Berlin Mathematics Research Center

MATH+

„Neural MRI“
Some remarks to a MR spektral analysis

Ariane Fillmer & Karsten Tabelow

Thematic Einstein Semester on Mathematics of Imaging in Real-World Challenges 2021/22

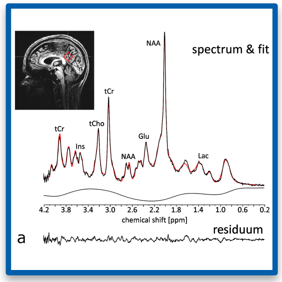
WIAS

Leibniz Association

MRS data analysis pipeline

Reconstruction

Artifact correction



Signal model

$$Y(\nu) = B(\nu) + \exp\left[i\left(\phi_0 + \nu\phi_1\right)\right] \sum_{g=1}^{N_G} \sum_{l=1}^{N_g} C_{l,g} M_{l,g}\left(\nu; \gamma_g, \sigma_g, \epsilon_g\right)$$

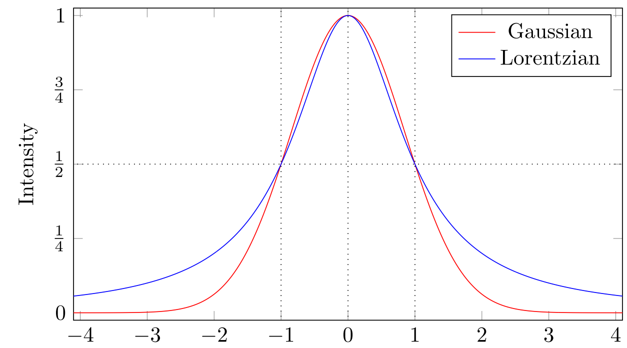
Statistics:
Estimates
Errors

Science
Questions

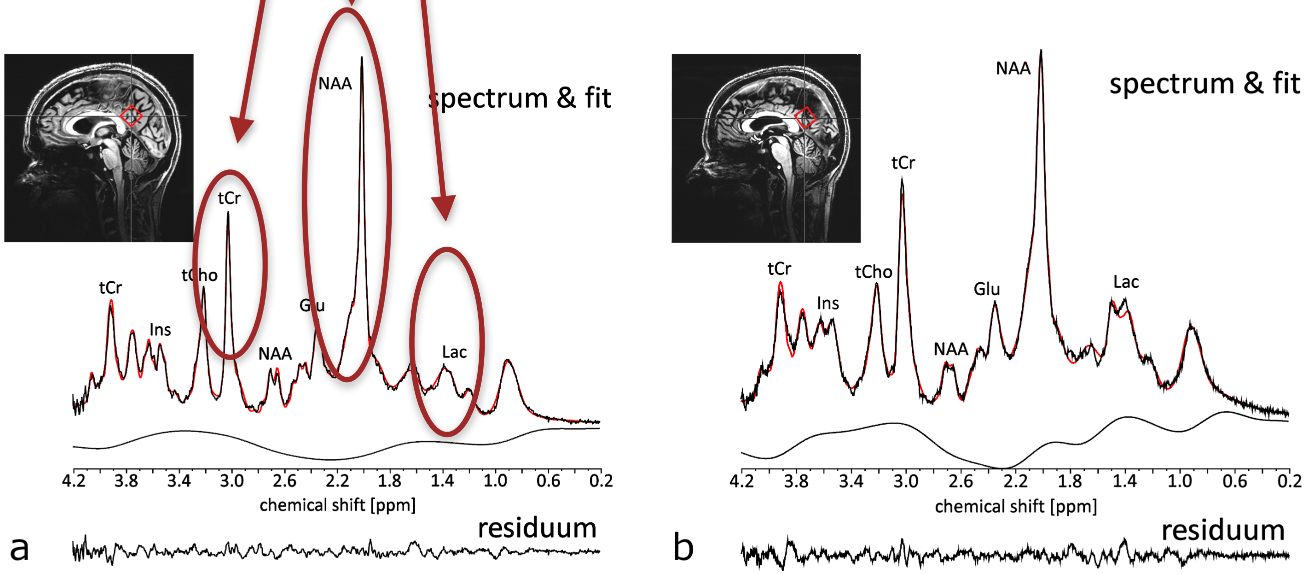
1. Model for spektral data
2. Spline interpolation
3. Cramér-Rao Bounds
4. Weighted mean

Spectral data: Basic model

Superposition of Gaussian and Lorentzian

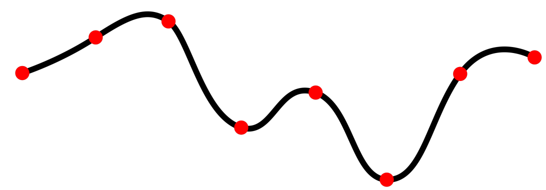


Multiple Peaks corresponding to different metabolites

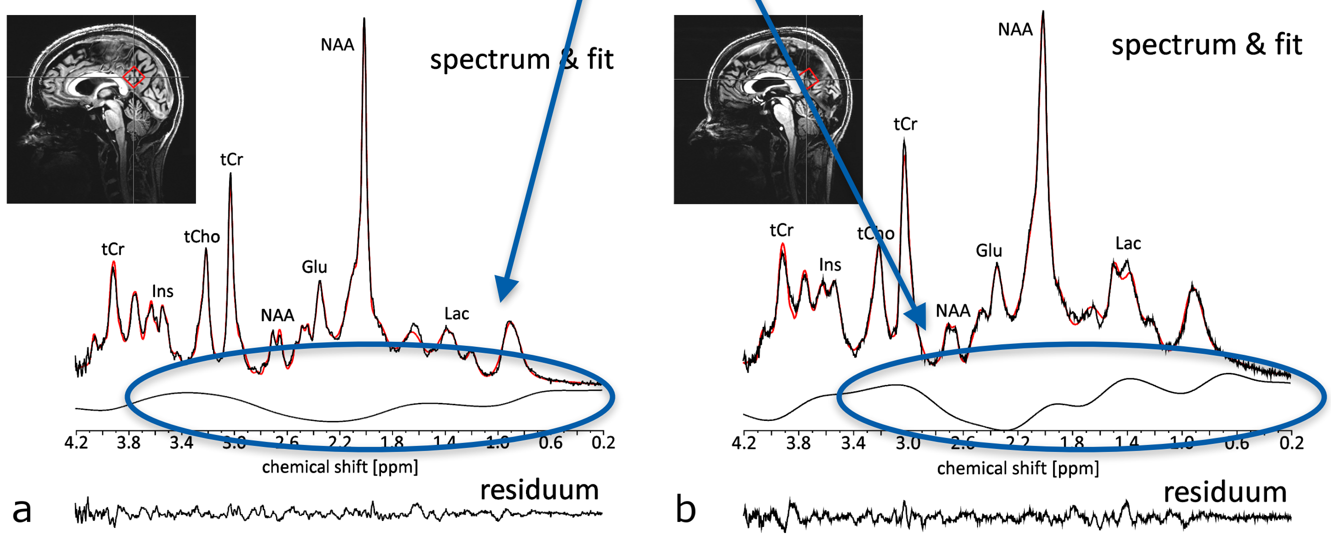


Spectral data: Basic model

Smooth function: Splines

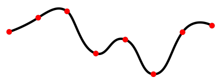


Baseline



Model for MR spectra

Spektral data — Baseline — Superposition of multiple peaks

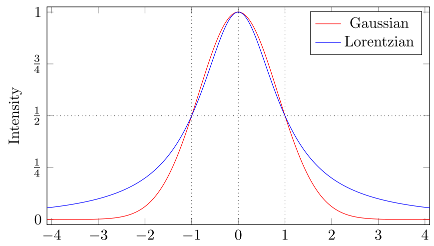


$$\mathrm{Y}(v) = \mathrm{B}(v) + \exp\left[i\left(\phi_0 + v\phi_1\right)\right] \sum_{g=1}^{N_G} \sum_{l=1}^{N_g} C_{l,g} M_{l,g}\left(v; \gamma_g, \sigma_g, \epsilon_g\right)$$

Phase shift

$$M_{l,g}\left(v; \gamma_g, \epsilon_g\right) = \mathscr{FFT}\left\{ m_{l,g}(t) \exp\left[-\left(\left(\gamma_g + \sigma_g^2 t \right) + i\epsilon_g \right) t \right] \right\}$$

A single peak is the superposition of a Gaussian and a Lorentzian



Polynomial approximation: Taylor expansion

(All derivatives exist)

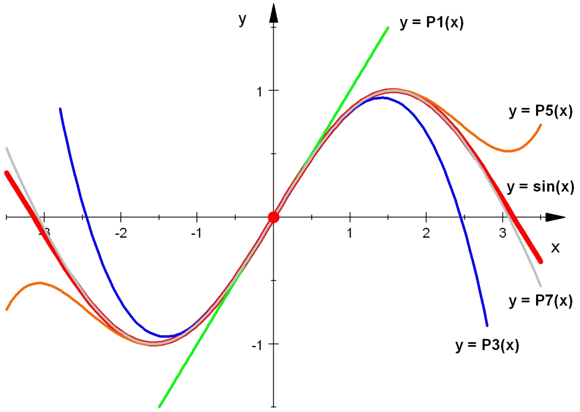
Interpolation of smooth functions by polynomials around some position a

$$\text{Taylor series } f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n$$

Examples:

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

$$\sin(x) = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!}$$



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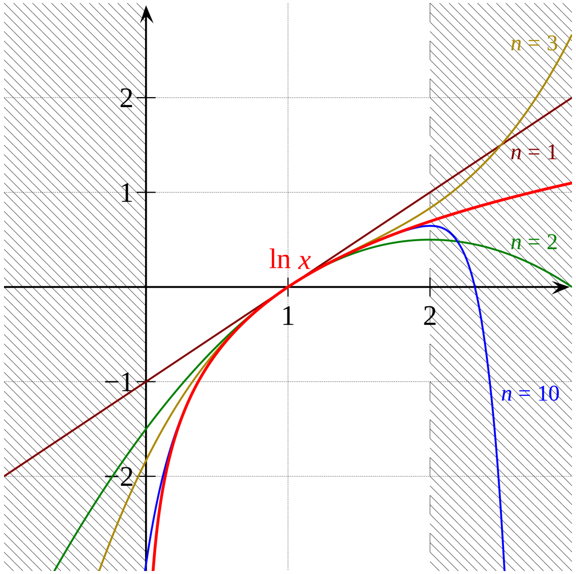
Examples:

$$\ln(x) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n}(x-1)^n$$



Convergence only for $0 < x < 2$

Polynomial approximation: Weierstrass theorem

Any continuous function $f(x)$ can be approximated by polynomials $P_n(x)$ on an interval $[a, b]$:

$$\lim_{n\to\infty}\left(\sup_{a\le x\le b}\ |f(x) - P_n(x)|\right) = 0$$

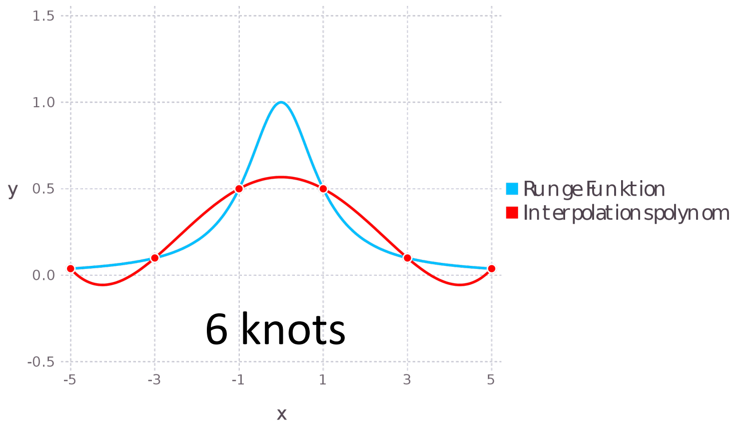
How to find $P_n(x)$?

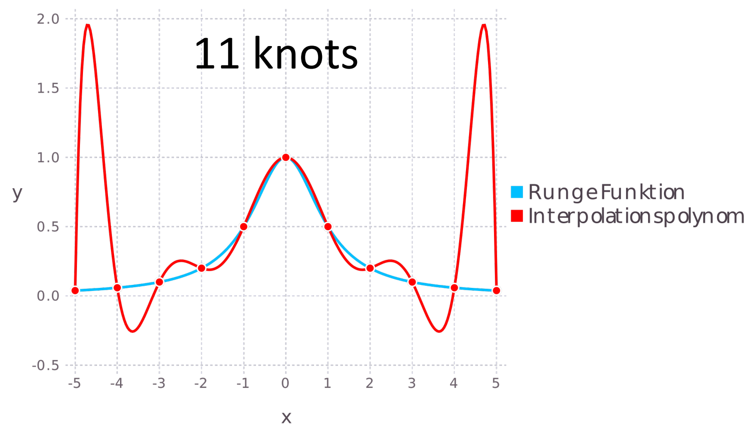
Choose $n + 1$ (equidistant) points?

However, this may fail miserably

Polynomial approximation: Runge function

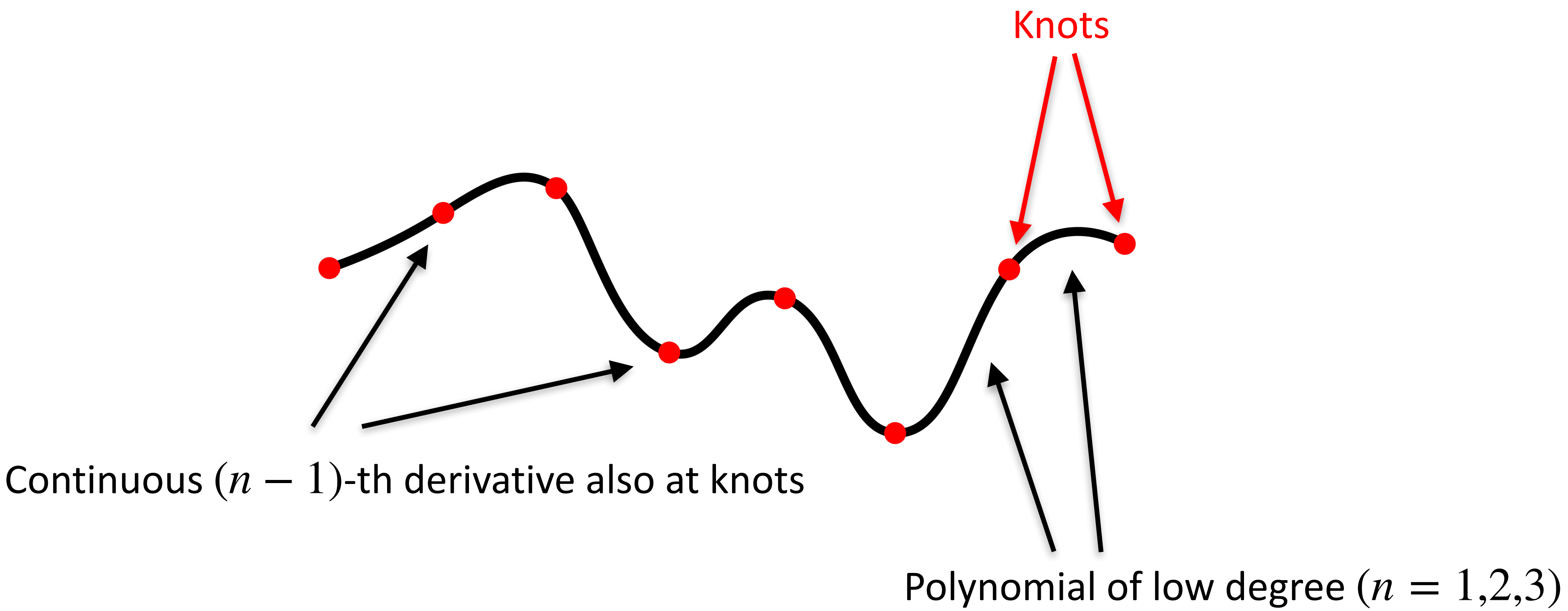
$$f(x) = \frac{1}{1+x^2}$$





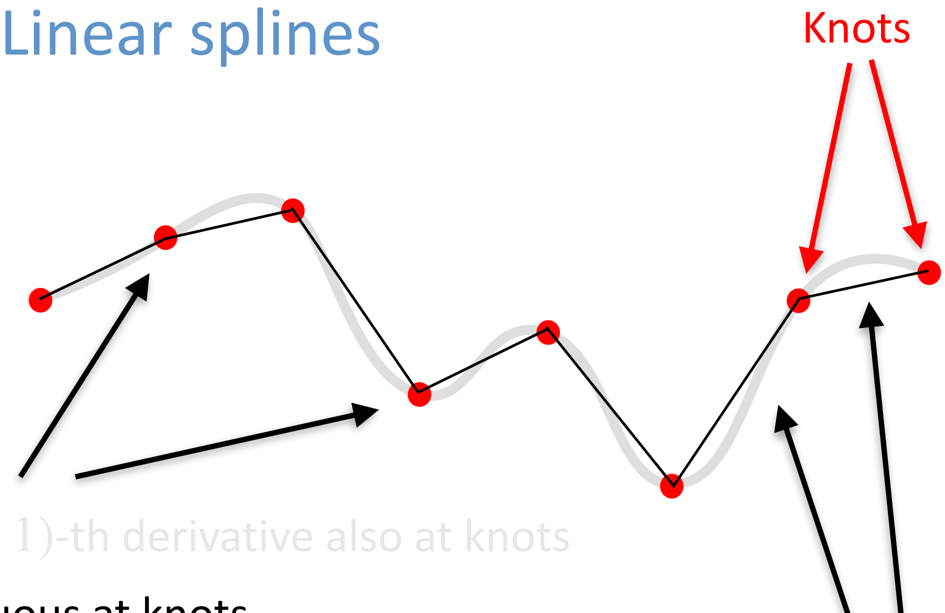
$$\lim_{n\to\infty} \left(\sup_{a\leq x\leq b} \, |f(x) - P_n(x)| \right) = \infty$$

Polynomial approximation: Spline interpolation



Polynomial approximation: Spline interpolation

Linear splines



Continuous $(n-1)$-th derivative also at knots

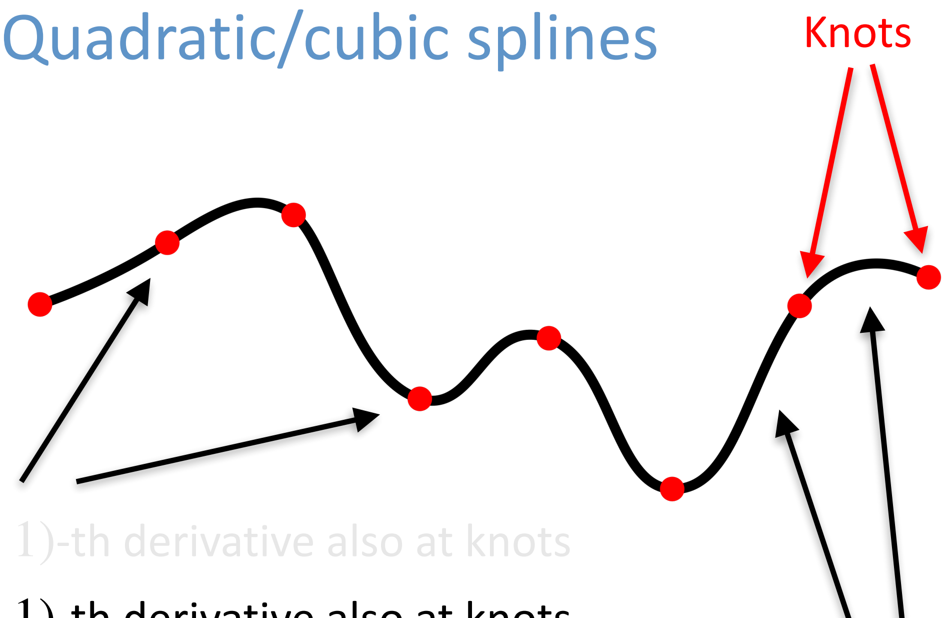
Continuous at knots

Polynomial of low degree $(n = 1,2,3)$

Polynomial of degree $n = 1$ (linear)

Polynomial approximation: Spline interpolation

Quadratic/cubic splines



Continuous $(n-1)$-th derivative also at knots

Continuous $(n-1)$-th derivative also at knots

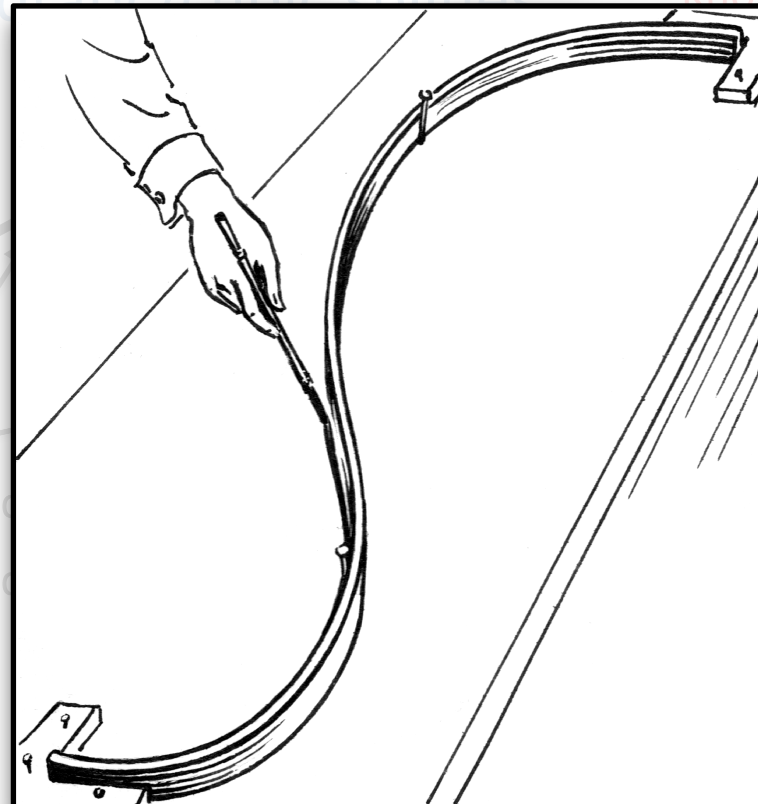
Polynomial of low degree $(n = 1{,}2{,}3)$

Polynomial of degree $n = 2,\ 3$

Polynomial approximation: Spline interpolation

Quadratic/cubic splines

Knots



Continuous $(n-1)$-th d

Continuous $(n-1)$-th d

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Polynomial approximation: Spline interpolation

Baseline

Quadratic/cubic splines

Knots

Continuous $(n-1)$-th de

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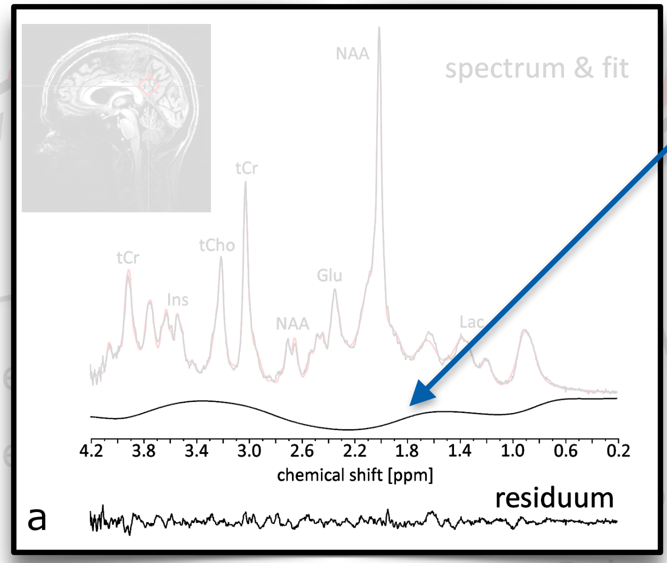


mial of low degree $(n = 1,2,3)$

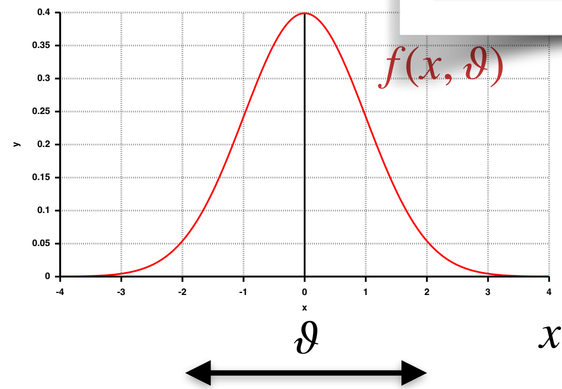
Polynomial of degree $n = 2,\ 3$

Fisher-Information

Observed random variable $X \sim P_{\vartheta_0}$ from a

Family of probability measures $(P_\vartheta)_{\vartheta \in \Theta}$ with density $f(x, \vartheta)$

Gaussian distributions with fixed variance σ^2 but varying mean ϑ



Score function $S_\vartheta(x) := \dfrac{\partial}{\partial \vartheta} \ln f(x, \vartheta)$

Fisher-Information $I(\vartheta) := \mathrm{Var}_\vartheta(S_\vartheta)$

$I(\vartheta) = 1/\sigma^2$

(If variance σ^2 and mean ϑ are unknown - 2 x 2 matrix)

„Amount of information in X about ϑ_0“ of the distribution P_{ϑ_0} of X

Cramér-Rao bounds

n observations of a random variable $X \sim P_{\vartheta_0}$ from a

Family of probability measures $(P_\vartheta)_{\vartheta \in \Theta}$ with density $f(x, \vartheta)$

n observations $x_1, \ldots x_n$

Estimator T for some function $g(\vartheta)$ with $E_\vartheta(T) = g(\vartheta)$ (unbiased)

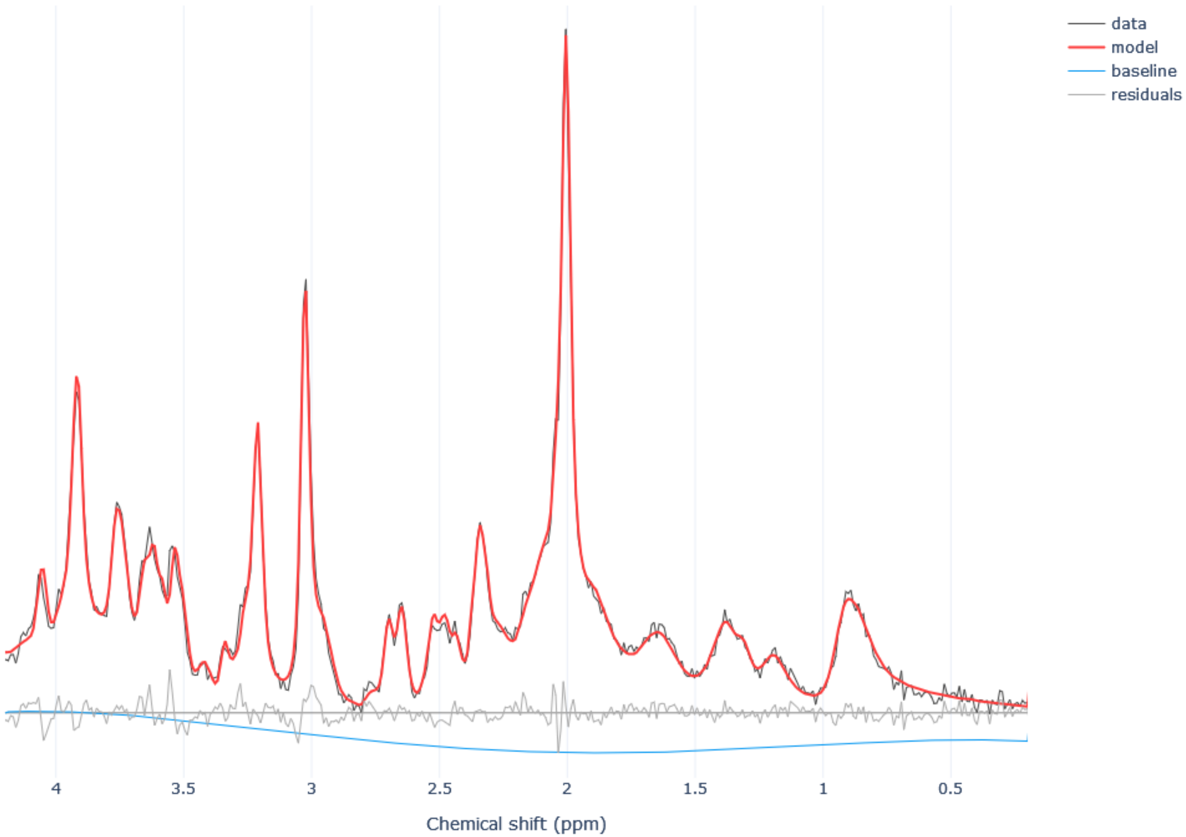
Estimator T of mean: $\dfrac{x_1 + \ldots + x_n}{n}$

Cramér-Rao bound $\mathrm{Var}(T) \geq \dfrac{g'(\vartheta)}{I(\vartheta)}$

Then, $\mathrm{Var}(T) \geq \dfrac{\sigma^2}{n}$

Cramér-Rao bounds

Metab	mMol/kg	CRLB	%CRLB	/Cr+PCr
Ala	0	0.2	999	0
Asc	0.16	0.36	223.9	0.02
Asp	1.76	0.58	32.9	0.17
Cr	6.77	0.53	7.8	0.65
GABA	2.13	0.28	13.4	0.2
GPC	1.46	0.23	15.6	0.14
GSH	1.8	0.19	10.4	0.17
Glc	0	0.54	999	0
Gln	1.73	0.36	20.5	0.17
Glu	11.16	0.37	3.3	1.06
Ins	8.17	0.35	4.2	0.78
Lac	0.82	0.19	22.8	0.08
Mac	0.78	0.07	8.4	0.07
NAA	14.57	0.42	2.9	1.39
NAAG	2.1	0.2	9.3	0.2
PCh	0.5	0.24	49	0.05
PCr	3.72	0.52	14	0.35
PE	1.78	0.38	21.2	0.17
Scyllo	0.73	0.09	12.6	0.07
Tau	2.07	0.34	16.4	0.2
Cr+PCr	10.48	0.35	3.3	1
NAA+NAAG	16.67	0.37	2.2	1.59
Glu+Gln	12.89	0.47	3.6	1.23
GPC+PCh	1.96	0.11	5.4	0.19
Glc+Tau	2.07	0.42	20.2	0.2



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SPECTROSCOPIC METHODOLOGY – Mini-Review

Magnetic Resonance in Medicine 75:15–18 (2016)

The Trouble With Quality Filtering Based on Relative Cramér-Rao Lower Bounds

Roland Kreis*

Cramér Rao Lower Bounds (CRLB) have become the standard for expression of uncertainties in quantitative MR spectroscopy. If properly interpreted as a lower threshold of the error associated with model fitting, and if the limits of its estimation are respected, CRLB are certainly a very valuable tool to give

factors, the method of Cramér Rao estimation of the lower bounds of measurement error (1) has become the standard way of determining the minimum error associated with a MRS measurement from a single spectrum. It reflects the maximum trust that can be associated with

Weighted means

Mean estimator with minimal variance

$$\bar{x} = \sum_{i=1}^{n} w_i x_i \qquad \text{Subject to } \sum_{i=1}^{n} w_i = 1 \text{ and } w_i \geq 0$$

$$\text{Variance is } \operatorname{Var} \bar{x} = \sum_{i=1}^{n} w_i^2 \operatorname{Var}(x_i)$$

$$\text{Optimal is } w_i = \frac{1}{\operatorname{Var}(x_i)} \sum_{i=j}^{n} \frac{1}{\operatorname{Var}(x_j)}$$