordinates of the simulation points are included in the table [4] below:

Table 4: *Input data of coordinates x and y for quadratic function.*

x	1	2	3	4	5	6	7	8	9	10
y	1.14	1.72	2.14	3.26	4.66	5.71	6.83	10.19	12.50	13.64

It was assumed that the simulation measurements were made in four cases: with constant standard absolute uncertainties $u(x_i) = 0.08$ and $u(y_i) = 0.17$ and also with constant standard relative uncertainties $\delta(x_i) = 1\ \%$ and $\delta(y_i) = 5\ \%$ also $\delta(x_i) = 2\ \%$ and $\delta(y_i) = 0.5\ \%$ and $\delta(x_i) = 0\ \%$ and $\delta(y_i) = 2\ \%$.

In order to use the Monte Carlo method for the propagation of x and y coordinate distributions, the equation of zero gradient over coordinates was partially solved analytically x_{pi} using formulas for the root of the equation of the third degree. In this way, we will be able to use analytical formulas contained in random variable symbols containing a series of samples processed directly in R or Matlab environments.

The form of the criterion function for its minimization for uncorrelated variables is as follows

$$\phi(\boldsymbol{x_p}) = \sum_{i=1}^{n} \frac{(x_{pi}-x_i)^2}{u^2(x_i)} + \frac{(f(x_{pi})-y_i)^2}{u^2(y_i)} \tag{28}$$

A gradient of the criterion function in *the* n-dimensional coordinate space x_{pi} conditions the achievement of the minimum function $\phi(\boldsymbol{x_p})$ when:

$$\nabla_{\boldsymbol{x_p}} \phi(\boldsymbol{x_p}) = 0 \tag{29}$$

The above condition leads to the equations of the third degree for every x_{pi}:

$$x_{pi}^3 + \frac{3a_1}{2a_2} x_{pi}^2 + \left(\frac{a_0-y_i}{a_2} + \frac{a_1^2}{2a_2^2} + \frac{u^2(y_i)}{2a_2^2 u^2(x_i)}\right) x_{pi} + \frac{a_1(a_0-y_i) - \frac{x_i u^2(y_i)}{u^2(x_i)}}{2a_2^2} = 0 \tag{30}$$

Which can be transformed to the equation $t^3 + Pt + Q = 0$, where $t = x_{pi} - \frac{a_1}{2a_2}$ and P, and Q are coefficients obtained from (30). The Monte Carlo method was applied to 10^6 samples drawn from the normal distribution for every both x_i coordinates and yi measurement points, while the solution for the least squares method was carried out iteratively, i.e. the initial values of a_2, a_1 and a_0 were assumed in order to use the analytical solution with one real root equal $t = \sqrt[3]{-\frac{Q}{2} + \sqrt{P^3/27 + Q^2/4}} + \sqrt[3]{-\frac{Q}{2} - \sqrt{P^3/27 + Q^2/4}}$ for the equation of the third degree (30) and thus it is easy to determine the probability density distributions of x_{pi}. In the final part of the determinant method (it is not possible to use library function in R for determinant), we need to solve a system of equations:

$$\begin{cases} \sum_{i=1}^{n} \frac{a_2 x_{pi}^2 + a_1 x_{pi} + a_0}{u^2(y_i)} = \sum_{i=1}^{n} \frac{y_i}{u^2(y_i)} \\ \sum_{i=1}^{n} x_{pi} \frac{a_2 x_{pi}^2 + a_1 x_{pi} + a_0}{u^2(y_i)} = \sum_{i=1}^{n} \frac{x_{pi} y_i}{u^2(y_i)} \\ \sum_{i=1}^{n} x_{pi}^2 \frac{a_2 x_{pi}^2 + a_1 x_{pi} + a_0}{u^2(y_i)} = \sum_{i=1}^{n} \frac{x_{pi}^2 y_i}{u^2(y_i)} \end{cases} \tag{31}$$

The output probability density distributions are obtained for a_2, a_1, and a_0. These distributions should be inserted into (30) and repeated iteratively until the output distributions of a_2, a_1, and a_0 are consistent with the input distributions. Euclide's distance of mean values of distributions between iteration for a_2, a_1, and a_0 less then 10^{-5} finishes iterations.

For the new approximate proposed method, a coordinate transformation has been used: x to the new function $\xi(x,p) = (x+p)^2$ and $y = a_2x^2 + a_1x + a_0 = a_2\left(x + \frac{a_1}{2a_2}\right)^2 + a_0 - \frac{a_1^2}{4a_2}$ that is $y = A\xi + B$ where A=a_2 and B=$a_0 - \frac{a_1^2}{4a_2}$, and $p = \frac{a_1}{2a_2}$. The expanded uncertainty of the new approximate method is determined by the following relation [16]:

$$U = t_{1-\frac{\alpha}{2},n-2}\sqrt{u^2(A_{global\ min})(x+p_{min})^4 + 2\rho_{AB}(x+p_{min})^2\, u(A_{global\ min})u(B_{global\ min}) + u^2(B_{global\ min})} \quad (32)$$

For $\alpha = 0.05$ coverage probability is 0.95. Calculations were also made using the Levenberg-Marquardt. The results of the match are presented in table 5a below.

Table 5a: *Comparison of new approximate method and Monte Carlo Method and Levenberg-Marquardt method for constant absolute uncertainties u(x) =0.08, u(y)=0.17– fitting parameters* a_2, a_1, *and* a_0.

Type of method	Fitted parameters							
	a_2		a_1		a_0		$\phi_{minglobal}$	
Monte Carlo method with iteration and solution for equation of third order	0.1320		0.0091		1.0473		34.81	
Proposed aproximate method	EXCEL	R	EXCEL	R	EXCEL	R	EXCEL	R
	0.1320	0.1321	0.0095	0.0095	1.0491	1.0472	34.77	34.77
Levenberg-Marguardt method	0.1320		0.0094		1.0483		34.82	

As we see from table 5a) the errors: for a_2 less than 0.1%, for a_1 less than 4.2% for a_0 less than 0.3%. Differences in the value of the criterion function of less than 0.12%.

Table 5b: *Comparison of new approximate method and Monte Carlo Method and Levenberg-Marquardt method for constant relative uncertainties δ(x) =1 % and δ (y)= 5% – fitting parameters* a_2, a_1, *and* a_0.

Type of method	Fitted parameters							
	a_2		a_1		a_0		$\phi_{minglobal}$	
Monte Carlo method with iteration and solution for equation of third order	0.1256		0.0578		0.979		12.74	
Proposed aproximate method	EXCEL	R	EXCEL	R	EXCEL	R	EXCEL	R
	0.1259	0.1256	0.0554	0.0578	0.982	0.979	12.75	12.75
Levenberg-Marguardt method	0.1255		0.0579		0.979		12.75	

From table 5b) the differences in the value of the criterion function are less than 0.2 %. The estimated values do not differ for the parameter a_0 below 0.24%, for a_1 below 4.1% in EXCEL (L-M method below 0.2%) and for a_0 less than 0.31 %.

Table 5c: *Comparison of new approximate method and Monte Carlo Method and Levenberg-Marquardt method for constant relative uncertainties δ(x) =2 % δ (y)= 0.5 % – fitting parameters* a_2, a_1, *and* a_0

Type of method	Fitted parameters							
	a_2		a_1		a_0		$\phi_{minglobal}$	
Monte Carlo method with iteration and solution for equation of third order	0.1196		0.1184		0.905		51.99	
Proposed approximate method	EXCEL	R	EXCEL	R	EXCEL	R	EXCEL	R
	0.1192	0.1191	0.1264	0.1272	0.899	0.898	51.17	51.17
Levenberg-Marguardt method	0.1194		0.1207		0.904		51.98	

In above table 5 c) the estimated values do not differ: for the parameter a_0 below 0.8%, for a_1 below 7.5% (L-M method 2%) and for a_2 less than 0.5%. Differences in the value of the criterion function of less than 1.6% for proposed method and 0.02%)

Table 5d: *Comparison of new approximate method and Monte Carlo Method and Levenberg-Marquardt method for constant relative uncertainties δ(x) =0% δ (y)= 2% – fitting parameters* a_2, a_1, *and* a_0.

Type of method	Fitted parameters							
	a_2		a_1		a_0		$\phi_{minglobal}$	
Monte Carlo method with iteration and equation of third order/ (Deteminant method)	0.1252		0.0586		0.979		86.99	
Proposed aproximate method	EXCEL	R	EXCEL	R	EXCEL	R	EXCEL	R
	0.1252	0.1254	0.0589	0.0577	0.979	0.967	86.99	86.99
Levenberg-Marguardt method	0.1252		0.0586		0.979		86.99	

In above table 5d) the estimated values do not differ for the parameter a_0 below 1.2 % for a_1 below 0.2 % % in R (L-M and EXCEL close to zero) for a_2 less than 0.2 % (Excel close to zero). The differences of values of the criterion function are negligible. The values for the L-M method are identical to those for Monte Carlo, but for the approximate method a close to zero but non-zero uncertainty value is used $u(x)= 10^{-11}$.

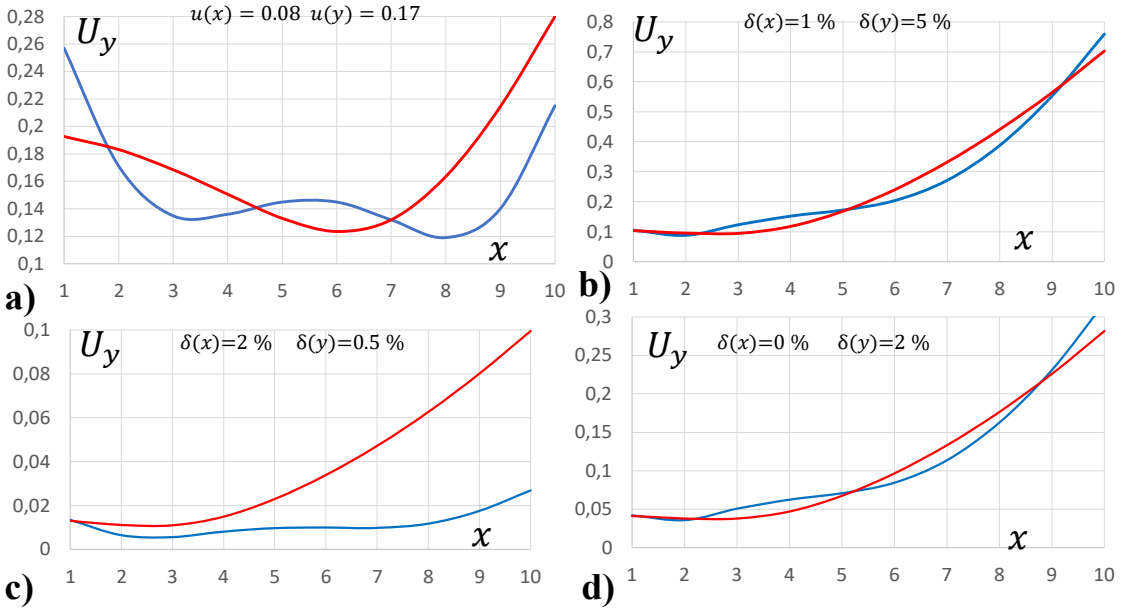

Figure 5: *The characteristic of expanded uncertainties (the half of coverage corridor) for fitted parabolic curve for Monte Carlo method – blue lines and new approximate method – red lines for considered cases: constant absolute uncertainties a) u(x) =0.08, u(y)=0.17, constant relative uncertainties: b) δ(x) =1 % , δ (y)= 5 % , c) δ(x) =2 % , δ (y)= 0.5 % , d) δ(x) =0 % δ (y)= 2 %.*

The largest deviations in relation to the Monte Carlo method occur for the parameter a_1 in Table 5 c) because as much as 7.5% for the proposed method, while the L-M method gives a deviation of 2%. Then the value of the global minimum of the criterion function is determined with an error of 1.6% for the proposed method, while for the L-M method this deviation is close to zero. In other cases, we have small errors of the criterion function below 0.2%. The results for the proposed approximate method are similar for implementation in woorbook Excel and in the R environment. In Table 5d) we have the smallest errors of the criterion function for the Levenberg-Marguardt method because it required writing a criterion function without the squares of the errors x because it could not start for settings of small uncertainties x. It coped without problems with a criterion function containing only the variable y (regression y to x).

The results of matching the parameters of the function for the approximate method can be considered consistent. They coincide with the results obtained iteratively using Monte Carlo and the L-M method.

In the case of the expanded uncertainty, the characteristics of which are illustrated in the diagrams of Figures 5a, b, c, d, the comparison concerned the results obtained by the Monte Carlo method and the approximate method from formula (32). The approximate method required numerical differentiation by x_i, y_i coordinates at the global minimum of criterial function point and determination of the parameters $u(A)$, $u(B)$ and ρ_{AB}, which fully take over the uncertainties of the coordinates x_i and y_i of the measurement points. Of course, it is not, because the other parameters of the function being adjusted are also in fact associated with uncertainties. The differences in underestimation included in Figure 5a) are half of the expanded uncertainty of the estimated Monte Carlo. More or less in the middle part of the measurement range, we have an underestimation of the corridor at the maximum level below 30%.

In fig 5 b and 5d cases we have areas of underestimation and overestimation – the lines constantly intersect at 4 points. Dashed lines on figures 5 a) and b) show expanded uncertainty for LPU method. The standard deviations of coefficients a_2, a_1, and a_0 and correlation coefficients between them are calculated in R from their distributions.

5.2 Example of adjustment to the sum of exponent and sinus functions

The second example investigates the fit of a nonlinear function given by the equation

$$y = b_1 \exp\left(-\frac{x}{b_2}\right) + b_3 \sin\left(\frac{x}{b_4}\right) \quad (33)$$

In [12] with four nominal parameters $b_4 = 6, b_3 = 20, b_2 = 1, b_1 = 5,$ The values of simulated measurement coordinates of x and y for n=10 with relative uncertainties of 2% are presented in the table 6.

Table 6: *The simulated coordinates for the nonlinear curve described by the equation (14).*

x	1	10	20	30	40	50	60	70	80	100
y	6.01	4.25	1.65	0.76	1.60	-0.15	-0.44	0.87	-0.38	-2.05

The results of calculations for the approximate and numerical methods of the L-M method were compared.

For the approximate method, the following variable swap was used: $\xi(x, \boldsymbol{p}) = \exp\left(\frac{x}{b_2}\right)\sin\left(\frac{x}{b_4}\right)$ and $\psi(y, x, p) = y\exp\left(\frac{x}{b_2}\right)$. Then the nonlinear equation can be represented in the form $\psi(y, x, p) = A\xi(x, p) + B$ where the relevant parameters are marked by $A = b_3, B = b_1$ oraz $p = [b_2, b_4]$. The uncertainties of the new coordinates based on the law of propagation of uncertainty are determined by:

$$u(\xi) \approx |\xi'|u(x) = \exp\left(\frac{x}{b_2}\right)\left|\frac{1}{b_2}\sin\left(\frac{x}{b_4}\right) + \frac{1}{b_4}\cos\left(\frac{x}{b_4}\right)\right|u(x), \quad (33a)$$

And

$$u(\psi) \approx \exp\left(\frac{x}{b_2}\right)\sqrt{u^2(y) + y^2u^2(x)/b_2^2} \quad (33b)$$

Since both new coordinates depend on the old x coordinate associated with the uncertainty $u(x)$, the new variables are correlated with the correlation coefficient described by:

$$\rho_{\xi\psi} = \frac{y}{b_2}\exp\left(\frac{2x}{b_2}\right)\left(\frac{1}{b_2}\sin\left(\frac{x}{b_4}\right) + \frac{1}{b_4}\cos\left(\frac{x}{b_4}\right)\right)u^2(x)/(u(\psi)u(\xi)) \quad (33c)$$

Therefore, the B4 formula was used for the inverse effective covariance matrix taking into account the correlation between the new coordinates. The results of the calculations are presented in the table below.

Table 7: *Results of coefficient obtained for approximate method and L-M.*

Type of method	Fitted parameters				
	b_1	b_2	b_3	b_4	$\phi_{minglobal}$
Proposed approximate method for coordinates ξ, ψ	5.17	0.93	18.27	6.10	53.58
Levenberg-Marguardt method for coordinates x, y	5,08	1.98	14.86	5.88	88.4

It shows in table 6 that the parameters b_1, b_2, b_3, b_4 determined by the L-M gradient method differ significantly from those obtained by the proposed approximate method, whose errors for the approximate method do not exceed the values of 3.4%, 7.1%, 8.7%, 1.7% respectively. Of course, it difficult to compare both criterial function because the one of the new coordinates ψ is depend on both coordinates x and y.

Figure 6 illustrates the arrangement of the measurement points, the ideal curve and the two curves after adjustment using the approximate method and the Levenberg-Marguardt method.

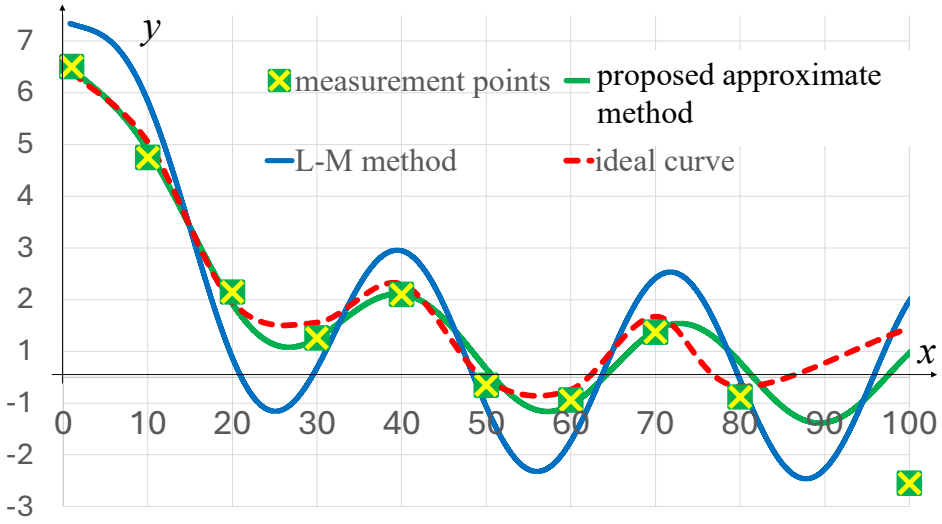

Figure 6: *Nominal curve and fitted curves using the approximate method and the L-M method with simulated measuring points.*

As we can see from Figure 6, the approximate fitting is closer to the nominal curve. However, the fit was based on measuring points, which could also represent a curve with slightly different parameters than the nominal ones.

6. Conclusion

The paper presents an approximate method of fitting any nonlinear curves (curves parameters) using the weight total least squares method, which is illustrated with examples. This method is based on the law of propagation of error and of uncertainty, i.e. the use of only the first derivatives determining analytically of the transforming functions the curve into the new coordinate system in which it is described by a straight line. Using an effective covariance matrix allows you to reduce the number of variables to optimize the criterion function. In such

a coordinate system, the criterion function depends solely on the parameters of the function represented by the vector $\boldsymbol{p}$ and the slope coefficient of the straight-line A, which greatly simplifies its minimization. By monitoring the minimum characteristics of the criterion function, the values of which are determined numerically depending on A, it is possible to obtain the global minimum with the free selection of other parameters. Calculation of the value of a function defined in this way is always possible, as long as the effective covariance matrix is correctly determined.

The methods used so far require a vector of initializing quantities, and numerically determined gradients of multivariate functions can lead to errors, which ends in the lack of iteration and, as a result, the lack of the final result of parameter matching.

The proposed approximate method does not have this feature and always determines the global minimum of the criterion function. The problem with numerical differentiation arises when determining the covering corridor.

The presented examples and the verification of the method for the quadratic function show that it allows for precise adjustment and estimation of the parameters of nonlinear curves and of the uncertainty corridor, taking into account all possible correlations of the measured coordinates. In most cases, we should expect an overestimation of the uncertainty corridor in relation to the Monte Carlo method, because we use the uncertainty propagation law with the expansion coefficient resulting from the student's t-distribution, although there will also be ranges in which the corridor will be slightly underestimated.

A comparison of the proposed approximate method with the classical Levenberg-Marguardt method implemented in the R environment showed its high accuracy and precision. The errors of comparable parameters did not exceed a single percent, which means that it can be used alternatively or dually in each case for comparison purposes.

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

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Appendix A Types of Least Squares Method

The formulas given by (5) can be expanded to the form

$$\phi(\Delta X,\Delta Y)=\sum_{i=1}^{n}Q_{ii}\frac{\Delta x_i{}^2}{u^2(x_i)}+\sum_{i=1}^{n}Q_{i+n,i+n}\frac{\Delta y_i{}^2}{u^2(y_{ii})}+2\sum_{i>j=1}^{n}Q_{ij}\frac{\Delta x_i\Delta x_j}{u(x_i)u(x_j)}+2\sum_{i>j=1}^{n}Q_{i+nj+n}\frac{\Delta y_i\Delta y_j}{u(y_i)u(y_j)}+$$
$$2\sum_{i,j=1}^{n}Q_{ij+n}\frac{\Delta x_i\Delta y_j}{u(x_i)u(y_j)}\rightarrow \min \quad \text{(A. 1)}$$

First case when measurement is carried out with coordinates x_i without uncertainties - $u(x_i)\rightarrow 0$ we get the WLS weighted method

$$\phi(\Delta Y)=\sum_{i=1}^{n}Q_{i+n,i+n}\frac{\Delta y_i{}^2}{u^2(y_{ii})}+2\sum_{i>j=1}^{n}Q_{i+nj+n}\frac{\Delta y_i\Delta y_j}{u(y_i)u(y_j)}=\Delta Y^T U_Y\Delta Y \quad \text{(A. 2)}$$

Of course, if the matrix $R^{-1}=R=I$ is diagonal – the case without correlations then $Q_{ii}=1$ and condition (1) is reduced to minimizing the sum of weighted squares (WTLS without correlations):

$$\phi(\Delta X,\Delta Y)=\sum_{i=1}^{n}\frac{\Delta x_i{}^2}{u^2(x_i)}+\frac{\Delta y_i{}^2}{u^2(y_i)}\rightarrow min \quad \text{(A. 3)}$$

When uncertainty $u(x_i)=u(y_i)$ as to the value the criterial function reduced to the form:

$$\phi(\Delta X,\Delta Y)=\sum_{i=1}^{n}\frac{\Delta x_i{}^2}{[unit(x_i)]^2}+\frac{\Delta y_i{}^2}{[unit(y_i)]^2}\rightarrow min \quad \text{(A. 4)}$$

It is called TLS (total last squares method). When $u(x_i)\rightarrow 0$ then we are dealing with the most well-known method of least squares OLS (ordinary least squares):

$$\phi(\Delta Y)=\sum_{i=1}^{n}\frac{\Delta y_i{}^2}{[unit(y_i)]^2}\rightarrow min \quad \text{(A. 5)}$$

which means $\sum_{i=1}^{n}\Delta y_i{}^2\rightarrow min$.

Appendix B Effective Inverse Covariance Matrix

To fit a straight-line $y=ax+b$, there are analytical solutions for zero gradient (10a) and we can easily determine the fitting errors for x and y coordinates. In this way we can replace equation (1) with matrix U_Z^{-1} by the equation for regression y on x with effective inverse symmetric matrix U_{Yeff}^{-1} [1].

In the special case where the matrix V_3 is symmetrical, i.e. $V_3=V_3^{\mathrm{T}}$, then

$$U_{Yeff}^{-1}=(V_1V_2-V_3V_3)V^{-1} \quad \text{(B.1)}$$

and when $V_3=0$ then

$$U_{Yeff}^{-1}=(a^2U_X+U_Y)^{-1} \quad \text{(B.2)}$$

As a result, for uncorrelated quantities, when matrices U_X and U_Y are diagonal U_{Yeff}^{-1} has only non-zero diagonal values equal to:

$[U_{Yeff}^{-1}]_{ii} = (u^2(y_i) + a^2u^2(x_i))^{-1}$ where and i=1,…,n. (B.3)

This is a special case in which the correlations between the measured at each point are uncorrelated.

If correlations are present, then a more general formula is used

$[U_{Yeff}^{-1}]_{ii} = (u^2(y_i) + a^2u^2(x_i) - 2\rho_{x_iy_i}au(x_i)u(y_i))^{-1}$, (B.4)

which is used in physical measurements – all matrixes that are components of the matrix $\boldsymbol{U_z}$ are diagonal. Special cases are dictated not only by the simplification and acceleration of calculations, but also by the possibility of performing them, because, as can be seen from the formula for the general form of the formula for the effective covariance matrix, there is an operation of inverting the covariance matrix $\boldsymbol{V}$, which, depending on the input data and the algorithm used, may lead to singularities and there may be problems with its numerical determination in general.

Appendix C Glossary of Principal Symbols

Symbol	Description
$\phi_{\xi\psi minglobal}$	global minimum of criterial function in new coordinates
a,A	slope of straight line
$A_{global\ min}$	slope of straight line at global minimum of criterial function
a_0, a_1, a_2	parameters of the function described by the eq. (27)
b,B	intercept of straight line
$B_{global\ min}$	intercept of straight line at global minimum of criterial function
u(A),u(B)	standard uncertainty of A and B determined numerically
ρ_{AB}	correlation coefficient between A and B
b_1, b_2, b_3, b_4	parameters of the function described by the eq (33)
C, C^T	matrix, transposition of matrix of sensitivity coefficient -element are first partial derivatives due to x_i and y_i coordinates
U_y	expanded uncertainty for y equal the half width of coverage corridor
U_{Yeff}^{-1}	Effective inverse covariance matrix size n x n for x,y coordinates
x_i y_i	coordinates of measurement points before transformation coordinates x to ξ
ρ_{xy}	correlation coefficient between x_i and y_i
x_i y_i	coordinates of measurement points before transformation coordinates x to ξ
p	m-dimensional vector of fitting parameters
p	scalar parameters
β	n x n in general non symmetric matrix obtained as local minimum due to vector $\mathbf{X_p}$
$u(x_i)$	standard uncertainty of measurement points for coordinates x
$u(y_i)$	standard uncertainty of measurement points for coordinates y
δ(x)	standard relative uncertainty of measurement points for coordinates x
δ(y)	standard relative uncertainty of measurement points for coordinates y
$u(\xi_i)$	standard uncertainty of measurement points after transformation coordinates x to ξ

$u(\psi_i)$	standard uncertainty of measurement points after transformation coordinates y to ψ
U_Z	symmetric covariance matrix size 2n x 2n for variable z
U_X	symmetric covariance matrix size n x n for variable x
U_Y	symmetric covariance matrix size n x n for variable y
U_{XY}	in general, non-symmetric covariance matrix size n x n for variable x and y
U_Z^{-1}	inverse covariance matrix for z
$V_1 V_2, V_3$	three parts of inverse covariance matrix U_Z^{-1}
U_{in}	input covariance matrix
U_{out}	output covariance matrix
$\phi(\Delta X, \Delta Y)$	criterial function for two vector of fitting error ΔX for x coordinate and ΔY for y coordinate
X	n-dimensional vector of coordinates x (measurement points)
Y	n-dimensional vector of coordinates y (measurement points)
ΔX	n-dimensional vector of fitting error for coordinates x
ΔY	n-dimensional vector of fitting error for coordinates y
ΔZ	2n-dimensional vector of fitting error for coordinates x and y
ξ_i, ψ_i	coordinates of measurement points after transformation coordinates y to ψ
$\rho_{\xi\psi}$	correlation coefficient between ξ_i and ψ_i
$\Delta\xi$	n-dimensional vector of fitting error for coordinates ξ
$\Delta\Psi$	n-dimensional vector of fitting error for coordinates ψ
U_ξ	symmetric covariance matrix size n x n for variable ξ
U_Ψ	symmetric covariance matrix size n x n for variable ψ
$U_{\xi\Psi}$	in general, non-symmetric covariance matrix size n x n for variable ξ and ψ
X_p x_p	n-dimensional vector of coordinates of points lying on the fitting curve
ξ, ξ'	transformation function for variable x and first derivative of the function ξ
ψ, ψ'	transformation function for variable y and first derivative of the function ψ
ξ	n-dimensional vector of coordinates ξ
ψ	n-dimensional vector of coordinates ψ
R	correlator matrix size 2n x 2n for x and y
R^{-1}	inverse of correlator matrix size 2n x 2n
Q_{ij}	element of inverse of correlator matrix for i row and j column
P, Q	coefficients in canonical equation of third degree
I	identity matrix
I	measured current
I_0	saturation current of diode
ε	constant characteristic of a particular diode and operating temperature
U	measured voltage
R	resistance of resistor
x′, y′	coordinates in the local cartesian system of CNN machines
λ_x, λ_y	half axis of ellipse for coordinates x and y
R	environment for statistical programing
$r_{min,}\alpha_{min}, \varphi_{min}$	parameters of translation and rotation two-dimensional object (ellipse)

S, S_{ξ}, $S_{\xi\xi}$, S_{ψ} , $S_{\psi\psi}S_{\xi\psi}$	auxiliary coefficient defined by the new coordinates and the new inverse effective covariance matrix
H	tension of the conductor at the lowest point of the conduit
L	distance of the first column from the x coordinate corresponding to the lowest overhang
h_{min}	the lowest overhang