Úvod do praktické fyziky, cvičení 10
Metoda nejmenších čtverců

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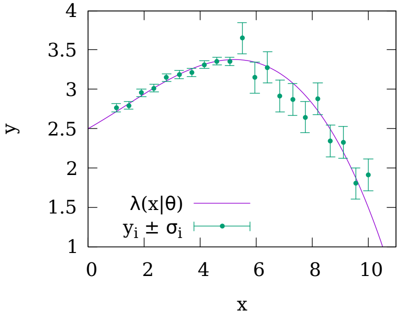
Jak odhadnout parametry modelu z experimentálních dat?

- Nechť mezi veličinou x a y platí vztah
$$y = \lambda(x|\boldsymbol{\theta}).$$
- *Modelová funkce* λ závisí na parametrech
$$\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots \theta_m).$$
- V bodech $x_1, x_2, \ldots, x_N$ jsme naměřili hodnoty $y_1, y_2, \ldots, y_N$ se standardními odchylkami $\sigma_1, \sigma_2, \ldots, \sigma_N$.
- $y_i \in N\big(\lambda(x_i|\boldsymbol{\theta}), \sigma_i\big)$
- Chceme odhad $\boldsymbol{\theta}$ – *fit* $\lambda(x|\boldsymbol{\theta})$ *to the data.*



Odhad $\boldsymbol{\theta}$ metodou maximální věrohodnosti

- Věrohodnostní funkce je součinem hustot pravděpodobnosti (zde normálních rozdělení)

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

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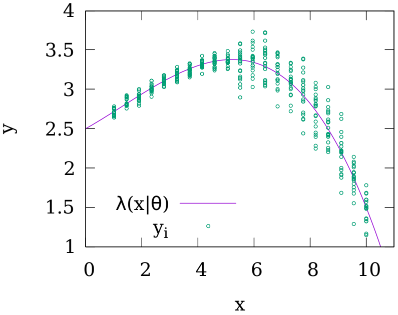

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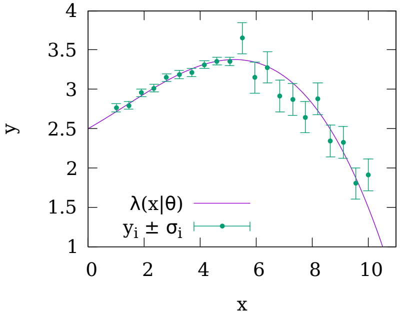

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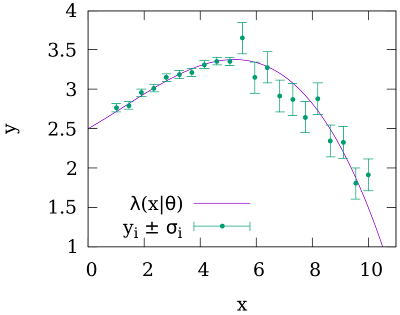

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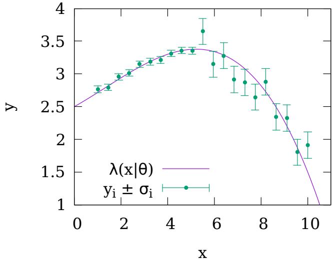
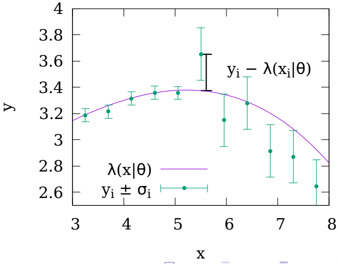
- Maximalizace $\ln L \Leftrightarrow$ minimalizace χ^2, kde

$$\chi^2(\boldsymbol{\theta}|\boldsymbol{x},\boldsymbol{y},\boldsymbol{\sigma}) = \sum_{i=1}^{N} \frac{\left[y_i - \lambda(x_i|\boldsymbol{\theta})\right]^2}{\sigma_i^2}$$

- Minimalizace: analyticky (pro funkci λ lineární v θ) nebo numericky.





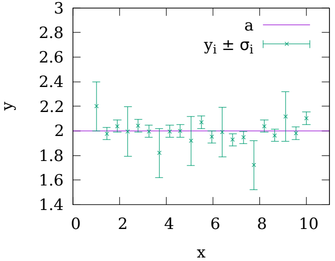
Fit konstantní funkce $\lambda(x|a) = a$

- Vlastně stejná situace jako ve cvičení 9.
- Chi-kvadrát:

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

- Je-li $\hat{a}$ minimum, platí:

$$0 = \frac{\partial \chi^2}{\partial a}(\hat{a}) = -2\sum_{i=1}^{N} \frac{y_i - \hat{a}}{\sigma_i^2} = -2\sum_{i=1}^{N}\frac{y_i}{\sigma_i^2} + 2\sum_{i=1}^{N}\frac{\hat{a}}{\sigma_i^2}.$$



- Vyjádříme $\hat{a}$

$$\hat{a} = \frac{\sum_{i=1}^{N} \frac{y_i}{\sigma_i^2}}{\sum_{i=1}^{N} \frac{1}{\sigma_i^2}} = \frac{\langle y \rangle}{\langle 1 \rangle}, \qquad \text{kde} \qquad \langle g \rangle = \sum_{i=1}^{N} \frac{g_i}{\sigma_i^2}.$$

- Standardní odchylka – metoda přenosu chyb:

$$\frac{\partial \hat{a}}{\partial y_j} = \frac{1}{\langle 1 \rangle}\frac{1}{\sigma_j^2} \qquad \sigma_{\hat{a}}^2 = \sum_{j=1}^{N}\left(\frac{\partial \hat{a}}{\partial y_j}\sigma_j\right)^2 = \sum_{j=1}^{N}\left(\frac{1}{\langle 1 \rangle}\frac{\sigma_j}{\sigma_j^2}\right)^2 = \frac{1}{\langle 1 \rangle}$$

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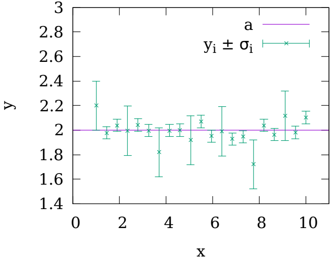

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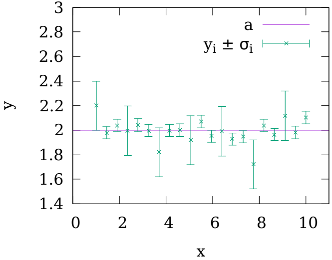

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Fit přímé úměrnosti $\lambda(x|b) = bx$

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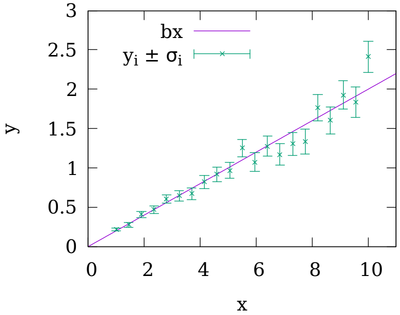

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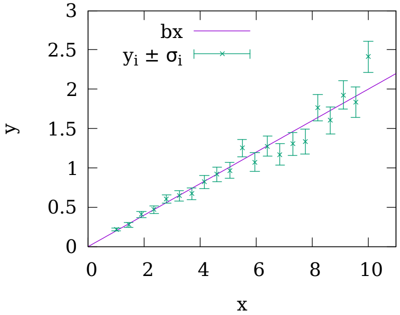

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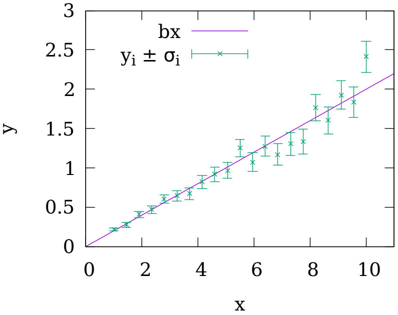

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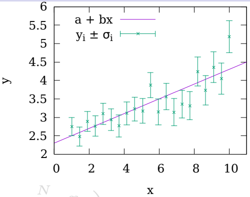
Fit lineární závislosti $\lambda(x|a,b) = a + bx$



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

- Takzvaná *lineární regrese.*
- Je-li v bodě $(\hat{a},\hat{b})$ minimum, platí

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- Soustavu rovnic zapíšeme přehledně pomocí $\langle\ldots\rangle$

$$\hat{a}\langle 1\rangle + \hat{b}\langle x\rangle = \langle y\rangle$$

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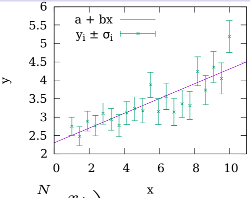

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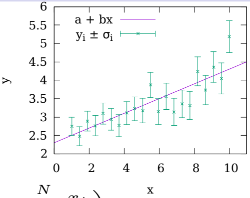
$$\hat b = \frac{\langle x\rangle\langle y\rangle - \langle 1\rangle\langle xy\rangle}{\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle}$$



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

- Takzvaná *lineární regrese*.
- Je-li v bodě $(\hat{a}, \hat{b})$ minimum, platí

$$0 = \frac{\partial \chi^2}{\partial a} = -2\sum_{i=1}^{N} \frac{y_i - \hat{a} - \hat{b}x_i}{\sigma_i^2} = 2\left(-\sum_{i=1}^{N}\frac{y_i}{\sigma_i^2} + \hat{a}\sum_{i=1}^{N}\frac{1}{\sigma_i^2} + \hat{b}\sum_{i=1}^{N}\frac{x_i}{\sigma_i^2}\right)$$

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- Soustavu rovnic zapíšeme přehledně pomocí $\langle \dots \rangle$

$$\hat{a}\langle 1\rangle + \hat{b}\langle x\rangle = \langle y\rangle$$
$$\hat{a}\langle x\rangle + \hat{b}\langle x^2\rangle = \langle xy\rangle$$

- Vyjádříme $\hat{a}$:

$$\hat{a}\langle 1\rangle\langle x^2\rangle + \hat{b}\langle x\rangle\langle x^2\rangle = \langle y\rangle\langle x^2\rangle$$
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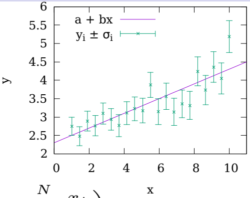
Fit lineární závislosti $\lambda(x|a,b) = a + bx$



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

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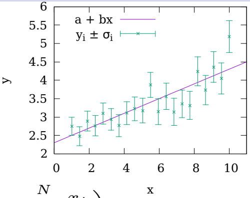

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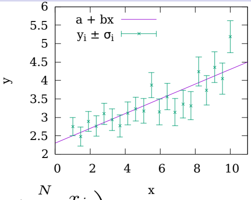

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$$\hat{a}\langle 1\rangle\langle x\rangle + \hat{b}\langle x\rangle\langle x\rangle = \langle y\rangle\langle x\rangle$$
$$\hat{a}\langle x\rangle\langle 1\rangle + \hat{b}\langle x^2\rangle\langle 1\rangle = \langle xy\rangle\langle 1\rangle$$
$$\hat{b}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

Fit lineární závislosti $\lambda(x|a,b) = a + bx$

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- $\hat{a}$ a $\hat{b}$ jsou náhodné proměnné (jsou vytvořené kombinací náhodných proměnných).
- Neurčitosti (standardní odchylky) spočítáme přenosem chyb.
- Nejdřív spočítáme derivace vážených sum podle y_i:

$$\frac{\partial\langle 1\rangle}{\partial y_i} = \frac{\partial\langle x\rangle}{\partial y_i} = \frac{\partial\langle x^2\rangle}{\partial y_i} = 0 \qquad \frac{\partial\langle y\rangle}{\partial y_i} = \frac{1}{\sigma_i^2} \qquad \frac{\partial\langle xy\rangle}{\partial y_i} = \frac{x_i}{\sigma_i^2}$$

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$$\frac{\partial\hat{a}}{\partial y_i} = \frac{\langle x\rangle\frac{x_i}{\sigma_i^2} - \langle x^2\rangle\frac{1}{\sigma_i^2}}{\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle}, \qquad \frac{\partial\hat{b}}{\partial y_i} = \frac{\langle x\rangle\frac{1}{\sigma_i^2} - \langle 1\rangle\frac{x_i}{\sigma_i^2}}{\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle},$$

- Standardní odchylka $\hat{a}$:

$$\sigma_{\hat{a}}^2 = \sum_{i=1}^{N}\left(\frac{\partial\hat{a}}{\partial y_i}\sigma_i\right)^2 = \frac{1}{\left(\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle\right)^2}\sum_{i=1}^{N}\left(\langle x\rangle^2\frac{x_i^2}{\sigma_i^4} - 2\langle x\rangle\langle x^2\rangle\frac{x_i}{\sigma_i^4} + \langle x^2\rangle^2\frac{1}{\sigma_i^4}\right)\sigma_i^2$$

$$= \frac{\langle x\rangle^2\langle x^2\rangle - 2\langle x\rangle^2\langle x^2\rangle + \langle x^2\rangle^2\langle 1\rangle}{\left(\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle\right)^2} = \frac{\langle 1\rangle\langle x^2\rangle^2 - \langle x\rangle^2\langle x^2\rangle}{\left(\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle\right)^2} = \frac{\langle x^2\rangle\left(\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2\right)}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2}$$

- Analogicky odvodíme pro $\hat{b}$ a dostaneme:

$$\sigma_{\hat{a}}^2 = \frac{\langle x^2\rangle}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2} \qquad \sigma_{\hat{b}}^2 = \frac{\langle 1\rangle}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2}$$

Fit lineární závislosti $\lambda(x|a,b) = a + bx$

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- Teď snadno určíme také derivace $\hat{a}$ a $\hat{b}$ podle y_i:

$$\frac{\partial\hat{a}}{\partial y_i} = \frac{\langle x\rangle\frac{x_i}{\sigma_i^2} - \langle x^2\rangle\frac{1}{\sigma_i^2}}{\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle}, \qquad \frac{\partial\hat{b}}{\partial y_i} = \frac{\langle x\rangle\frac{1}{\sigma_i^2} - \langle 1\rangle\frac{x_i}{\sigma_i^2}}{\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle},$$

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$$\sigma_{\hat{a}}^2 = \sum_{i=1}^{N}\left(\frac{\partial\hat{a}}{\partial y_i}\sigma_i\right)^2 = \frac{1}{\left(\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle\right)^2}\sum_{i=1}^{N}\left(\langle x\rangle^2\frac{x_i^2}{\sigma_i^4} - 2\langle x\rangle\langle x^2\rangle\frac{x_i}{\sigma_i^4} + \langle x^2\rangle^2\frac{1}{\sigma_i^4}\right)\sigma_i^2$$

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- Analogicky odvodíme pro $\hat{b}$ a dostaneme:

$$\sigma_{\hat{a}}^2 = \frac{\langle x^2\rangle}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2} \qquad \sigma_{\hat{b}}^2 = \frac{\langle 1\rangle}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2}$$

Fit lineární závislosti $\lambda(x|a,b) = a + bx$

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

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- Teď snadno určíme také derivace $\hat{a}$ a $\hat{b}$ podle y_i:

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$$\frac{\partial\langle 1\rangle}{\partial y_i} = \frac{\partial\langle x\rangle}{\partial y_i} = \frac{\partial\langle x^2\rangle}{\partial y_i} = 0 \qquad \frac{\partial\langle y\rangle}{\partial y_i} = \frac{1}{\sigma_i^2} \qquad \frac{\partial\langle xy\rangle}{\partial y_i} = \frac{x_i}{\sigma_i^2}$$

- Teď snadno určíme také derivace $\hat{a}$ a $\hat{b}$ podle y_i:

$$\frac{\partial\hat{a}}{\partial y_i} = \frac{\langle x\rangle\frac{x_i}{\sigma_i^2} - \langle x^2\rangle\frac{1}{\sigma_i^2}}{\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle}, \qquad \frac{\partial\hat{b}}{\partial y_i} = \frac{\langle x\rangle\frac{1}{\sigma_i^2} - \langle 1\rangle\frac{x_i}{\sigma_i^2}}{\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle},$$

- Standardní odchylka $\hat{a}$:

$$\sigma_{\hat{a}}^2 = \sum_{i=1}^{N}\left(\frac{\partial\hat{a}}{\partial y_i}\sigma_i\right)^2 = \frac{1}{\left(\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle\right)^2}\sum_{i=1}^{N}\left(\langle x\rangle^2\frac{x_i^2}{\sigma_i^4} - 2\langle x\rangle\langle x^2\rangle\frac{x_i}{\sigma_i^4} + \langle x^2\rangle^2\frac{1}{\sigma_i^4}\right)\sigma_i^2$$

$$= \frac{\langle x\rangle^2\langle x^2\rangle - 2\langle x\rangle^2\langle x^2\rangle + \langle x^2\rangle^2\langle 1\rangle}{\left(\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle\right)^2} = \frac{\langle 1\rangle\langle x^2\rangle^2 - \langle x\rangle^2\langle x^2\rangle}{\left(\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle\right)^2} = \frac{\langle x^2\rangle\left(\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2\right)}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2}$$

- Analogicky odvodíme pro $\hat{b}$ a dostaneme:

$$\sigma_{\hat{a}}^2 = \frac{\langle x^2\rangle}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2} \qquad \sigma_{\hat{b}}^2 = \frac{\langle 1\rangle}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2}$$

Fit lineární závislosti $\lambda(x|a,b) = a + bx$

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

- Kovarianci $\mathrm{cov}(\hat{a},\hat{b})$ spočítáme podobně, jako σ „přenosem“ (viz Dodatky),

$$\mathrm{cov}\big(A(\boldsymbol{x}), B(\boldsymbol{x})\big) = \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{\partial A}{\partial x_i}\bigg|_{\boldsymbol{\mu_x}} \frac{\partial B}{\partial x_j}\bigg|_{\boldsymbol{\mu_x}} \mathrm{cov}(x_i, x_j).$$

- Dosadíme derivace z předchozí strany a využijeme, že měření jsou nezávislá,

$$\begin{aligned}
\mathrm{cov}(\hat{a},\hat{b}) &= \frac{1}{\big(\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle\big)^2} \sum_{i=1}^{N} \left(\langle x\rangle \frac{x_i}{\sigma_i^2} - \langle x^2\rangle \frac{1}{\sigma_i^2}\right)\left(\langle x\rangle \frac{1}{\sigma_i^2} - \langle 1\rangle \frac{x_i}{\sigma_i^2}\right)\sigma_i^2 \\
&= \frac{1}{\big(\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle\big)^2} \sum_{i=1}^{N} \left(\langle x\rangle^2 \frac{x_i}{\sigma_i^2} - \langle x\rangle\langle 1\rangle \frac{x_i^2}{\sigma_i^2} - \langle x^2\rangle\langle x\rangle \frac{1}{\sigma_i^2} + \langle x^2\rangle\langle 1\rangle \frac{x_i}{\sigma_i^2}\right) \\
&= \frac{\langle x\rangle^3 - \langle x\rangle\langle 1\rangle\langle x^2\rangle - \cancel{\langle x^2\rangle\langle x\rangle\langle 1\rangle} + \cancel{\langle x^2\rangle\langle 1\rangle\langle x\rangle}}{\big(\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle\big)^2} = \frac{\langle x\rangle}{\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle}
\end{aligned}$$

- Nyní už známe standardní odchylky i kovarianci parametrů lineární závislosti:

$$\sigma_{\hat{a}}^2 = \frac{\langle x^2\rangle}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2} \qquad \sigma_{\hat{b}}^2 = \frac{\langle 1\rangle}{\langle 1\rangle\langle x^2\rangle - \langle x\rangle^2} \qquad \mathrm{cov}(\hat{a},\hat{b}) = \frac{\langle x\rangle}{\langle x\rangle^2 - \langle 1\rangle\langle x^2\rangle}$$

Dodatky: Odvození přenosu kovariance

- Funkce $A(\boldsymbol{x})$ a $B(\boldsymbol{x})$ aproximujeme dvěma členy Taylorovy řady:

$$A(\boldsymbol{x}) \approx A(\boldsymbol{\mu_x}) + \sum_{i=1}^{N} \frac{\partial A}{\partial x_i}\bigg|_{\boldsymbol{\mu_x}} (x_i - \mu_{x_i}) \qquad B(\boldsymbol{x}) \approx B(\boldsymbol{\mu_x}) + \sum_{i=1}^{N} \frac{\partial B}{\partial x_i}\bigg|_{\boldsymbol{\mu_x}} (x_i - \mu_{x_i})$$

- Kovariance je $\mathrm{cov}(A, B) = E[AB] - E[A]E[B]$ (viz lekce 7)

$$E[AB] = E\Bigg[A(\boldsymbol{\mu_x})B(\boldsymbol{\mu_x}) + A(\boldsymbol{\mu_x}) \sum_{i=1}^{N} \frac{\partial B}{\partial x_i}\bigg|_{\boldsymbol{\mu_x}} (x_i - \mu_{x_i}) + B(\boldsymbol{\mu_x}) \sum_{i=1}^{N} \frac{\partial A}{\partial x_i}\bigg|_{\boldsymbol{\mu_x}} (x_i - \mu_{x_i})$$
$$+ \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial A}{\partial x_i}\bigg|_{\boldsymbol{\mu_x}} \frac{\partial B}{\partial x_j}\bigg|_{\boldsymbol{\mu_x}} (x_i - \mu_{x_i})(x_j - \mu_{x_j})\Bigg]$$

- Uvědomíme si, že $E[x_i - \mu_{x_i}] = 0$ a $E\big[(x_i - \mu_{x_i})(x_j - \mu_{x_j})\big] = \mathrm{cov}(x_i, x_j)$,

$$E[AB] = A(\boldsymbol{\mu_x})B(\boldsymbol{\mu_x}) + \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial A}{\partial x_i}\bigg|_{\boldsymbol{\mu_x}} \frac{\partial B}{\partial x_j}\bigg|_{\boldsymbol{\mu_x}} \mathrm{cov}(x_i, x_j).$$

- Po odečtení $E[A]E[B] = A(\boldsymbol{\mu_x})B(\boldsymbol{\mu_x})$ dostaneme

$$\mathrm{cov}\big(A(\boldsymbol{x}), B(\boldsymbol{x})\big) = \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial A}{\partial x_i}\bigg|_{\boldsymbol{\mu_x}} \frac{\partial B}{\partial x_j}\bigg|_{\boldsymbol{\mu_x}} \mathrm{cov}(x_i, x_j).$$