MathMet 2022
Paris | France | 2-4 November 2022

Matching the parabolic curve to both correlated coordinates of tested points by the linear regression method

2022

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1.Introduction

A few historical facts:

- The least squares method (abbreviation LSM) was introduced by most likely **Adrien-Marie Legendre** mathematician as early as 1805.

- **Carl Friedrich Gauss** german mathematician and physicist has already used LSM since 1794 (according to Wikipedia data) In addition, in 1809 he introduced the assumption of compatibility of the error distribution with normal distribution (Gaussian or Gaussian-Laplace distribution),

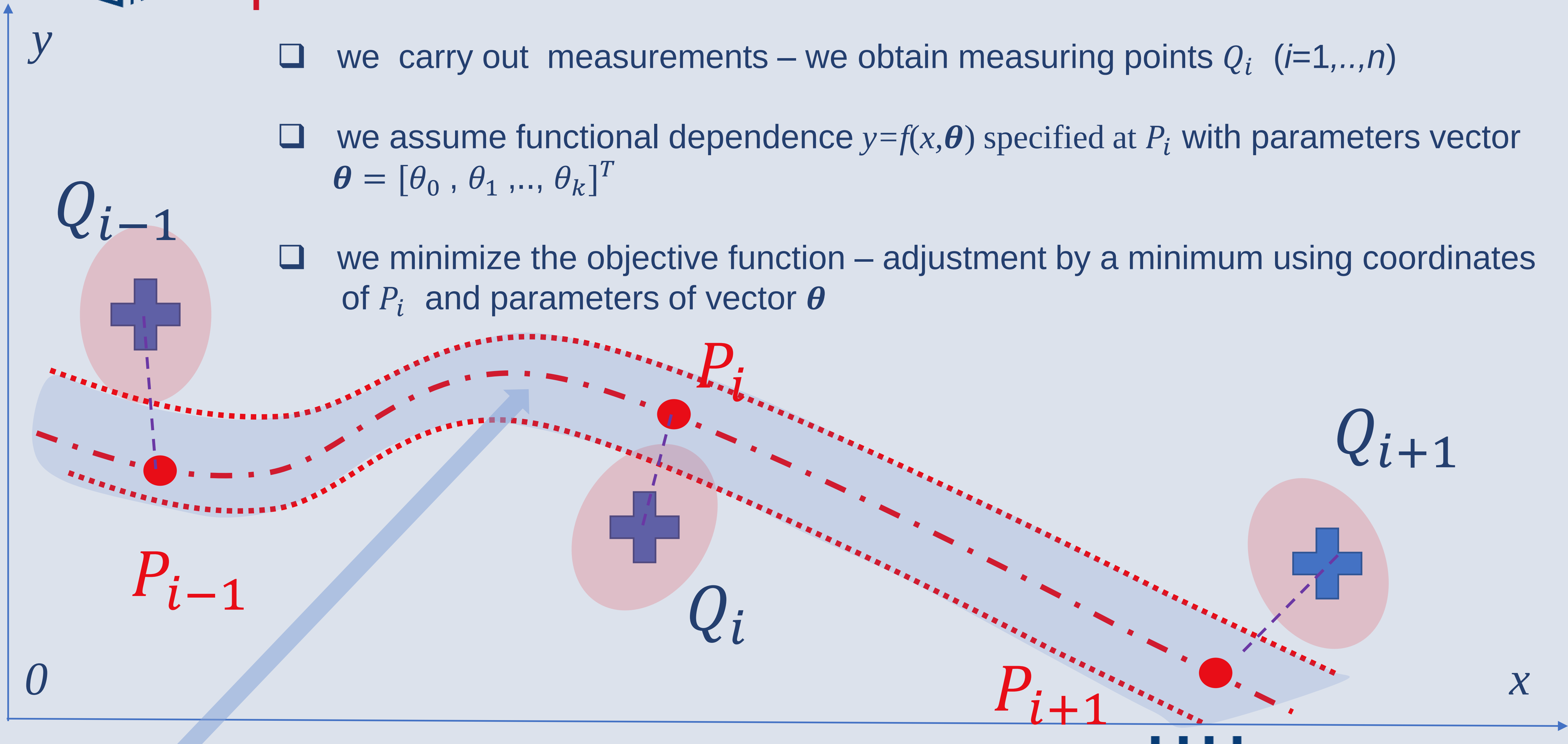
- **Auguste Bravais** – french physicist, in 1844 introduced the concept of correlation coefficient, later called the Pearson coefficient, from **Karl Pearson**, who at the turn of the nineteenth and twentieth centuries developed the theory of correlation as linear statistical relationships between variables.

Multivariate Gaussian (Normal) density distribution is defined as ($N=2n$):

$$g(\Delta \boldsymbol{Z}) = \frac{1}{(2\pi)^{N/2}\sqrt{\det(\boldsymbol{U}_Z)}} \cdot exp\left(-\frac{1}{2}\Delta \boldsymbol{Z}^{\mathrm{T}}\, \boldsymbol{U}_{\boldsymbol{Z}}^{-1}\Delta \boldsymbol{Z}\right)$$

2. Least squares method for linear regression

- we carry out measurements – we obtain measuring points Q_i (i=1,..,n)
- we assume functional dependence $y=f(x,\boldsymbol{\theta})$ specified at P_i with parameters vector $\boldsymbol{\theta} = [\theta_0 , \theta_1 ,.., \theta_k]^T$
- we minimize the objective function – adjustment by a minimum using coordinates of P_i and parameters of vector $\boldsymbol{\theta}$



$$y=f(x,\boldsymbol{\theta})=\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \ldots + \theta_k x^k$$

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3. Linear regression- notation and elementary equation

$\boldsymbol{Z}= [\boldsymbol{X}^{\mathrm{T}}, \boldsymbol{X}^{\mathrm{T}}]^{\mathrm{T}}$, $\boldsymbol{Z}=[z_1,\ldots, z_{2n}]^{\mathrm{T}} = [x_1,\ldots, x_n, y_1,\ldots, y_n]^{\mathrm{T}}$,

$\boldsymbol{Z_p}= [\boldsymbol{X_p^{\mathrm{T}}}, \boldsymbol{Y_p^{T}}]^{\mathrm{T}}$, $\boldsymbol{Z_p} =[z_{p1},\ldots, z_{p2n}]^{\mathrm{T}} = [x_{p1},\ldots, x_{pn}, y_{p1},\ldots, y_{pn}]^{\mathrm{T}}$,

$\Delta\boldsymbol{Z}= \boldsymbol{Z}-\boldsymbol{Z_p}$,

$$\boldsymbol{U_Z} = \begin{bmatrix} u^2(z_1) & \cdots & \rho_{1,2n}u(z_1)u(z_{2n}) \\ \vdots & \ddots & \vdots \\ \rho_{1,2n}u(z_1)u(z_{2n}) & \cdots & u^2(z_{2n}) \end{bmatrix} = \begin{bmatrix} \boldsymbol{U_X} & \boldsymbol{U_{XY}} \\ \boldsymbol{U_{XY}^T} & \boldsymbol{U_Y} \end{bmatrix} \Longrightarrow \boldsymbol{U_Z^{-1}} = \begin{bmatrix} \boldsymbol{U_{11}} & \boldsymbol{U_{12}} \\ \boldsymbol{U_{12}^T} & \boldsymbol{U_{22}} \end{bmatrix},$$

$$\phi(\Delta\boldsymbol{Z}) = \Delta\boldsymbol{Z}^{\mathrm{T}}\boldsymbol{U_Z^{-1}}\Delta\boldsymbol{Z} \rightarrow min$$

$$\phi(\boldsymbol{\Delta Z}) = \boldsymbol{\Delta Z^T}\ \boldsymbol{U_Z^{-1}}\boldsymbol{\Delta Z} = \Delta\boldsymbol{X}^T\boldsymbol{U}_{11}\Delta\boldsymbol{X} + \Delta\boldsymbol{X}^T\boldsymbol{U}_{12}\Delta\boldsymbol{Y} + \boldsymbol{\Delta Y^T}\boldsymbol{U_{12}^T}\Delta\boldsymbol{X} + \boldsymbol{\Delta Y^T}\boldsymbol{U}_{22}\boldsymbol{\Delta Y}$$

4. Types of linear regression due to the nature of the U_Z covariance matrix

$\boldsymbol{U_Z}=\sigma^2\boldsymbol{I}$

$u_x = u_y = \sigma$

I- identity matrix

1. TLS (Total Least Squares) - $u_x = u_y$ uncertainties may be known or unknown – extention of Ordinary Least Squares (OLS) by adding variable x

$$\phi(\Delta\boldsymbol{X},\Delta\boldsymbol{Y}) = \sum_{i=1}^{n} \Delta x_i^2 + \Delta y_i^2 \rightarrow min$$

$\rho_{ij} = 0$

$\boldsymbol{U_Z}$ - diagonal

2. WTLS-non correlated e.g. extension of Weighted Least Squares (WLS) by adding variable x and $u_{x_i} \neq u_{y_i}$ *i*=1,…,*n*

$$\phi(\Delta\boldsymbol{X},\Delta\boldsymbol{Y}) = \sum_{i=1}^{n} \frac{\Delta x_i^2}{u_{x_i}^2} + \frac{\Delta y_i^2}{u_{y_i}^2} \rightarrow min$$

3.WTLS (Weighted Total Least Squares) $\Delta\boldsymbol{Z} = [\Delta\boldsymbol{X}^{\boldsymbol{T}}, \Delta\boldsymbol{X}^{\boldsymbol{T}}]^{\boldsymbol{T}}$

$$\phi(\Delta\boldsymbol{Z}) = \Delta\boldsymbol{Z}^{\mathrm{T}}\boldsymbol{U}_{\boldsymbol{z}}^{-1}\Delta\boldsymbol{Z} \rightarrow min$$

5. Mathematical formulation of the optimalization problem (minimum ϕ)

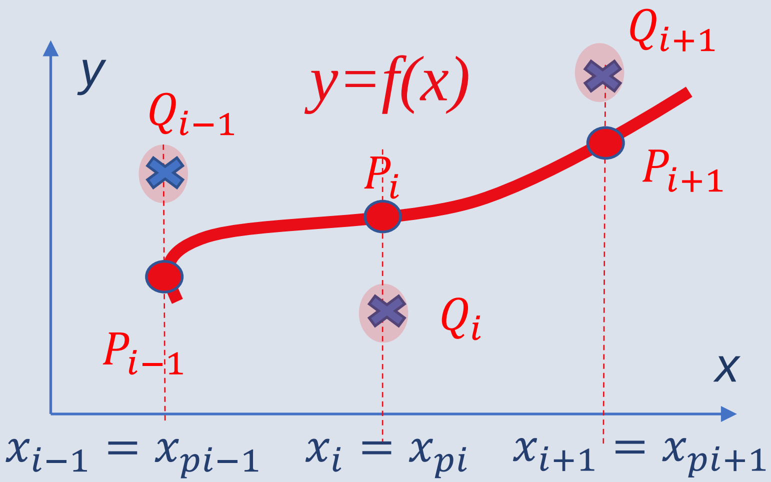
$$\begin{cases} \phi(\Delta \boldsymbol{Z}) = \Delta \boldsymbol{Z}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{z}}^{-1} \Delta \boldsymbol{Z} \rightarrow min \\ \boldsymbol{Y}_{\boldsymbol{p}} = \boldsymbol{F}(\boldsymbol{X}_{\boldsymbol{p}}, \boldsymbol{\theta}) = \begin{bmatrix} f(x_{p1}, \boldsymbol{\theta}) \\ \dots \\ f(x_{pk}, \boldsymbol{\theta}) \end{bmatrix} \\ \text{where } \boldsymbol{\theta} = [\theta_0, \dots, \theta_k]^{\mathrm{T}} \end{cases}$$

$$\boldsymbol{\nabla}_{\boldsymbol{X_p}} \phi = \boldsymbol{0}$$

$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} \phi = \boldsymbol{0}$$

$n+k+1$ – nonliner equations

6. Linear regression-special case



$\boldsymbol{U_X} \to \mathbf{0}, \boldsymbol{U_Z} \to \boldsymbol{U_Y}$ and $\boldsymbol{U_Y}$ – diagonal

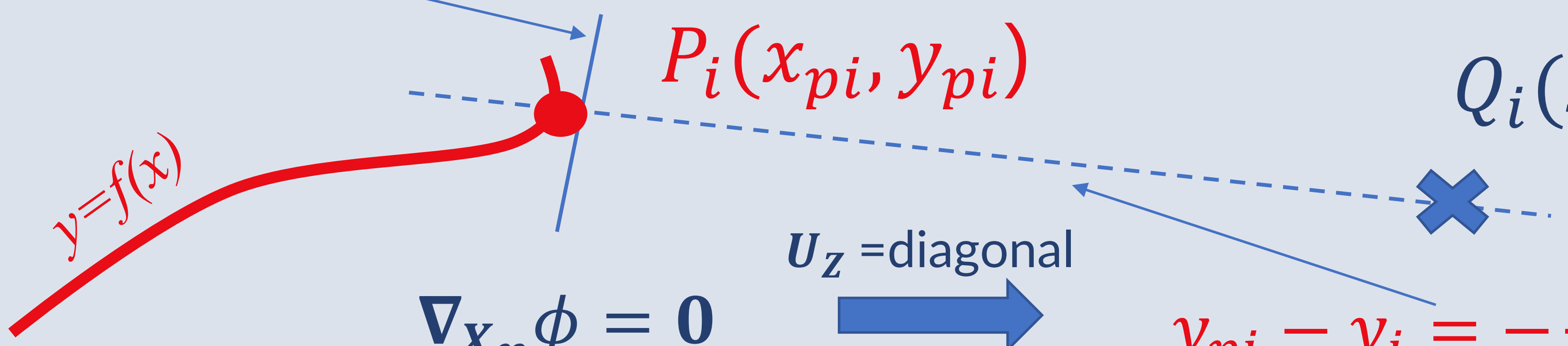
$$\cancel{\nabla_{\boldsymbol{x_p}} \phi = \mathbf{0}}$$

$$\downarrow$$

$$\boldsymbol{\nabla_\theta} \phi = \mathbf{0}$$

System of linear *k*+1- equations solved by determinant method.
This case will be used for validation of scripts, EXCEL macro.

7. The interpretation of minimalized condition $\nabla_{X_p}\phi = 0$



$$\nabla_{X_p}\phi = 0 \xrightarrow{\boldsymbol{U_Z}\text{ =diagonal}} y_{pi} - y_i = -\frac{1}{f'(y_{pi})}\frac{u^2(y_i)}{u^2(x_i)}(x_{pi} - x_i)$$

The crossing line between points Q_i and P_i is perpendicular to the tangential line at P_i if $u(y_i)$= $u(x_i)$ and $\boldsymbol{U_Z}$ is diagonal matrix

8. Linear regression for straight line

$$\begin{cases}\phi(\Delta \boldsymbol{Z}) = \Delta \boldsymbol{Z}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{z}}^{-1} \Delta \boldsymbol{Z} \rightarrow min \\ \boldsymbol{Y}_{\boldsymbol{p}} = a\boldsymbol{X}_{\boldsymbol{p}} + \boldsymbol{b}\end{cases} \Rightarrow \begin{cases}\phi(\Delta \boldsymbol{Z}) = \Delta \boldsymbol{Z}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{z}}^{-1} \Delta \boldsymbol{Z} \rightarrow min \\ \Delta \boldsymbol{Y} = \boldsymbol{a} \Delta \boldsymbol{X} + \boldsymbol{Y} - a\boldsymbol{X} - \boldsymbol{b}\end{cases}$$

$$\boldsymbol{\nabla}_{\boldsymbol{X}_{\boldsymbol{p}}} \phi = \boldsymbol{0} \quad - \boldsymbol{analytical\ solution}$$

Local minimum for $\boldsymbol{\Delta X}$ $(\boldsymbol{X}_{\boldsymbol{p}})$

$$\phi(\boldsymbol{\Delta X}, a, b) \geq [\boldsymbol{Y} - a\boldsymbol{X} - \boldsymbol{b}]^{T}\ \boldsymbol{U}_{\boldsymbol{Yeff}}^{-1}\ [\boldsymbol{Y} - a\boldsymbol{X} - \boldsymbol{b}]$$

9.Linear regression for straight line – inverse effective covariance matrix

$$\boldsymbol{U}_{\boldsymbol{Y}\boldsymbol{eff}}^{-1} = \boldsymbol{U}_{22} - \left(\boldsymbol{U}_{12}^{\mathrm{T}} + a\boldsymbol{U}_{22}\right)\boldsymbol{U}^{-1}(\boldsymbol{U}_{12} + a\boldsymbol{U}_{22}),$$

$$\boldsymbol{U} = a^{2}\boldsymbol{U}_{11} + a\left(\boldsymbol{U}_{12}^{T} + \boldsymbol{U}_{12}\right) + \boldsymbol{U}_{22} \ ,$$

Positive definite matrixes

Vectors of errors:

$$\boldsymbol{\Delta X}^{\mathrm{T}} = -\boldsymbol{E}\left(\boldsymbol{U}_{12}^{\mathrm{T}} + a\boldsymbol{U}_{22}\right)\boldsymbol{U}^{-1}, \qquad \boldsymbol{\Delta Y}^{\mathrm{T}} = \boldsymbol{E}\left(\boldsymbol{U}_{11} + a\boldsymbol{U}_{12}\right)\boldsymbol{U}^{-1}$$

$$\boldsymbol{E} = \boldsymbol{Y} - a\boldsymbol{X} - \boldsymbol{b}$$

10.1 One input parameter objective function

$S = \mathbf{1}^{\mathrm{T}}\, \boldsymbol{U}_{\boldsymbol{eff}}^{-1} \mathbf{1} = \sum_{i=1}^{n} \sum_{j=1}^{n} [\, u_{yeff}^{-1}]_{ij} > 0,\qquad S_x = \boldsymbol{X}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{Yeff}}^{-1} \mathbf{1} = \mathbf{1}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{Yeff}}^{-1} \boldsymbol{X},\ S_{xx} = \boldsymbol{X}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{Yeff}}^{-1} \boldsymbol{X},$

$S_y = \boldsymbol{Y}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{Yeff}}^{-1} \mathbf{1} = \mathbf{1}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{Yeff}}^{-1} \boldsymbol{Y},\ S_{yy} = \boldsymbol{Y}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{Yeff}}^{-1} \boldsymbol{Y},\ S_{xy} = \boldsymbol{X}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{Yeff}}^{-1} \boldsymbol{Y} = \boldsymbol{Y}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{Yeff}}^{-1} \boldsymbol{X}.$

Local minimum for b $\quad b = (S_y - aS_x)/S$ and then $\quad \phi(\boldsymbol{\Delta X}, a, b) \geq \phi(a, b) \geq \phi(a)$

$$\boxed{\phi(a) = a^2 \left(S_{\boldsymbol{xx}} - \frac{S_x^2}{S}\right) + 2\left(\frac{S_x S_y}{S} - S_{\boldsymbol{xy}}\right) a + S_{\boldsymbol{yy}} - \frac{S_y^2}{S}}$$

$$M(a) = \sum_{i=1}^{n} \frac{[(y_i - \bar{y}) - (x_i - \bar{x})]^2}{u^2(y_i) + a^2 u^2(x_i)} \qquad \boldsymbol{U}_{\boldsymbol{Yeff}\,\boldsymbol{ii}}^{-1} = w_i = \frac{1}{u^2(y_i) + a^2 u^2(y_i)} \qquad \bar{x} = \frac{\sum_{i=1}^{n} w_i x_i}{\sum_{i=1}^{n} w_i}, \qquad \bar{y} = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i},$$

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$\phi(a) = M(a)$ if $\boldsymbol{U}_{\mathrm{Z}}$ *diagonal*

10.2 One input parameter objective function

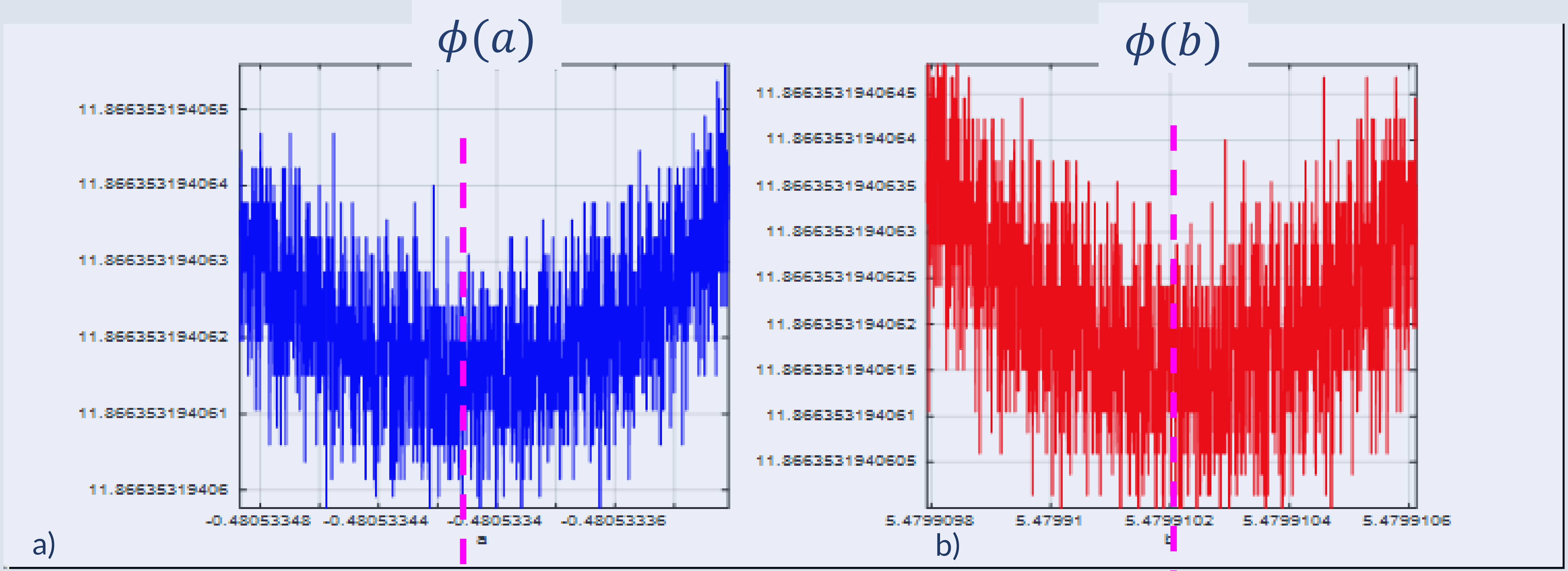


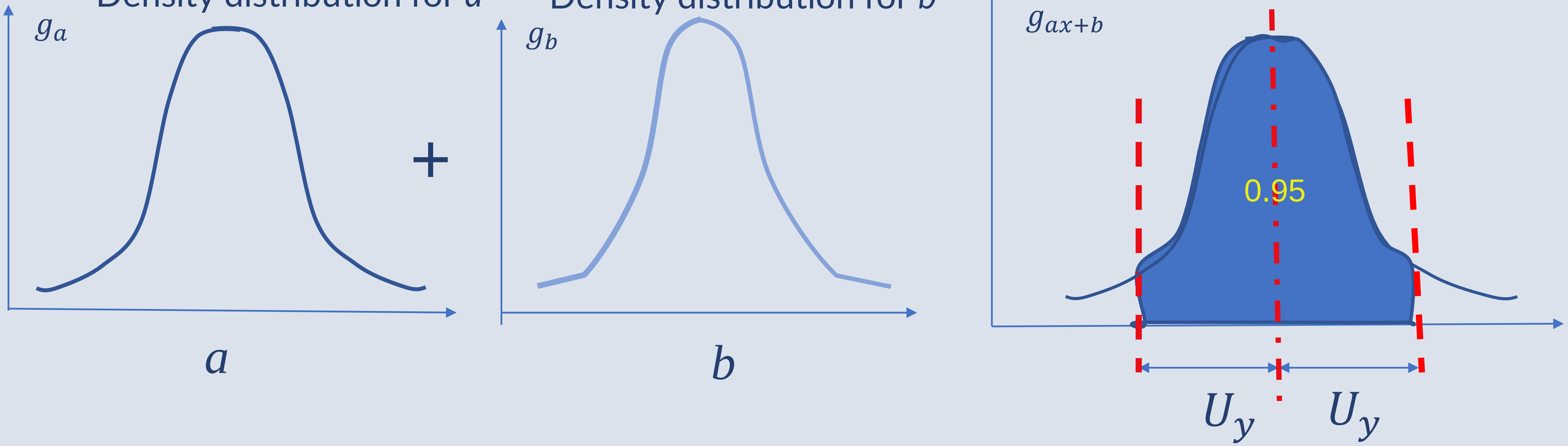
Fig. 1 Numerical characteristics of: a) $\phi(a)$ and *b)* $\phi(b)$, global min at ϕ = 11,8663531940615 for Pearson's Data with York's Weights (increment step $\Delta\, a{=}10^{-10}$).

11. 1 Coverage corridor of straight line regression

$$y = ax + b$$

At given x its sum of two distributions in general correlated –

Density distribution for a Density distribution for b Density distribution for $ax + b$

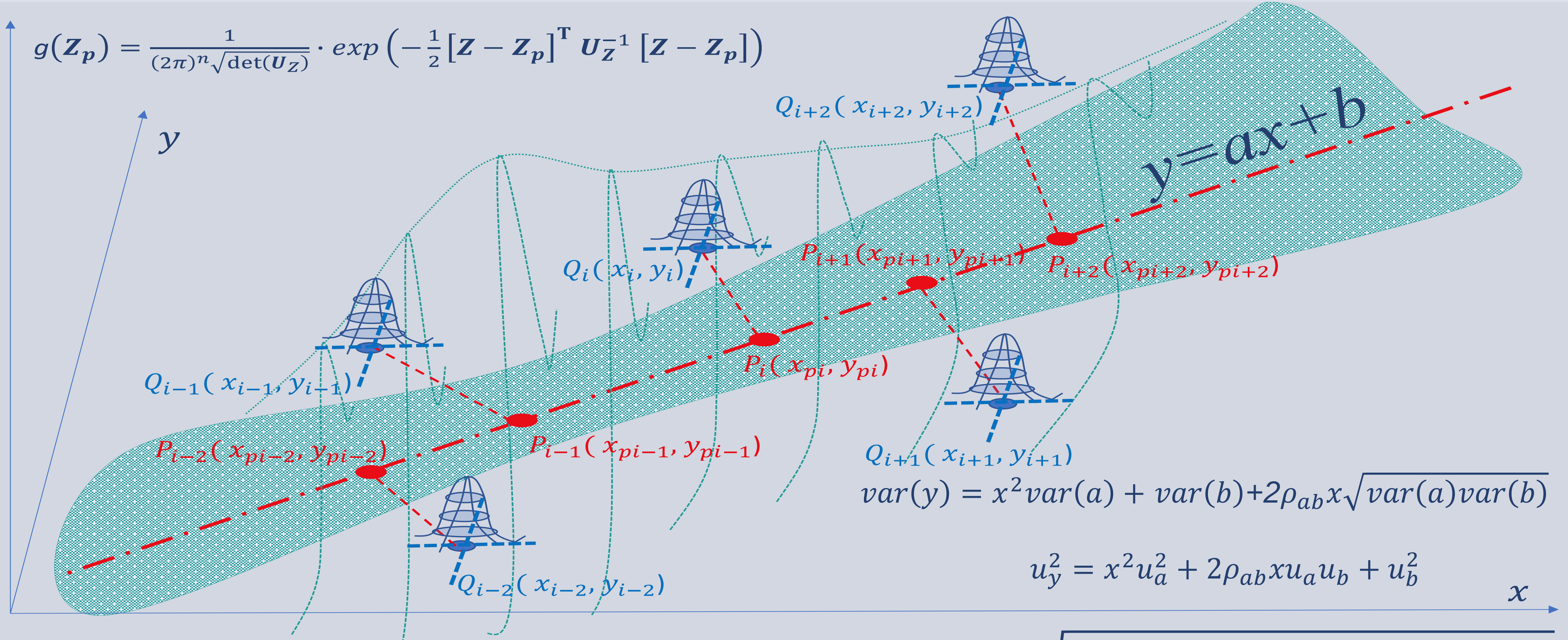


Propagation of distributions based on the simulation of samples – Monte Carlo Method

Cholesky decomposition $U_Z = HH^T$ $Z_S = Z + H^T D$ D – 2 x n dimensional vector of elements from N(0,1)

11. 2 Coverage corridor of straight line regression

$$g(\boldsymbol{Z_p}) = \frac{1}{(2\pi)^n\sqrt{\det(\boldsymbol{U_Z})}} \cdot exp\left(-\frac{1}{2}\left[\boldsymbol{Z}-\boldsymbol{Z_p}\right]^{\mathrm{T}} \boldsymbol{U_Z^{-1}} \left[\boldsymbol{Z}-\boldsymbol{Z_p}\right]\right)$$



$$var(y) = x^2 var(a) + var(b) + 2\rho_{ab} x\sqrt{var(a)var(b)}$$

$$u_y^2 = x^2u_a^2 + 2\rho_{ab}xu_au_b + u_b^2$$

$$\boldsymbol{U_{ab}} = \boldsymbol{C\,U_Z\,C^{\mathrm{T}}}, \boldsymbol{U_{ab}} = \begin{bmatrix} u_a^2 & \rho_{ab}u_au_b \\ \rho_{ab}u_au_b & u_b^2 \end{bmatrix}, \quad U_y = t_{1-\alpha/2,n-2}\sqrt{x^2u_a^2 + 2\rho_{ab}xu_au_b + u_b^2}$$

LPU –Law of Propagation of Uncertainty

12.A new proposed estimated method for more complicated fitting curve

$$\begin{cases} \phi(\Delta \boldsymbol{Z}) = \Delta \boldsymbol{Z}^{\mathrm{T}} \boldsymbol{U}_{\boldsymbol{z}}^{-1} \Delta \boldsymbol{Z} \rightarrow min \\ \boldsymbol{Y}_{\boldsymbol{p}} = \boldsymbol{F}(\boldsymbol{X}_{\boldsymbol{p}}, \boldsymbol{\theta}) \end{cases} \quad => \quad \boldsymbol{X}_{\boldsymbol{p}} \Rightarrow \boldsymbol{\xi}(\boldsymbol{X}_{\boldsymbol{p}} + \boldsymbol{\nu})$$

$$\boldsymbol{Y}_{\boldsymbol{p}} = \theta_1 \cdot \boldsymbol{\xi}(\boldsymbol{X}_{\boldsymbol{p}} + \boldsymbol{\nu}) + \boldsymbol{\theta}_{\boldsymbol{o}}$$

$$\boldsymbol{Y}_{\boldsymbol{p}} = \boldsymbol{F}(\boldsymbol{X}_{\boldsymbol{p}}, \boldsymbol{\theta}) = \begin{bmatrix} f(x_{p1}, \boldsymbol{\theta}) \\ \dots \\ f(x_{pk}, \boldsymbol{\theta}) \end{bmatrix} \longrightarrow f(x, \theta_0, \theta_1, \nu) = \theta_1 \xi(x + \nu) + \theta_0$$

Assuming very small matching errors $\Delta\xi_i = \xi'(x_i + \nu)\Delta x_i$ and the fulfillment of the law of propagation of uncertainty $u(\xi_i) \approx |\frac{\partial \xi}{\partial x_i}| u(x_i)$ the above approximate relationship is valid because of both sides multiplication by a unit matrix leads to:

13.Derivation of the new proposed method

$$\phi(\Delta X,\Delta Y) = [\Delta \boldsymbol{X}^{\mathrm{T}},\Delta \boldsymbol{Y}^{\mathrm{T}}]\boldsymbol{L}\boldsymbol{L}^{-1}\begin{bmatrix} \boldsymbol{U}_X & \boldsymbol{U}_{XY} \\ \boldsymbol{U}_{XY}^T & \boldsymbol{U}_Y \end{bmatrix}^{-1}\boldsymbol{L}^{-1}\boldsymbol{L}[\Delta \boldsymbol{X}^{\mathrm{T}},\Delta \boldsymbol{Y}^{\mathrm{T}}]^{\mathrm{T}} =$$

$$[\Delta \boldsymbol{X}^{\mathrm{T}},\Delta \boldsymbol{Y}^{\mathrm{T}}]\boldsymbol{L}\left[\boldsymbol{L}\begin{bmatrix} \boldsymbol{U}_X & \boldsymbol{U}_{XY} \\ \boldsymbol{U}_{XY}^T & \boldsymbol{U}_Y \end{bmatrix}\boldsymbol{L}\right]^{-1}\boldsymbol{L}[\Delta \boldsymbol{X}^{\mathrm{T}},\Delta \boldsymbol{Y}^{\mathrm{T}}]^{\mathrm{T}} \approx [\Delta \boldsymbol{\xi}^{\mathrm{T}},\Delta \boldsymbol{Y}^{\mathrm{T}}]\begin{bmatrix} \boldsymbol{U}_\xi & \boldsymbol{U}_{\xi Y} \\ \boldsymbol{U}_{\xi Y}^T & \boldsymbol{U}_Y \end{bmatrix}^{-1}[\Delta \boldsymbol{\xi}^{\mathrm{T}},\Delta \boldsymbol{Y}^{\mathrm{T}}]^{\mathrm{T}} = \phi_\xi\,(\Delta \boldsymbol{\xi},\Delta \boldsymbol{Y})$$

when we define the elements of the diagonal matrix (2*n*x2*n*) :

$$\boldsymbol{L} = \begin{bmatrix} \xi'(x_1+\nu) & 0 & 0 & 0 & 0 & 0 \\ 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & \xi'(x_n+\nu) & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

and the first *n* diagonal elements are equal to: $\boldsymbol{L}_{ii} = \xi'(x_i+\nu) \neq 0$ if $i \leq n$ and $\boldsymbol{L}_{ii} = 1$ if $i > n$ the others are ones. Of course $\boldsymbol{L}\boldsymbol{L}^{-1} = \boldsymbol{L}^{-1}\boldsymbol{L} = \boldsymbol{I}$ and therefore from LPU $u(\xi_i) \approx |\frac{\partial \xi}{\partial x_i}|\, u(x_i)$ and hence

$$\phi(\Delta \boldsymbol{Z}) = \Delta \boldsymbol{Z}\,\boldsymbol{U}_z^{-1}\Delta \boldsymbol{Z}^{\mathrm{T}} \approx \Delta \boldsymbol{Z}_\xi\,\boldsymbol{U}_{\xi Z}^{-1}\,\Delta \boldsymbol{Z}_\xi{}^{\mathrm{T}} = \phi_\xi\,(\Delta \boldsymbol{Z}_\xi) \quad \text{where } \Delta \boldsymbol{Z}_\xi = [\Delta \boldsymbol{\xi}^{\mathrm{T}},\Delta \boldsymbol{Y}^{\mathrm{T}}]^{\mathrm{T}}$$

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14.Limitations of the new proposed method

1) $f(x, \theta_0, \theta_1, v) = \theta_1 \xi(x+v) + \theta_0$ - the function f must be represented by only three parametrs θ_0, θ_1, v

2) $x_i \longrightarrow \xi_i$, $\xi(x+v)$, $\xi'(x_i + v) = \frac{d\xi}{dx}|_{x=x_i} = \frac{\partial \xi}{\partial x}|_{x=x_i} \neq 0$

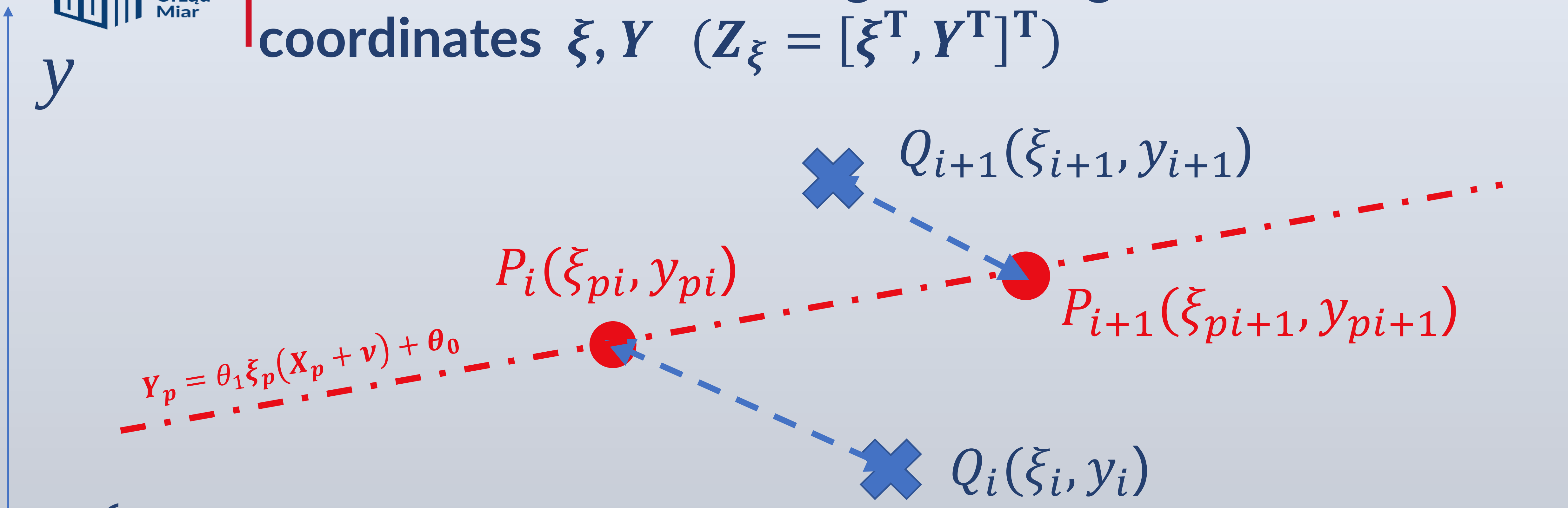
3) $\Delta\xi_i \approx \xi'(x_i+v)\Delta x_i$ the law of propagation of errors

4) $u(\xi_i) \approx |\frac{\partial \xi}{\partial x}|_{x=x_i} u(x_i)$ the law of propagation of uncertainty

$$\boldsymbol{U_Z, U_X, U_Y, U_{XY}, Z \longrightarrow U_{\xi Z} = L\, U_Z L,\ U_\xi,\ U_Y,\ U_{\xi Y},\ Z_\xi}$$

$$\phi \approx \phi_\xi$$

15.New method as a stright line regression in the new coordinates ξ, Y $\left(Z_\xi = [\xi^{\mathrm{T}}, Y^{\mathrm{T}}]^{\mathrm{T}}\right)$



$$\begin{cases} \phi_\xi = \Delta \boldsymbol{Z}_\xi{}^T \boldsymbol{U}_{\xi Z}^{-1} \Delta \boldsymbol{Z}_\xi \rightarrow min \\ \boldsymbol{Y}_p = \theta_1 \xi_p + \boldsymbol{\theta}_0 \end{cases}$$

$\nabla_{\xi_p} \phi_\xi = \mathbf{0}$ – *analitycally*

θ_0, θ_1,v – *minimalization*

16. Numerical scheme – algorithm for manually fitting or hybrid method with matlab,R scripts or macro EXCEL

1) Choose value of ν and set up interval range $[\nu_{low}\ ,\nu_{high}]$ for ν for example $\nu = \nu_{low} < \nu_{high}$,

2) Calculate the new coordinates for measurements points $\xi(x_i + \nu)$ and the new uncertainties $u(\xi_i) \approx |\frac{\partial \xi}{\partial x_i}|\, u(x_i)$= $|\xi'(x_i + \nu)|u(x_i)$ and finally the new matrix $\boldsymbol{U_{\xi Z}} = \boldsymbol{L U_Z L}$,

3) Determine characteristic $\phi(\theta_1, \nu_{low})$ at few series points with step $\Delta\theta_1$ between $\theta_{1low} < \theta_{1high}$ to find local minimum ϕ=local_min for θ_1 and determine θ_0= $(S_y(\theta_1, \nu_{low}) - \theta_1 S_x(\theta_1, \nu_{low}))/S(\theta_1, \nu_{low})$,

4) Calculate the new parameter ν=ν_{low} + $i\ \Delta\nu$ with step $\Delta\nu$ to find global minimum for $\phi(\theta_{1min}, \nu_{min})$ =global_min monitoring the characteristic $\phi(\theta_1, \nu)$ at any ν.

In Excel workbook it can be changing value ν by button of control Active X and simultaneously observing characteristic $\phi(\theta_1, \nu)$ sampled on the few points θ_1= θ_{1low}+$j\ \Delta\theta_1$ (in our simulations we used eight points for θ_1) to obtain global minimum.

17.1 LPU for coverage corridor – determining numerically matrix C of sensitivity coefficients

$$\boldsymbol{U}_{\theta_1\theta_0} = \begin{bmatrix} u_{\theta_1}^2 & \rho_{\theta_0\theta_1} u_{\theta_0} u_{\theta_1} \\ \rho_{\theta_0\theta_1} u_{\theta_0} u_{\theta_1} & u_{\theta_0}^2 \end{bmatrix} = \boldsymbol{C}\,\boldsymbol{U}_{\xi Z}\,\boldsymbol{C}^{\mathrm{T}}$$

where $\boldsymbol{U}_{\theta_1\theta_0}$ covariance matrix for straight line regression parameters $u_{\theta_0}, u_{\theta_1}, \rho_{\theta_1\theta_0}$- uncertainty of its parameters θ_0 and θ_1 and their correlation coefficient ρ, **C** – matrix of sensitivity coefficients of the form:

$$\boldsymbol{C} = \left[\frac{\partial\theta_1}{\partial \boldsymbol{Z}_\xi}, \quad \frac{\partial\theta_0}{\partial \boldsymbol{Z}_\xi}\right]^{\mathrm{T}} = \begin{bmatrix} \frac{\partial\theta_1}{\partial z_{\xi 1}}, & \dots, & \frac{\partial\theta_1}{\partial z_{\xi 2n}} \\ \frac{\partial\theta_0}{\partial z_{\xi 1}}, & \dots, & \frac{\partial\theta_0}{\partial z_{\xi 2n}} \end{bmatrix}$$

The matrix of sensivity coefficient **C** is determined numerically by differences quotients which estimated the first partial derivatives:

$$\frac{\partial\theta_{1_N}}{\partial z_{\xi i}} \cong \frac{\theta_{1_N}\left(z_{\xi i_i} + h\right) - \theta_{1_N}\left(z_{\xi i} - h\right)}{2h}, \qquad \frac{\partial\theta_{0_N}}{\partial \xi z_i} \cong \frac{\theta_{0_N}\left(z_{\xi i} + h\right) - \theta_{0_N}\left(z_{\xi i} - h\right)}{2h}$$

where: $\theta_{1_N}$and θ_{0_N} are values determined numerically from the modification of the coordinates of the measuring points $\xi(x_i + v)$ and y_i by $\pm\, h$.

17.2 LPU for coverage corridor – determining numerically matrix C of sensitivity coefficients

$$\boldsymbol{U}_{\theta_{1N}\theta_{0N}} \approx \begin{bmatrix} u^2_{\theta_{1N}} & \rho_{\theta_{01N}} u_{\theta_{0N}} u_{\theta_{1N}} \\ \rho_{\theta_{01N}} u_{\theta_{0N}} u_{\theta_{1N}} & u^2_{\theta_{0N}} \end{bmatrix} = \begin{bmatrix} \frac{\partial \theta_{1N}}{\partial z_{\xi 1}}, & \frac{\partial \theta_{1N}}{\partial z_{\xi 2n}} \\ \cdots & \cdots \\ \frac{\partial \theta_{0N}}{\partial z_{\xi 1}}, & \frac{\partial \theta_{0N}}{\partial z_{\xi 2n}} \end{bmatrix} \boldsymbol{U}_{\xi Z} \begin{bmatrix} \frac{\partial \theta_{1N}}{\partial z_{\xi 1}}, & \frac{\partial \theta_{0N}}{\partial z_{\xi 1}} \\ \cdots & \cdots \\ \frac{\partial \theta_{1N}}{\partial z_{\xi 2n}}, & \frac{\partial \theta_{0N}}{\partial z_{\xi 2n}} \end{bmatrix}$$

where the uncertainties of the intercept u_{θ_0} and slope u_{θ_1} are determined by the propagation method uncertainty by numerical determination of the sensitivity matrix and multiplication by the covariance matrix $\boldsymbol{U}_{\xi Z}$:

$$u_y \approx \sqrt{[\xi(x+v_{min})]^2 u^2_{\theta_{1N}} + 2|\xi(x+v_{min})| \rho_{\theta_{10N}} u_{\theta_{0N}} u_{\theta_{1N}} + u^2_{\theta_{0N}}}$$

As a result, after taking into account the calculated parameters of the curve, the uncertainty band around the adjusted curve is expressed by the equation

$$y \approx \theta_{1minN} \xi(x+v_{min}) + \theta_{0minN} \pm t_{1-\alpha/2,n-2} \sqrt{[\xi(x+v_{min})]^2 u^2_{\theta_{1N}} + 2|\xi(x+v_{min})| \rho_{\theta_{10N}} u_{\theta_{0N}} u_{\theta_{1N}} + u^2_{\theta_{0N}}}$$

18. Fitting parabolic curve (example)

In the special case of matching with a second degree curve:

$$y = Ax^2 + Bx + C = A\left(x + \frac{B}{2A}\right)^2 + C - B^2/4A$$

is obtained: $\xi = (x + v_{min})^2$, $\theta_{1min} = A$, $v_{min} = B/2A$ and $\theta_{0min} = C - B^2/4A$.

So $A = \theta_{1min}$, $B = 2Av_{min} = 2\theta_{1min}v_{min}$, $\theta_{0min} = C - \frac{B^2}{4A}$, and $C = \theta_{0min} + \theta_{1min}v_{min}^2$

Uncertainty $u(\xi_i) \approx \left|\frac{\partial\xi}{\partial x_i}\right| u(x_i) = 2|x_i + v_{min}|u(x_i) \neq 0$ $i=1,\ldots,n$ and hence the uncertainty corridor

is expressed as follows:

$$y \approx \theta_{1min}(x + v_{min})^2 + \theta_{0min} \pm t_{t_{1-\alpha/2,n-2}}\sqrt{(x + v_{min})^4 u_{\theta_1}^2 + 2(x + v_{min})^2 \rho_{\theta_{10}} u_{\theta_1} u_{\theta_0} + u_{\theta_0}^2}$$

If sensitve coefficients are numerically zero it can be applied Monte Carlo method with Cholesky decomposition.

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19. Three numerical cases

1) Fitting to ideal curve:

$$y = 0,2(x-3)^2 + 1 = 0,2x^2 - 1,2x + 2,8$$

with relative uncertainty 2 % of measurement points without correlations

2) Fitting to ideal curve

$$y = 0,2(x-3)^2 + 1 = 0,2x^2 - 1,2x + 2,8$$

with relative uncertainty 2 % of measurement points with correlations ***Ux, Uy***(0,2) , ***Uxy*** (-0,2)

Table 1. Slightly scattered measuring points

x	1	2	3	4	5	6	7	8	9	10
y	1,81	1,19	0,99	1,27	1,79	2,7	4,19	4,9	8,19	9,29

3) Fitting to the temperature dependence of density of reference material (CRM): $At^2 + Bt + C$

Table 2. Measurement of density (CRM) as function of temperature

t[°C]	15	20	30	35	40	45	50
density [kg/m3]	1254,75	1249,51	1239,04	1233,8	1228,56	1223,32	1218,08

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19.1. Fitting to ideal curve with the same relative uncertainty $\delta_x = \delta_y = 2$ % without correlations

a) $\phi(\theta_1)$, θ_{1min}=0,1881

b) $\phi(\theta_0)$, θ_{0min}=1,0127

Fig. 2 Numerical characteristics of: a) $\phi(\theta_1)$ and *b)* $\phi(\theta_0)$ for v_{min}=-3,0 , global min at $\phi \approx \phi_\xi$=16,8203 $\Delta v = 0{,}1$.

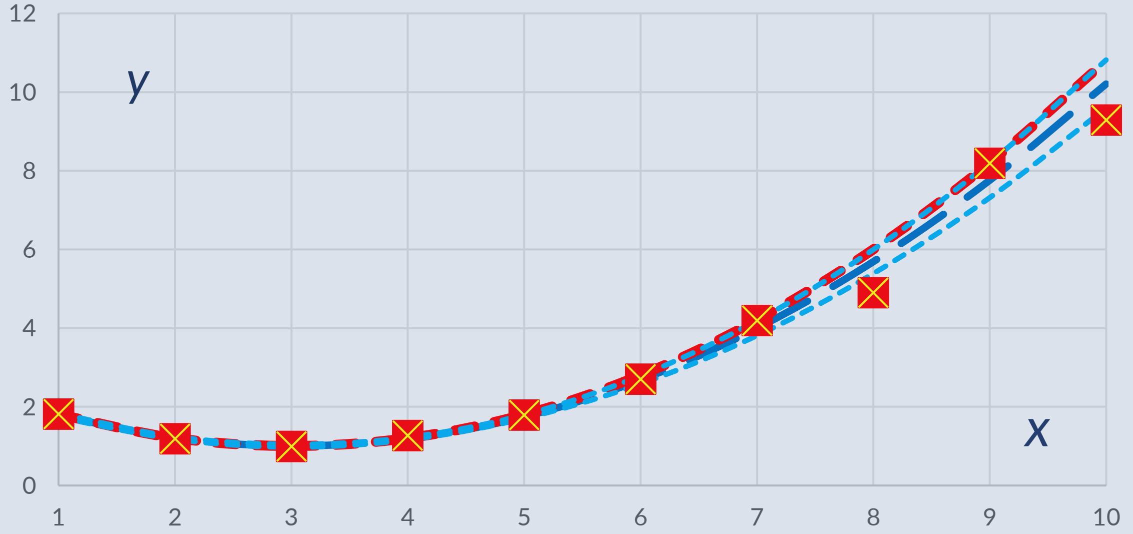

Fig. 3 Measurements points, ideal parabola:
$y = 0{,}2(x-3)^2 + 1 = 0{,}2x^2 - 1{,}2x + 2{,}8$ - red,
and curve adjusted to:
$y = 0{,}188x^2 - 1{,}140x + 2{,}732$ - blue,
and coverage corridor – light blue (0.95).

19.2 Fitting to ideal curve with the same relative uncertainty $\delta_x = \delta_y = 2$ % with correlations

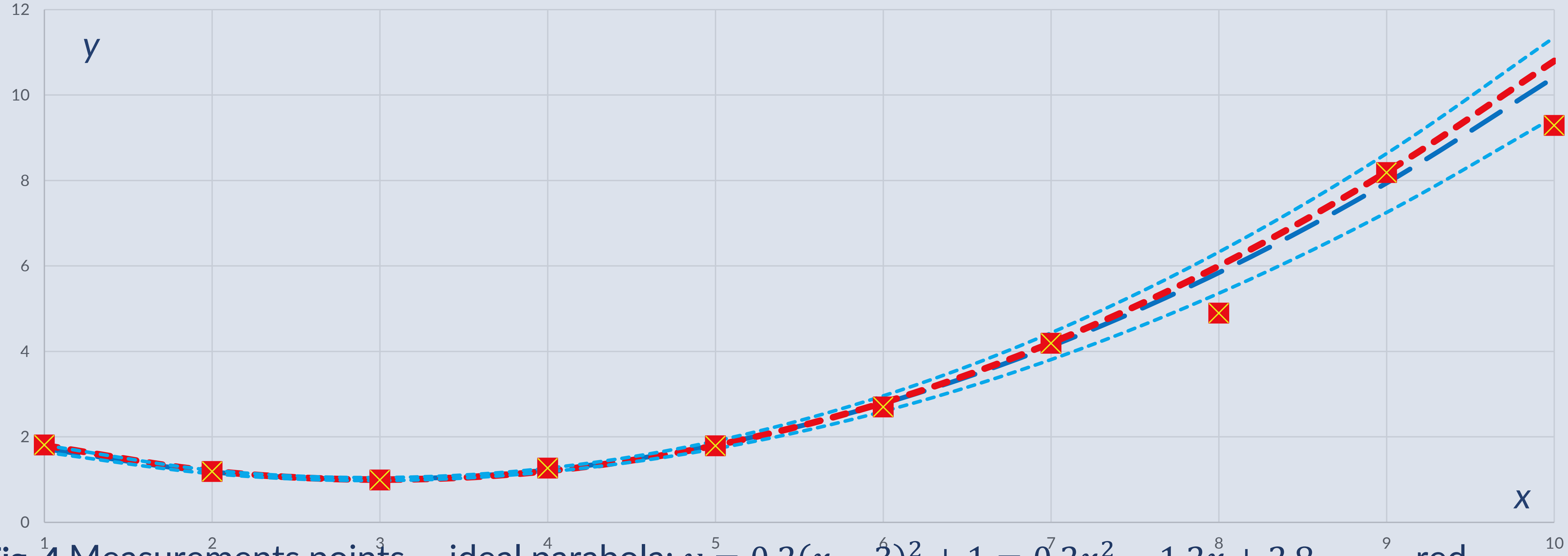

Fig. 4 Measurements points, ideal parabola: $y = 0{,}2(x-3)^2 + 1 = 0{,}2x^2 - 1{,}2x + 2{,}8$ - red, and curve adjusted to: $y = 0{,}1902x^2 - 1{,}141x + 2{,}726$ - blue, and coverage corridor – light blue (0.95), correlated variables ***Ux,(0,2) Uy***(0,2) , ***Uxy*** (-0,2) , v_{min} =-3,0, Δν=0,1, θ_{1min} =0,1902, θ_{0min} =1,0144, global min at $\phi \approx \phi_\xi$=20,8236.

19.3 Matching the parabolic curve to a certified standard CRM 2,4-Dichlorotoluen

Fitting to the dependence of density of Certified Refrence Materials (CRM) as function of temperature:

$$At^2 + Bt + C.$$

Density C7 H6 Cl2 2,4-Dichlorotoluen 1.251 g/mL at 25 °C, liquid 2,4-Dichlorotoluen 1250 kg/m3 standard uncertainty: for density 0,025 kg/m3, for temperature 0,29 °C .

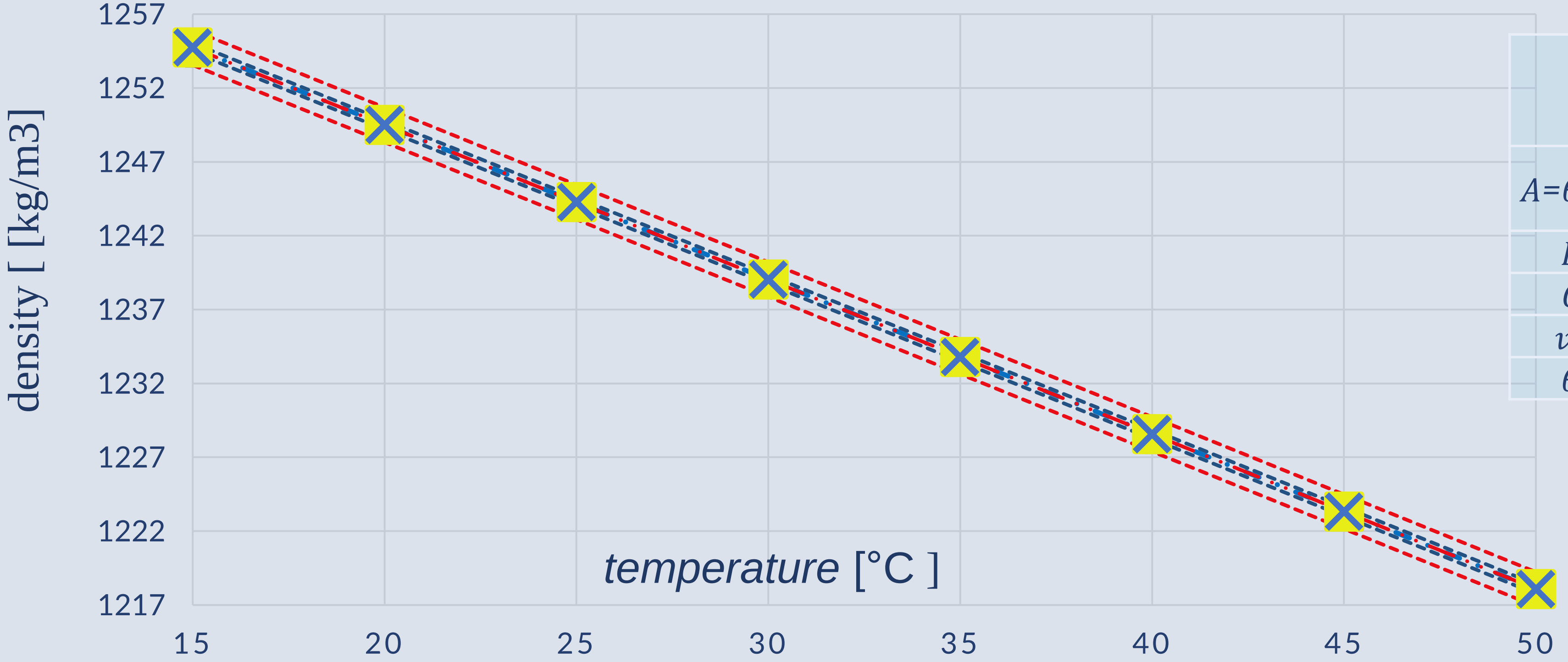

Fig. 4 Measurements points, density as function of temperature, global min at $\phi \approx \phi_\xi < 0.01$ coverage corridor (0.95) for correlated (red) and non correlated (blue) model.

Table 3. Results of simulations

	Non correlated	Correlated ***Ux*,*Uy***(0,2) ***Uxy***(-0,2)
$A=\theta_{1min}$	-5,55899E-05	-5,62000E-05
B	-1,04409	-1,04430
C	1270,42	1270,42
v_{min}	9391,6	9298,6
θ_{0min}	6155,44	6123,87

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20. Summary

A method of adjusting the parameters of the assumed curve to measurement points using the linear regression method is presented.

The method consists the adjustment of nonlinear curve to measurement points with coordinates (x, y) in a new coordinate system, in which the x coordinate is replaced by ξ (x+v) and as a result, due to the propagation of errors and the resulting of law of propagation of uncertainty, lead to the approximation of the criterion function by minimization like in the straight line regression.

During the minimization of the criterion function for adjusting the curve, the covariance matrix is also modified – the change of uncertainty for the coordinate ξ(x+v). Uncertainty corridors can be determined from the law of propagation of uncertainty (LPU)– numerically determined from the differences quotient for sensitivity coefficients. If their values are numerically close to zero, the uncertainty corridor can be determined by the Monte Carlo method using the generation of samples from the normal distribution N(0.1) and the decomposition of the covariance matrix by the Cholesky method determine both density distributions of the slope coefficient and the intercept. An algorithm was used to minimize the objective function dependent only on the slope of straight line and position constant.

The method was successfully tested for the simulation of a quadratic function with slightly scattered measurement points measured with uncertainties of 2 % for correlated and uncorrelated quantities as well as for CMR material 2,4-Dichlorotoluene.

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Thank You For Attention