Simulation of Nanosystems for Energy Conversion
Department of Electrical and Computer Engineering
Technical University of Munich

Python for Engineering Data Analysis

Least squares fitting

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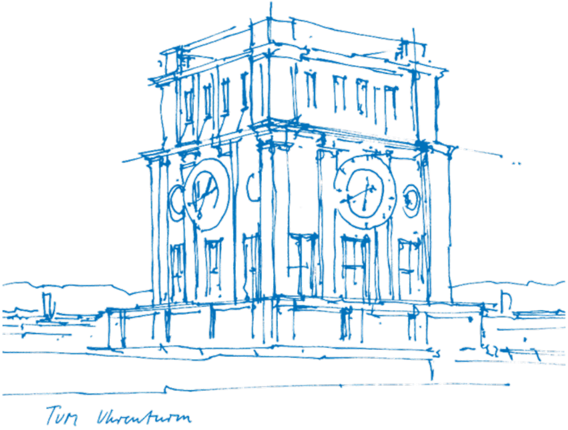
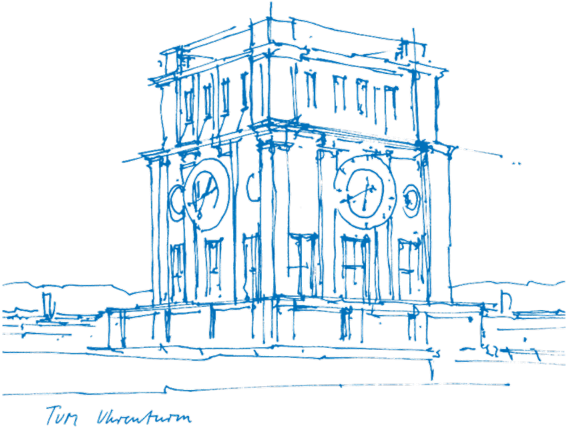


Linear least squares

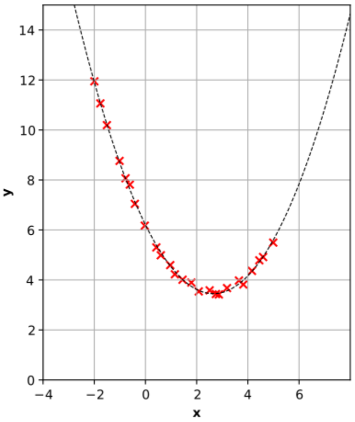


Linear least squares

- given a set of N measurements $(\vec{x}_i, y_i)$ with $i = 1, 2, \ldots, N$.
- find the best fitting curve $f(\vec{x}, \vec{\beta})$ with a set of parameters $\vec{\beta}$.
- in other words: find the parameters $\vec{\beta}$ that minimize the squared error ϵ^2.

$$\epsilon_i = y_i - f(\vec{x}_i, \vec{\beta}) \tag{1}$$

$$\epsilon^2 = \sum_{i=1}^{N} \epsilon_i^2 = \vec{\epsilon}^{\mathrm{T}} \cdot \vec{\epsilon} \tag{2}$$



Linear least squares

- define a target function $f(\vec{x}, \vec{\beta})$.
- if the target function is linear in the parameters $\vec{\beta}$ one can decompose f into

$$f(\vec{x}, \vec{\beta}) = \beta_0 + \beta_1 f_1(\vec{x}) + \beta_2 f_2(\vec{x}) + \ldots \tag{3}$$

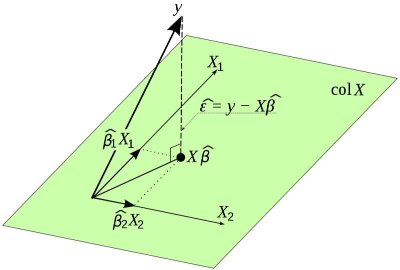
$$= (1, f_1, f_2, \ldots) \cdot \vec{\beta} = \boldsymbol{X} \cdot \vec{\beta} \tag{4}$$

- $\Longrightarrow$ solve (approximate) the linear system

$$\boldsymbol{X} \cdot \vec{\beta} \approx \vec{y} = \vec{y}_{\parallel} + \vec{y}_{\perp} \tag{5}$$

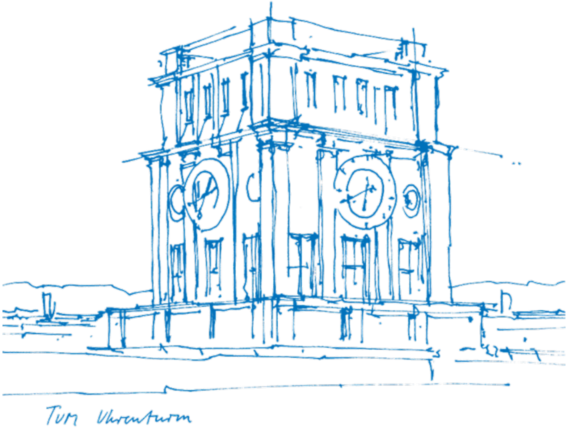
$$\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X} \cdot \vec{\beta} = \boldsymbol{X}^{\mathrm{T}} \cdot \vec{y}_{\parallel} + \cancel{\boldsymbol{X}^{\mathrm{T}} \cdot \vec{y}_{\perp}} \tag{6}$$

$$\vec{\beta} = (\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1} \cdot \boldsymbol{X}^{\mathrm{T}}\vec{y} \tag{7}$$



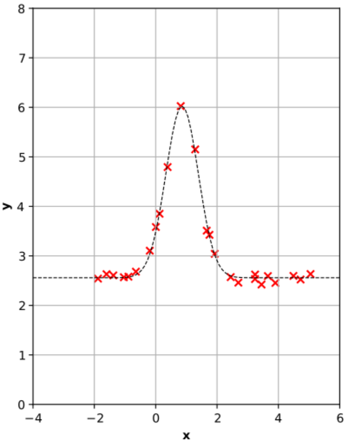
Geometric interpretation:
Find the closest point in the column space of $\boldsymbol{X}$ to the point $\vec{y}$.

Non-linear least squares



Non-linear least squares

- for non-linear problems the parameters $\vec{\beta}$ are not independent and a decomposition of f is not possible.
- an iterative algorithm is necessary to find the solution.
  - Gradient descent method
  - Gauss-Newton method
  - Levenberg-Marquardt method
- start with an initial set of parameters β_0 and update them by a step $\Delta\beta$ minimizing the error function ϵ^2 step by step.



Gradient descent method

- Compute the gradient of the error function ϵ^2 with respect to each parameter β_i

$$\frac{\partial \epsilon^2}{\partial \beta_i} = -2 \sum_{j=1}^{N} \epsilon_j \cdot \frac{\partial f(\vec{x}_j, \vec{\beta})}{\partial \beta_i} \tag{8}$$

$$\nabla_\beta \epsilon^2 = -2 \vec{\epsilon}^{\mathrm{T}} \cdot \boldsymbol{J} \tag{9}$$

- with the jacobian matrix $\boldsymbol{J}$ collecting all the derivatives with respect to β_i (columns) evaluated at all measurement points x_j (rows).
- advance a (small) step α along the negative gradient to update the parameters.

$$\Delta \vec{\beta} = \alpha \boldsymbol{J}^{\mathrm{T}} \vec{\epsilon} \tag{10}$$

Gauss-Newton method

- linearize the problem at the current parameter set β^k and find the best fitting parameters for the linearized problem. (k is the iteration counter)
- update the parameters and repeat the linearization at the new position β^{k+1}.

$$f(x, \vec{\beta}^{k+1}) = f(x, \vec{\beta}^k) + \frac{\partial f}{\partial \beta_1} \Delta\beta_1 + \frac{\partial f}{\partial \beta_2} \Delta\beta_2 + \cdots = y \tag{11}$$

$$\boldsymbol{J} \Delta\vec{\beta} = \vec{y} - f(x, \vec{\beta}^k) = \vec{\epsilon} \tag{12}$$

$$\Delta\vec{\beta} = (\boldsymbol{J}^{\mathrm{T}} \boldsymbol{J})^{-1} \cdot \boldsymbol{J}^{\mathrm{T}} \vec{\epsilon} \tag{13}$$

- the Gauss-Newton method converges fast, but only for "well behaving" functions $f(x, \vec{\beta})$.
- the start position β_0 has to be fairly close to the minimum already.

Levenberg-Marquardt method

- combination of the Gauss-Newton method and the gradient descent method.
- A prose description would be: "use small gradient descent steps towards the minimum when necesary and use larger Gauss-Newton steps when possible".

$$(\boldsymbol{J}^{\mathrm{T}}\boldsymbol{J} + \lambda \boldsymbol{I}) \cdot \Delta\vec{\beta} = \boldsymbol{J}^{\mathrm{T}}\vec{\epsilon} \tag{14}$$

- for $\lambda = 0$ the method is similar to the Gauss-Newton method.
- for large λ the method is similar to the gradient descent method, because $\boldsymbol{J}^{\mathrm{T}}\boldsymbol{J}$ will become negligible.
- the choice of λ can be optimized according to the particular problem.
- literature suggests a starting value according to the 2-norm of the matrix $\boldsymbol{J}^{\mathrm{T}}\boldsymbol{J}$.

$$\lambda^0 = ||\boldsymbol{J}^{\mathrm{T}}\boldsymbol{J}||_2 \tag{15}$$

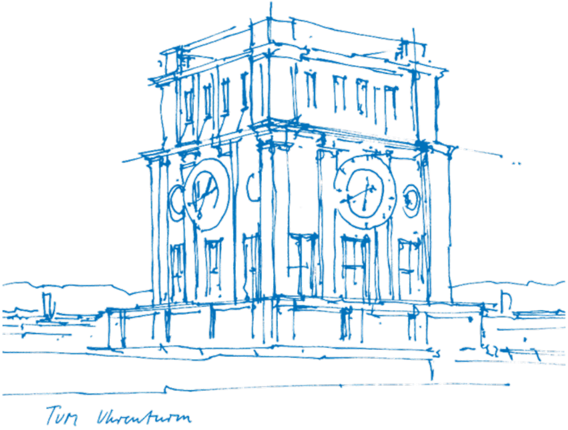
Levenberg-Marquardt method

- Marquardt developed a strategy to update λ every step.
- he introduced a measure for the improvement of an iteration step $\Delta\beta$

$$\rho^k = \frac{\epsilon^2(x, \vec{\beta}^k) - \epsilon^2(x, \vec{\beta}^{k+1})}{\Delta\vec{\beta}^{\mathrm{T}} \cdot (\lambda^k \Delta\vec{\beta} + \boldsymbol{J}^{\mathrm{T}} \vec{\epsilon}(x, \vec{\beta}^k))}, \tag{16}$$

  where the numerator represents the error reduction by the iteration step, and the denominator represents the predicted error reduction by the local linear model.
- if $\rho^k > 0.75$ then $\lambda^{k+1} = \lambda^k/3$.
- if $\rho^k < 0.25$ then $\lambda^{k+1} = 2\lambda^k$.
- otherwise $\lambda^{k+1} = \lambda^k$.
- only perform update step $\beta^{k+1} = \beta^k + \Delta\beta$ if $\rho^k > 0$. (if there is improvement at all)

Links



Some links with further information

- http://people.duke.edu/~hpgavin/ce281/lm.pdf
- http://people.compute.dtu.dk/pcha/LSDF/NonlinDataFit.pdf
- https://www.youtube.com/watch?v=lsKIhNkzpbw
- https://www.youtube.com/watch?v=8evmj2L-iCY
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