G. Least squares methods

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2. Linear least squares

The model of Linear Least Squares: $\boldsymbol{y} = \boldsymbol{A}\,\boldsymbol{a}$

$$\begin{aligned}
\boldsymbol{y} &= \text{vector of measured data} \\
\boldsymbol{A} &= \text{matrix (fixed)} \\
\boldsymbol{a} &= \text{vector of parameters} \\
\boldsymbol{r} &= \boldsymbol{y} - \boldsymbol{A}\boldsymbol{a} = \text{vector of residuals} \\
\boldsymbol{V}[\boldsymbol{y}] &= \text{covariance matrix of the data} \\
\boldsymbol{W} &= \boldsymbol{V}[\boldsymbol{y}]^{-1} \quad \text{weight matrix}
\end{aligned}$$

Least Squares Principle: minimize the expression

$$S(\boldsymbol{a}) = \boldsymbol{r}^T \boldsymbol{W} \boldsymbol{r} = (\boldsymbol{y} - \boldsymbol{A}\boldsymbol{a})^T \; W \; (\boldsymbol{y} - \boldsymbol{A}\boldsymbol{a})$$

with respect to $\boldsymbol{a}$.

Least Squares solution

Derivatives of expression $S(\boldsymbol{a})$:

$$\begin{aligned} \frac{\partial S}{\partial \boldsymbol{a}} &= 2\left(-\boldsymbol{A}^T\boldsymbol{W}\boldsymbol{y} + \left(\boldsymbol{A}^T\boldsymbol{W}\boldsymbol{A}\right)\boldsymbol{a}\right) \\ \frac{\partial^2 S}{\partial \boldsymbol{a}^2} &= \left(\boldsymbol{A}^T\boldsymbol{W}\boldsymbol{A}\right) \qquad = \text{constant} \end{aligned}$$

Solution (from $\partial S/\partial \boldsymbol{a} = 0$) is linear transf. of the data vector $\boldsymbol{y}$:

$$\hat{\boldsymbol{a}} = \left(\boldsymbol{A}^T\boldsymbol{W}\boldsymbol{A}\right)^{-1} \boldsymbol{A}^T\boldsymbol{W}\,\boldsymbol{y} \qquad = \boldsymbol{B}\boldsymbol{y}$$

Covariance matrix of $\boldsymbol{a}$ by "error" propagation ($\boldsymbol{V}[\boldsymbol{y}] = \boldsymbol{W}^{-1}$):

$$\boldsymbol{V}[\hat{\boldsymbol{a}}] = \boldsymbol{B}\,\boldsymbol{V}[\boldsymbol{y}]\,\boldsymbol{B}^T = \left(\boldsymbol{A}^T\boldsymbol{W}\boldsymbol{A}\right)^{-1}$$

(identical to inverse of second derivate of S).

Properties of solution

General scheme

Starting from **Principles** properties of the solution are derived, which are valid under certain conditions.

Conditions:

- Data are unbiased: $E[\boldsymbol{y}] = \boldsymbol{A}\,\bar{\boldsymbol{a}}$ ($\bar{\boldsymbol{a}}$ = true parameter vector
- Covariance matrix $\boldsymbol{V}[\boldsymbol{y}]$ is known (correct) and finite

Properties:

- Estimated parameters are unbiased: $E[\boldsymbol{a}] = \hat{\boldsymbol{a}}$

$$E[\hat{\boldsymbol{a}}] = \left(\boldsymbol{A}^T\boldsymbol{W}\boldsymbol{A}\right)^{-1} \boldsymbol{A}^T\boldsymbol{W}\,E[\boldsymbol{y}] = \bar{\boldsymbol{a}}$$

- In the class of unbiased estimates $\boldsymbol{a}^*$, which are linear in the data, the Least Squares estimates $\hat{\boldsymbol{a}}$ have the smallest variance (Gauß-Markoff theorem)

Properties are not valid, if conditions violated.

Straight line fit

Example: track fit of y (measured) vs. abscissa x

$$y_i = a_0 + a_1 \cdot x_i$$

Matrix $\boldsymbol{A}$ and parameter vector $\boldsymbol{a}$

$$\boldsymbol{A} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \qquad \boldsymbol{a} = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$$

Weight matrix is diagonal (*independent* measurements):

$$\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A} = \begin{pmatrix} \sum w_i & \sum w_i x_i \\ \sum w_i x_i & \sum w_i x_i^2 \end{pmatrix} \qquad \boldsymbol{A}^T \boldsymbol{W} \boldsymbol{y} = \begin{pmatrix} \sum w_i y_i \\ \sum w_i x_i y_i \end{pmatrix}$$

If one measured y_i-value is shifted (biased), then

- parameters biased, and
- χ^2-value very high.

Normal equations for uncorrelated data

Usually the direct measurements, which are input to a least squares problem, are *uncorrelated*, i.e. the covariance matrix $\boldsymbol{V}(\boldsymbol{y})$ and the weight matrix $\boldsymbol{W}$ are *diagonal*. This property, which is assumed here, simplifies the computation of the matrix products

$$\boldsymbol{C} = \boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A} \qquad \text{and} \qquad \boldsymbol{b} = \boldsymbol{A}^T \boldsymbol{W} \boldsymbol{y}$$

which are necessary for the solution

$$\hat{\boldsymbol{a}} = \boldsymbol{C}^{-1} \boldsymbol{b}$$

Normal equations for uncorrelated data contnd.

The diagonal elements of the weight matrix $\boldsymbol{W}$ are denoted by w_i, with $w_i = 1/\sigma_i^2$. Each data value y_i with its weight w_i makes an independent contribution to the final matrix products. Calling the i-th row $\boldsymbol{A}_i$, with

$$i\text{-th row of } \boldsymbol{A} \qquad \boldsymbol{A}_i = (d_1, d_2, \ldots, d_p)$$

the contributions of this row to $\boldsymbol{C}$ and $\boldsymbol{b}$ can be written as the $p \times p$-matrix $w_i \boldsymbol{A}_i^T \cdot \boldsymbol{A}_i$ and the p-vector $w_i \boldsymbol{A}_i^T \cdot y_i$. The contributions of a single row are:

$$\begin{array}{c|cccc} & d_1 & d_2 & \ldots & d_p \\ \hline d_1 & w_i d_1^2 & w_i d_1 d_2 & \ldots & w_i d_1 d_p \\ d_2 & & w_i d_2^2 & \ldots & w_i d_2 d_p \\ \ldots & & & \ldots & \ldots \\ d_p & & & & w_i d_p^2 \end{array} \qquad \begin{array}{c|c} & y_i \\ \hline d_1 & w_i d_1 z_i \\ d_2 & w_i d_2 z_i \\ \ldots & \ldots \\ d_p & w_i d_p z_i \end{array} ,$$

where the symmetric elements in the lower half are not shown.

Robust least square fit

Least square fit on observations y_i, yielding fitted values $\hat{y}_i$, and residuals $r_i = y_i - \hat{y}_i$. Estimate for the standard error of y_i (or of the r_i) is s_i.

- ”Clean” the data by pulling outliers towards their fitted values: winsorize the observations y_i and replace them by pseudo-observations y_i^*:

$$\begin{aligned} y_i^* &= y_i \,, & &\text{if} \quad |r_i| \leq c\, s_i \,, \\ &= \hat{y}_i - c\, s_i \,, & &\text{if} \quad r_i < -c\, s_i \,, \\ &= \hat{y}_i + c\, s_i \,, & &\text{if} \quad r_i > +c\, s_i \,. \end{aligned}$$

  The factor c regulates the amount of robustness, a goid choice is $c = 1.5$.

- Refit iteratively: the pseudo-observations y_i^* are used to calculate new parameters and new fitted values $\hat{y}_i$.

5. Orthogonal polynomials

If data interpolation required, but no parametrization known: Fit of normal general p-th polynomial to the data

$$f(x_i) \cong y_i \qquad \text{with} \quad f(x) = \sum_{j=0}^{p} a_j \, x^j$$

Generalization of straight-line fit to general p-th order polynomial straightforward: matrix $\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A}$ contains sum of all powers of x_i up to x_i^{2p}.

Disadvantage:

- fit numerically unstable
- determination of optimal order p difficult
- value of coefficients a_j depend on highest exponent p

Better: fit of orthogonal polynomial.

Straight line fit

Parametrization

$$f(x) = a_0 + a_1 x \quad \text{replaced by} \quad f(x) = a_0 \cdot p_0(x) + a_1 \cdot p_1(x)$$

The orthogonal polynomials $p_0(x)$ and $p_1(x)$ are defined by

$$\begin{aligned} p_0(x) &= b_{00} \\ p_1(x) &= b_{10} + b_{11} x = b_{11} \left(x - \langle x \rangle \right) \quad . \end{aligned}$$

with coefficients b_{00} and b_{11}

$$b_{00} = \left(\sum_{i=1}^{n} w_i \right)^{-1/2} \qquad b_{11} = \left(\sum_{i=1}^{n} w_i \left(x_i - \langle x \rangle \right)^2 \right)^{-1/2}$$

with the coefficient $b_{10} = -\langle x \rangle \, b_{11}$.

Advantage of new ansatz

$$\boldsymbol{A}^T\boldsymbol{W}\boldsymbol{A} = \begin{pmatrix} \sum w_i p_0^2(x_i) & \sum w_i p_0(x_i)p_1(x_i) \\ \sum w_i p_0(x_i)p_1(x_i) & \sum w_i p_1^2(x_i) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\boldsymbol{A}^T\boldsymbol{W}\boldsymbol{y} = \begin{pmatrix} \sum w_i p_0(x_i) y_i \\ \sum w_i p_1(x_i) y_i \end{pmatrix} = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$$

i.e. covariance matrix is unit matrix and parameters $\boldsymbol{a}$ are calculated by sums (no matrix inversion).

General orthogonal polynomial polynomial:

$$f(x) = \sum_{j=1}^{p} a_j p_j(x)$$

Title

Construction of higher order polynomial $p_j(x)$ by recurrence relation:

$$\boxed{\gamma p_j(x) = (x_i - \alpha)\, p_{j-1}(x) - \beta p_{j-2}(x)}$$

from the two previous functions $p_{j-1}(x)$ and $p_{j-2}(x)$ with parameters α and β defined by

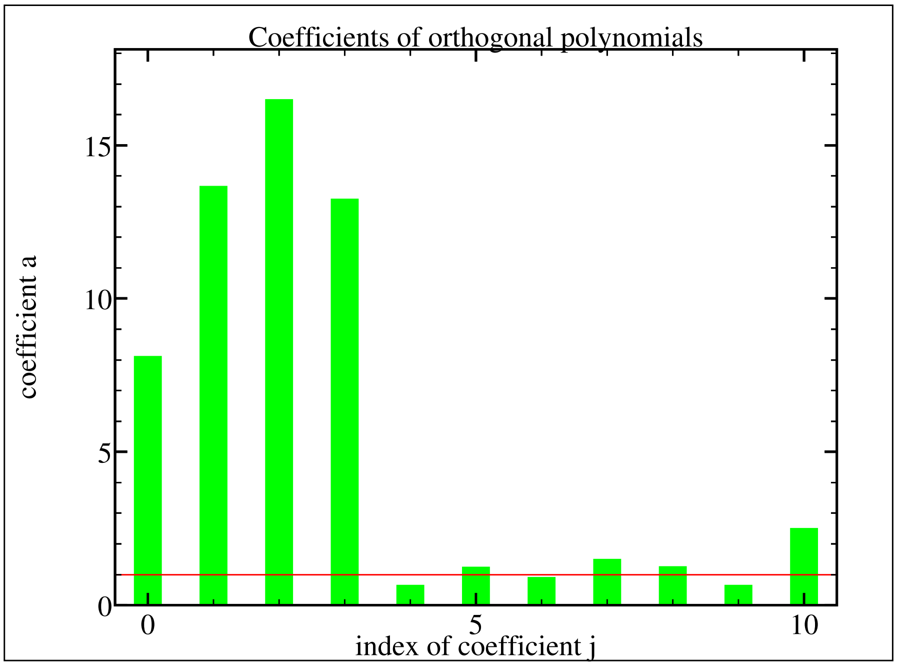
$$\alpha = \sum_{i=1}^{n} w_i x_i p_{j-1}^2(x_i) \qquad \beta = \sum_{i=1}^{n} w_i x_i p_{j-1}(x_i) p_{j-2}(x_i)$$

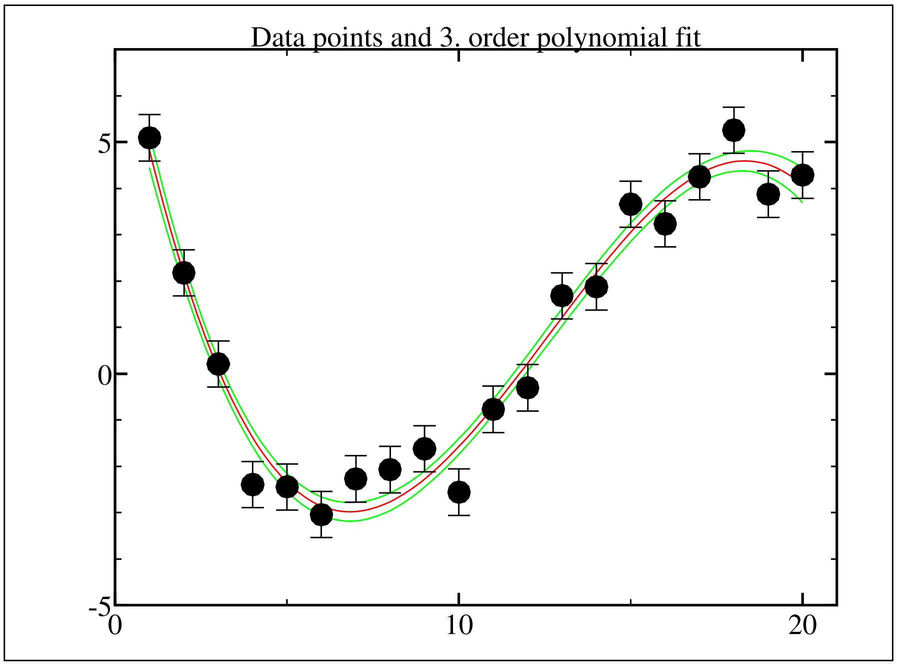
Normalization factor γ given by

$$\gamma^2 = \sum_{i=1}^{n} w_i \left[(x_i - \alpha)\, f_{j-1}\,(x_i) - \beta f_{j-2}\,(x_i)\right]^2$$

Parameters $\widehat{a}_j$ are determined from data by

$$\widehat{a}_j = \sum_{i=1}^{n} w_i p_j(x_i)\; y_i$$


Coefficients of orthogonal polynomials
coefficient a
index of coefficient j
0
5
10
15


Data points and 3. order polynomial fit
-5
0
5
10
20