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

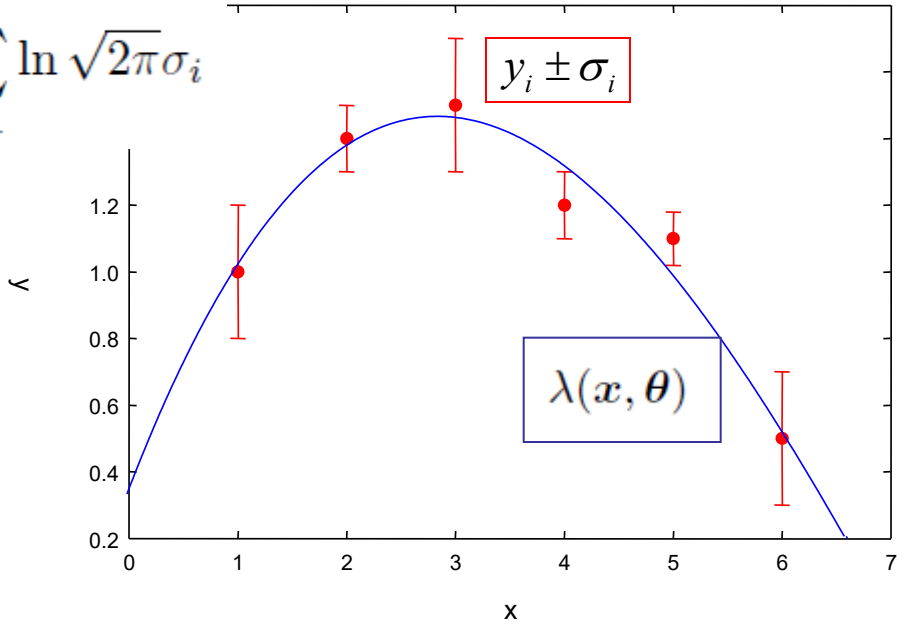
$\lambda(x, \boldsymbol{\theta})$ $\quad \boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_m)$ • modelová funkce

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



Rozdělení χ^2

$$f(y|N) = \frac{1}{2^{N/2}\Gamma(N/2)} y^{N/2-1} e^{-y/2} \qquad y \in \langle 0, \infty), \quad N = 1,2,...$$

N – počet stupňů volnosti

$$z_i \in N(0,1)$$

$$y = \sum_{i=1}^{N} z_i^2 \longrightarrow y \in \chi^2(N)$$

$$x_i \in N(\mu, \sigma)$$

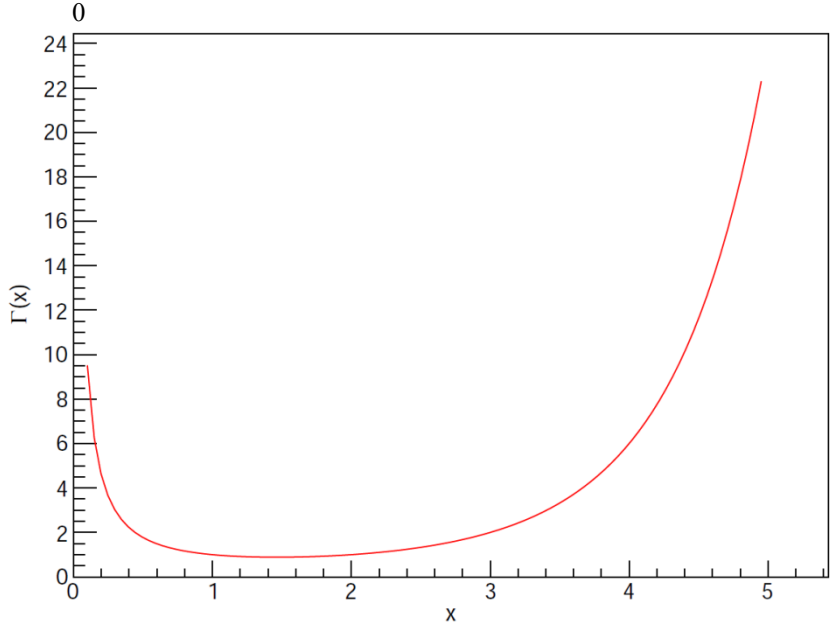
$$y = \sum_{i=1}^{N} \frac{(x_i - \mu_i)^2}{\sigma_i^2} \longrightarrow y \in \chi^2(N)$$

- gama funkce: $\Gamma(x) = \int_0^\infty e^{-t} t^{x-1}\, \mathrm{d}t$

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

$$\Gamma(x+1) = x\Gamma(x)$$

$$\Gamma(N) = (N-1)!$$



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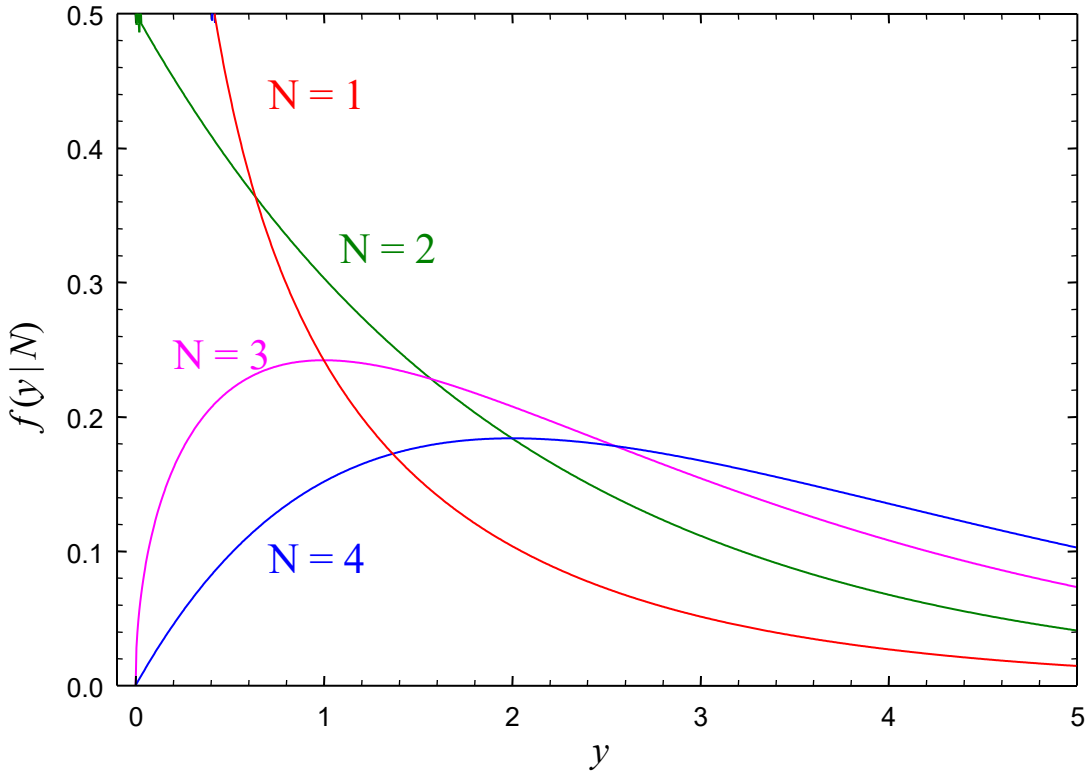
- momenty χ^2 rozdělení:

$$E[y] = N$$

$$V[y] = 2N$$



χ^2 test kvality fitu

- $y_1, y_2, \ldots, y_N$ naměřené hodnoty (nezávislé)
- normální rozdělení $y_i \in N(\mu_i, \sigma_i)$
- parametry: $\theta_1, \theta_2, \ldots, \theta_m$
- modelová funkce: $\lambda(x, \theta)$

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

- počet stupňů volnosti: *N*-*m*

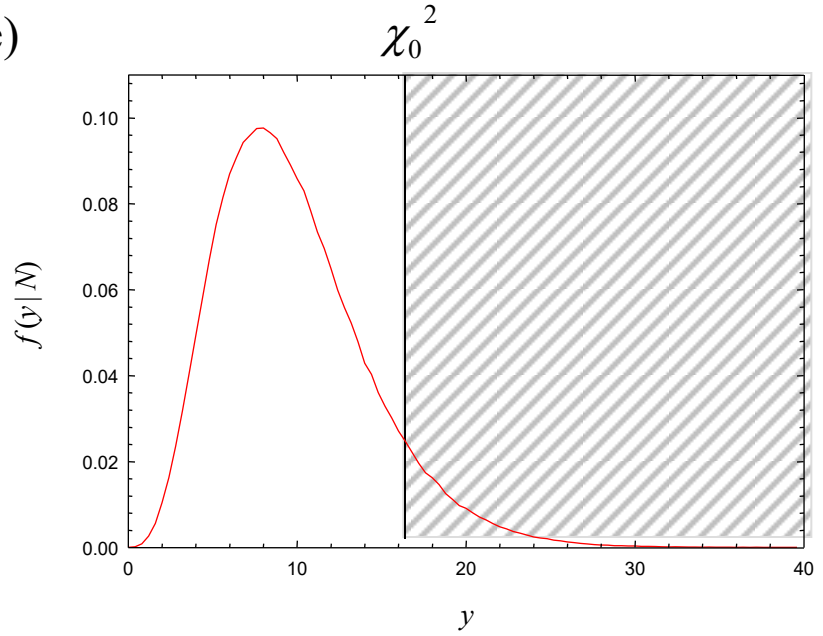
$$E\left[\chi^2\right] = N - m$$

$$V\left[\chi^2\right] = 2(N - m)$$

- χ^2 na počet stupňů volnosti: $\chi^2/(N-m)$

$$E\left[\chi^2/(N-m)\right] = 1$$

$$V\left[\chi^2/(N-m)\right] = 2/(N-m)$$



$$P\left[y \geq \chi_0^2\right] = \int_{\chi_0^2}^{\infty} f(y|N-m)\,dy$$

- pokud je $P\left[y \geq \chi_0^2\right] < \alpha$ zamítneme nulovou hypotézu
- α – **hladina signifikance**
- typicky volíme $\alpha = 0.05$ nebo 0.01

χ^2 test kvality fitu

- tabulka hodnot $P[y \geq \chi^2]$ pro počet stupňů volnosti $k = 1$ - 10

Počet stupňů volnosti	χ^2								hladina signifikance $\alpha = 5\ \%$ ↓	hladina signifikance $\alpha = 1\ \%$ ↓	
1	0.004	0.02	0.06	0.15	0.46	1.07	1.64	2.71	3.84	6.64	10.83
2	0.10	0.21	0.45	0.71	1.39	2.41	3.22	4.60	5.99	9.21	13.82
3	0.35	0.58	1.01	1.42	2.37	3.66	4.64	6.25	7.82	11.34	16.27
4	0.71	1.06	1.65	2.20	3.36	4.88	5.99	7.78	9.49	13.28	18.47
5	1.14	1.61	2.34	3.00	4.35	6.06	7.29	9.24	11.07	15.09	20.52
6	1.63	2.20	3.07	3.83	5.35	7.23	8.56	10.64	12.59	16.81	22.46
7	2.17	2.83	3.82	4.67	6.35	8.38	9.80	12.02	14.07	18.48	24.32
8	2.73	3.49	4.59	5.53	7.34	9.52	11.03	13.36	15.51	20.09	26.12
9	3.32	4.17	5.38	6.39	8.34	10.66	12.24	14.68	16.92	21.67	27.88
10	3.94	4.87	6.18	7.27	9.34	11.78	13.44	15.99	18.31	23.21	29.59
$P[y \geq \chi^2]$	0.95	0.90	0.80	0.70	0.50	0.30	0.20	0.10	0.05	0.01	0.001

- pro počet stupňů volnosti $k > 10$ rozdělení $\chi^2(k)$ konverguje k $N\left(k, \sqrt{2k}\right)$

χ^2 test kvality fitu

N = 10

$m = 2,\ \chi^2 = 47.04$

$\chi^2 / (N\text{-}m) = 5.88$

$P < 0.001$

$m = 3,\ \chi^2 = 36.47$

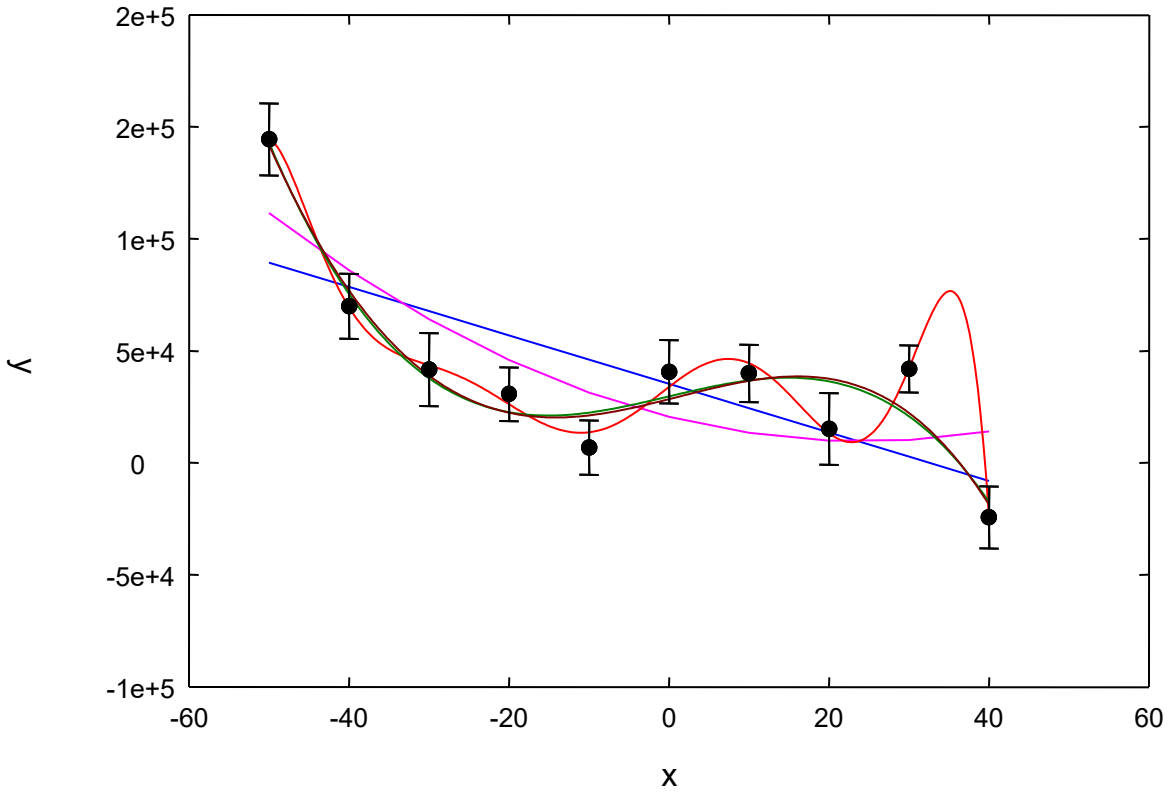
$\chi^2 / (N\text{-}m) = 5.21$

$P < 0.001$

$m = 4,\ \chi^2 = 9.06$

$\chi^2 / (N\text{-}m) = 1.51$

$0.1 < P < 0.2$



$m = 5,\ \chi^2 = 8.60$

$\chi^2 / (N\text{-}m) = 1.72$

$0.1 < P < 0.2$

$m = 9,\ \chi^2 = 0.84$

$\chi^2 / (N\text{-}m) = 0.84$

$P > 0.95$

rezidua

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$$r_i = \frac{y_i - \lambda(x_i|\boldsymbol{\theta})}{\sqrt{y_i}}$$

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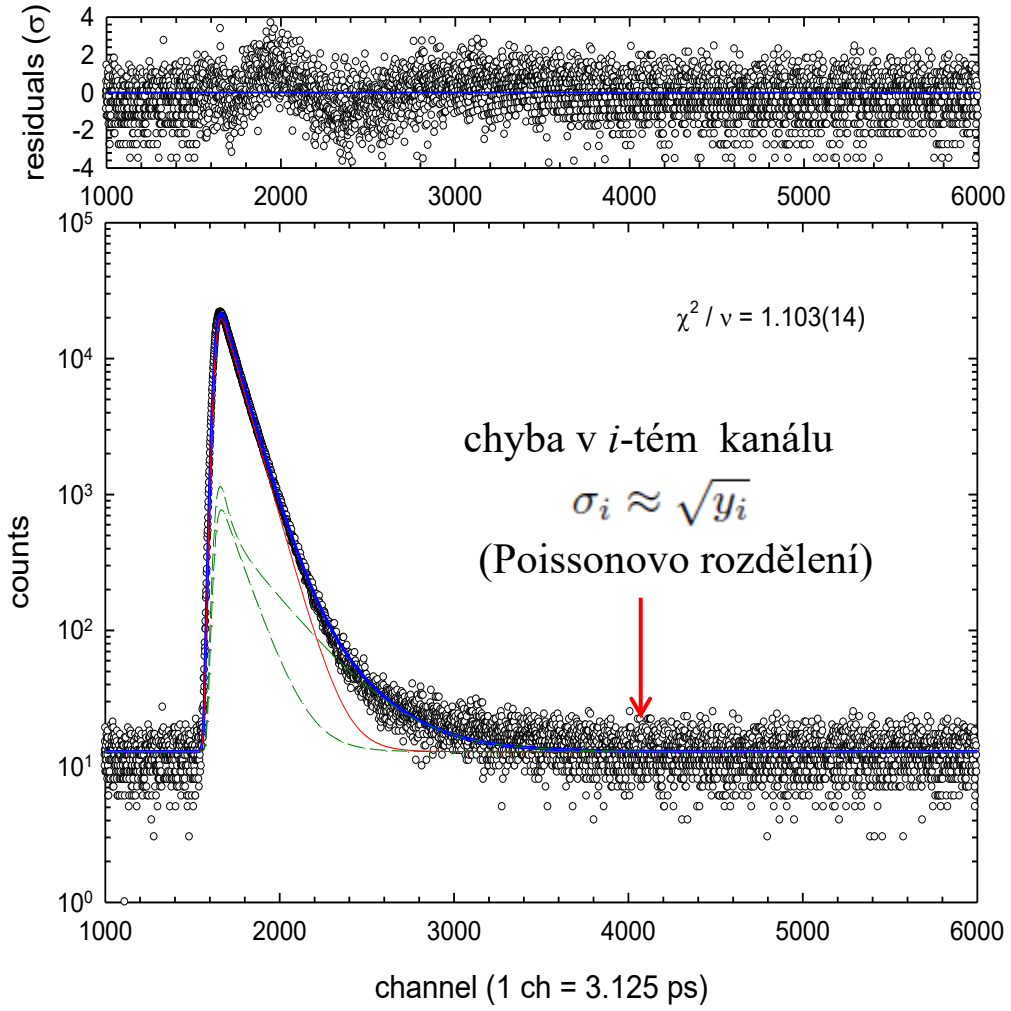
$$r_i \in N(0,1)$$

spektrum života pozitronů, CdTe krystal dopovaný In
jednokomponentní fit, τ_1 = 300(1) ps



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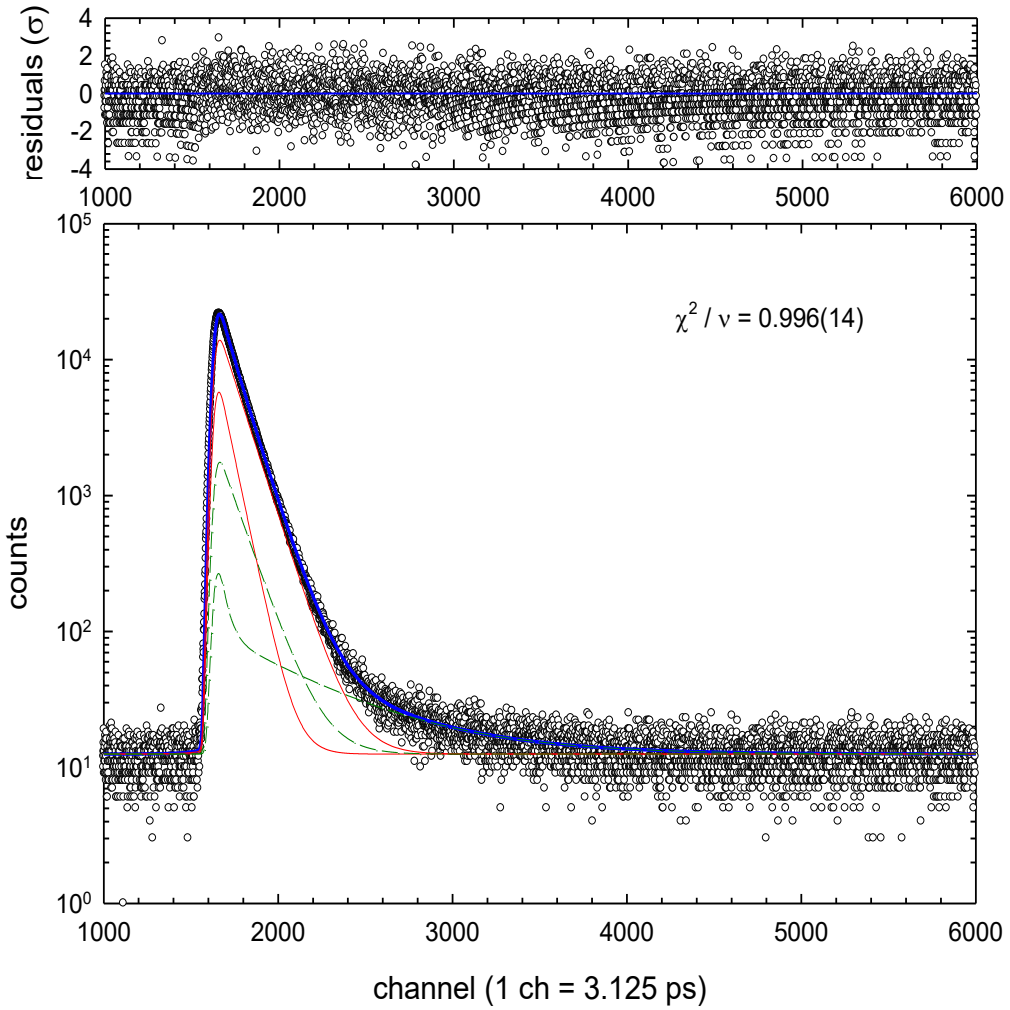
spektrum života pozitronů, CdTe krystal dopovaný In
jednokomponentní fit, τ_1 = 220(10) ps, τ_2 = 341(5) ps



V_{Cd} - In