Metoda nejmenších čtverců

$x_1, x_2, \ldots, x_N$

$y_1, y_2, \ldots, y_N$ $\quad y_i \in N(\lambda_i, \sigma_i)$ • experimentální data

x – nezávislá proměnná

y – závislá proměnná

$\lambda(\boldsymbol{x}, \boldsymbol{\theta}) \qquad \boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_m)$ • modelová funkce

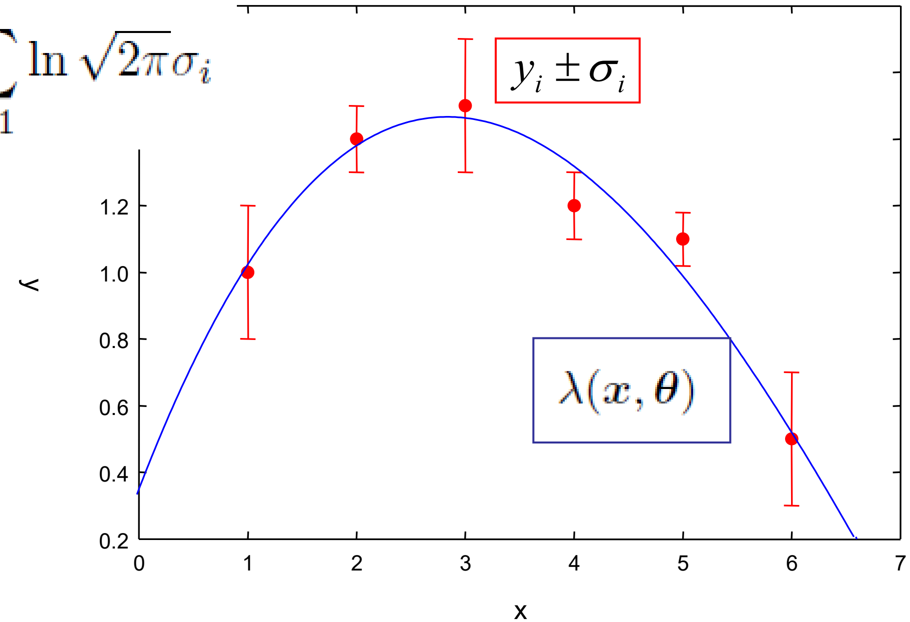
$$L(\boldsymbol{\theta}|\boldsymbol{y}) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left[-\frac{(y_i - \lambda(x_i|\boldsymbol{\theta}))^2}{2\sigma_i^2}\right]$$

• věrohodnostní funkce

$$\ln L(\boldsymbol{\theta}|\boldsymbol{y}) = -\sum_{i=1}^{N} \frac{(y_i - \lambda(x_i|\boldsymbol{\theta}))^2}{2\sigma_i^2} - \sum_{i=1}^{N} \ln \sqrt{2\pi}\sigma_i$$

$$\chi^2(\boldsymbol{\theta}|\boldsymbol{y}) = \sum_{i=1}^{N} \frac{(y_i - \lambda(x_i|\boldsymbol{\theta}))^2}{\sigma_i^2}$$

• minimalizace χ^2



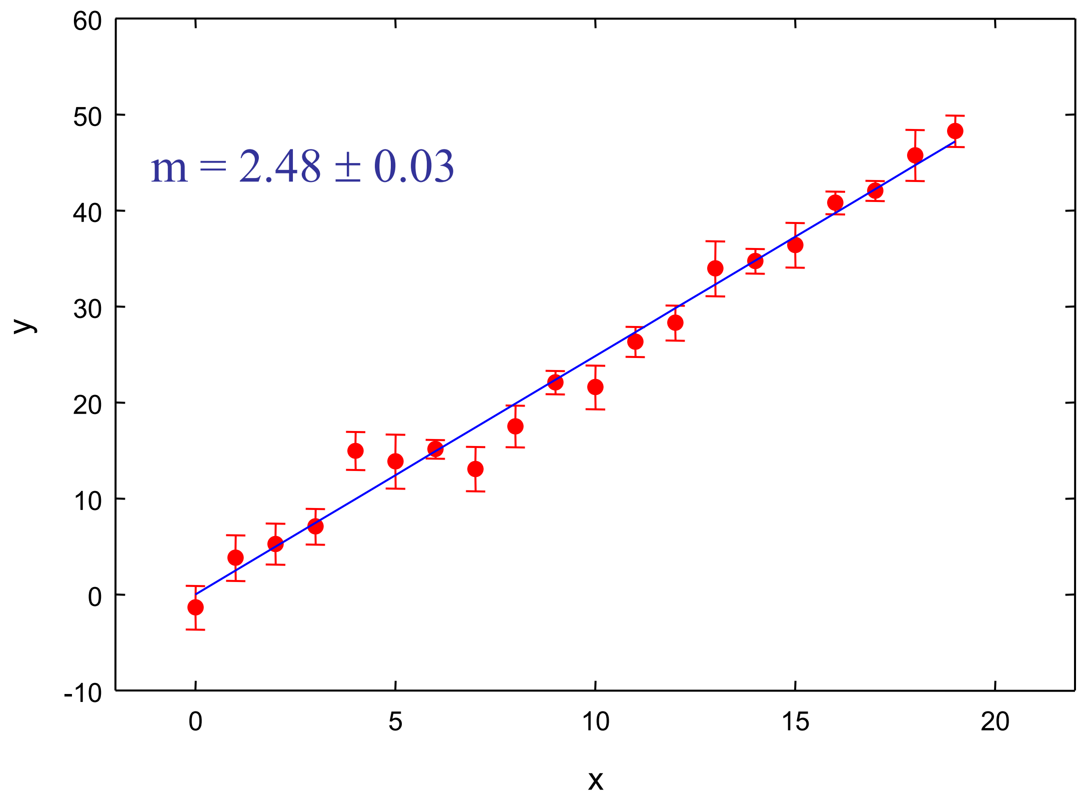
Metoda nejmenších čtverců – přímá úměrnost $y = m\,x$

$$\lambda(x|m) = mx$$

$$\chi^2(m|\boldsymbol{y}) = \sum_{i=1}^{N} \frac{(y_i - mx_i)^2}{\sigma_i^2}$$

$$\hat{m} = \frac{\sum_{i=1}^{N} \frac{x_i y_i}{\sigma_i^2}}{\sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2}} = \frac{\langle xy \rangle}{\langle x^2 \rangle}$$

$$\sigma_{\hat{m}} = \frac{1}{\sqrt{\sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2}}} = \frac{1}{\sqrt{\langle x^2 \rangle}}$$



označení: $\langle a \rangle \equiv \sum_{i=1}^{N} \frac{a_i}{\sigma_i^2}$

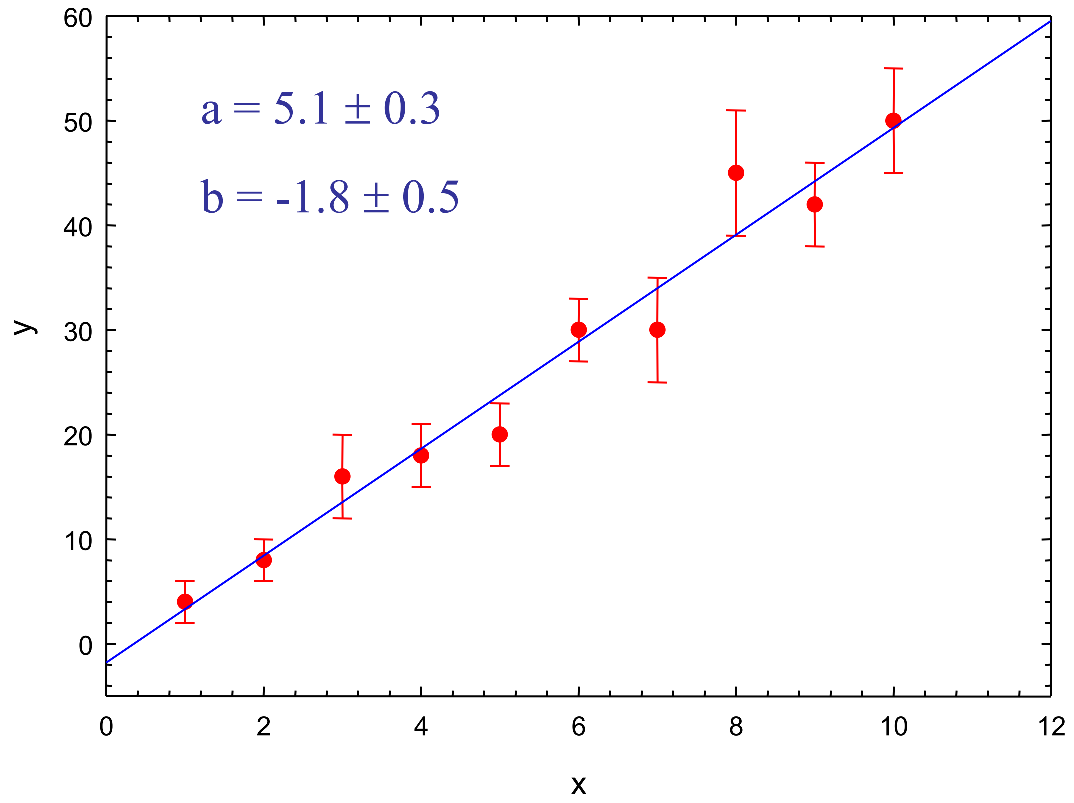
Metoda nejmenších čtverců – lineární regrese $y = a\,x + b$

$$\lambda(x|a,b) = ax + b$$

$$\chi^2(a,b|\boldsymbol{y}) = \sum_{i=1}^{N} \frac{(y_i - ax_i - b)^2}{\sigma_i^2}$$

$$\hat{a} = \frac{\langle 1\rangle\langle xy\rangle - \langle x\rangle\langle y\rangle}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2}$$

$$\hat{b} = \frac{\langle y\rangle\langle x^2\rangle - \langle x\rangle\langle xy\rangle}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2}$$



označení: $\langle a\rangle \equiv \sum_{i=1}^{N} \frac{a_i}{\sigma_i^2}$

Metoda nejmenších čtverců – vyjádření pomocí matic

$x_1, x_2, \ldots, x_N$

$y_1, y_2, \ldots, y_N \qquad y_i \in N(\lambda_i, \sigma_i)$

$\lambda(\boldsymbol{x}, \boldsymbol{\theta}) \qquad \boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_m)$ lineární model

$$\lambda(x_i|\boldsymbol{\theta}) = \sum_{j=1}^{m} a_j(x_i)\theta_j = \sum_{j=1}^{m} A_{ij}\theta_j$$

$$\boldsymbol{\lambda} = \boldsymbol{A\theta}$$

$$\chi^2 = \sum_{i=1}^{N} \frac{\left(y_i - \sum_{j=1}^{m} A_{ij}\theta_j\right)^2}{\sigma_i^2}$$

pokud $\sigma_i = \sigma$

$$\boxed{\chi^2 = \frac{1}{\sigma^2}(\boldsymbol{y} - \boldsymbol{A\theta})^T(\boldsymbol{y} - \boldsymbol{A\theta})}$$

obecně $\boldsymbol{V}, \quad V_{ij} = \mathrm{cov}(y_i, y_j)$

$$\chi^2 = (\boldsymbol{y} - \boldsymbol{A\theta})^T \boldsymbol{V}^{-1}(\boldsymbol{y} - \boldsymbol{A\theta})$$

$$\frac{\partial \chi^2}{\partial \theta_k} = -\frac{2}{\sigma^2}\sum_{i=1}^{N}\left(y_i - \sum_{j=1}^{m} A_{ij}\theta_j\right) A_{ik}$$

$$\frac{\partial \chi^2}{\partial \theta_k} = 0$$

$$\sum_{i=1}^{N} A_{ik} y_i = \sum_{i=1}^{N}\sum_{j=1}^{m} A_{ik}A_{ij}\theta_j$$

$$\boldsymbol{A}^T\boldsymbol{y} = \boldsymbol{A}^T\boldsymbol{A\theta}$$

$$\hat{\boldsymbol{\theta}} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{y} \equiv \boldsymbol{By}$$

$$\hat{\boldsymbol{\theta}} = (\boldsymbol{A}^T\boldsymbol{V}^{-1}\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{V}^{-1}\boldsymbol{y} \equiv \boldsymbol{By}$$

$\boldsymbol{U}, \quad U_{ij} = \mathrm{cov}(\hat{\theta}_i, \hat{\theta}_j)$

$$\boldsymbol{U} = \boldsymbol{BVB}^T$$

$$U_{ij}^{-1} = \frac{1}{2}\left[\frac{\partial^2 \chi^2}{\partial \theta_i \partial \theta_j}\right]_{\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}}$$

Metoda nejmenších čtverců – fit polynomu

$$\lambda(x_i|\boldsymbol{\theta}) = \sum_{j=1}^{m} a_j(x_i)\theta_j = \sum_{j=1}^{m} A_{ij}\theta_j$$

$$\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_m) \qquad \sigma_i \equiv \sigma$$

$$A_{ij} = x_i^j$$

$$\boldsymbol{A} = \begin{pmatrix} 1 & x_1 & x_1^2 & \ldots & x_1^m \\ 1 & x_2 & x_2^2 & \ldots & x_2^m \\ & \ldots & & & \\ 1 & x_N & x_N^2 & \ldots & x_N^m \end{pmatrix} \quad N \times m + 1$$

$$\boxed{\hat{\theta} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{y}}$$

$$\boldsymbol{A}^T\boldsymbol{A} = \begin{pmatrix} N & \sum_{i=1}^N x_i & \sum_{i=1}^N x_i^2 & \ldots & \sum_{i=1}^N x_i^m \\ \sum_{i=1}^N x_i & \sum_{i=1}^N x_i^2 & \sum_{i=1}^N x_i^3 & \ldots & \sum_{i=1}^N x_i^{m+1} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \sum_{i=1}^N x_i^m & \sum_{i=1}^N x_i^{m+1} & \sum_{i=1}^N x_i^{m+2} & \ldots & \sum_{i=1}^N x_i^{m+m} \end{pmatrix} \quad m + 1 \times m + 1$$

Metoda nejmenších čtverců – fit paraboly

$$A^T V^{-1} A = \begin{pmatrix} \sum_{i=1}^N \frac{1}{\sigma_i^2} & \sum_{i=1}^N \frac{x_i}{\sigma_i^2} & \sum_{i=1}^N \frac{x_i^2}{\sigma_i^2} \\ \sum_{i=1}^N \frac{x_i}{\sigma_i^2} & \sum_{i=1}^N \frac{x_i^2}{\sigma_i^2} & \sum_{i=1}^N \frac{x_i^3}{\sigma_i^2} \\ \sum_{i=1}^N \frac{x_i^2}{\sigma_i^2} & \sum_{i=1}^N \frac{x_i^3}{\sigma_i^2} & \sum_{i=1}^N \frac{x_i^4}{\sigma_i^2} \end{pmatrix}$$

$$\hat{\theta} = (A^T V^{-1} A)^{-1} A^T V^{-1} y \equiv B y$$

$$U, \quad U_{ij} = \mathrm{cov}(\hat{\theta}_i, \hat{\theta}_j)$$

$$U = B V B^T$$

$$\lambda(x|\theta) = \theta_0 + \theta_1 x + \theta_2 x^2$$

$\theta_0 = 140 \pm 50$

$\theta_1 = 92 \pm 5$

$\theta_2 = -1.8 \pm 0.1$