Introduction into Linear Regression

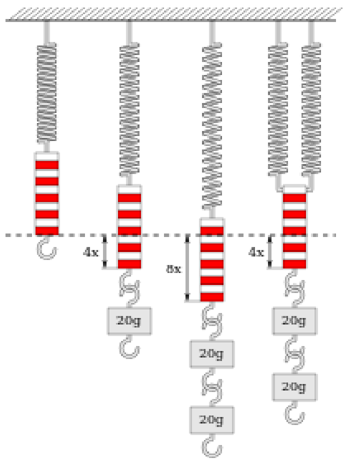
- Theory and experiment:
  How to confirm the congruence?

- Example:
  Elongation y [cm] of a spring subject to a force t [N]

  Hooke's law:

$$y = y_0 + \frac{1}{D} t$$

  (D spring constant, describes stiffness of spring, y_0 pre-elongation of spring due to own weight)



Source: Wikipedia

- Are the free parameters D, y_0 constant over different experiments?

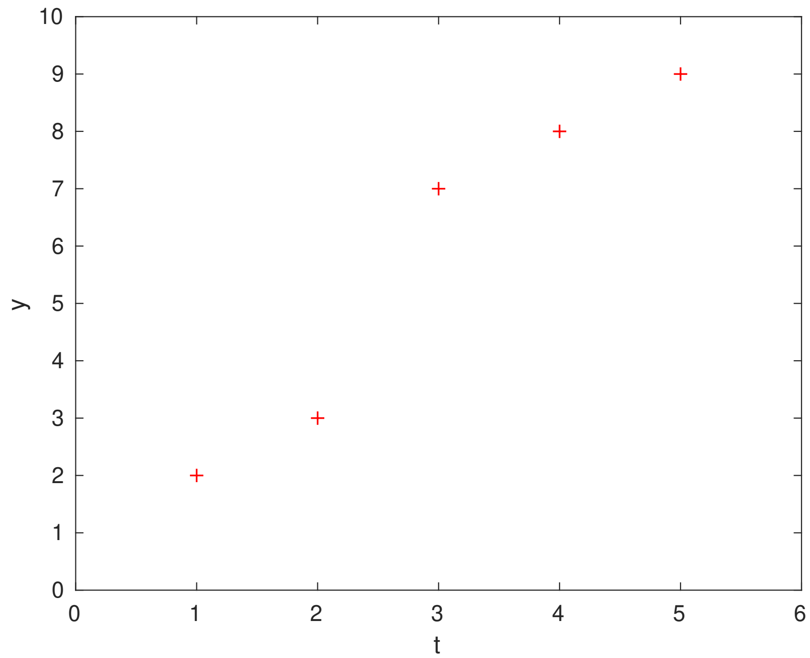
Linear Regression - Intro

$$\text{Theory: } y(t) = x_1 + x_2\, t$$

$$\text{Data: } (t_i, y_i)$$

$$\text{Error (residuum): } r_i = y_i - y(t_i)$$

i	t_i	y_i	$y(t_i)$	r_i	r_i^2
1	1	2			
2	2	3			
3	3	7			
4	4	8			
5	5	9			



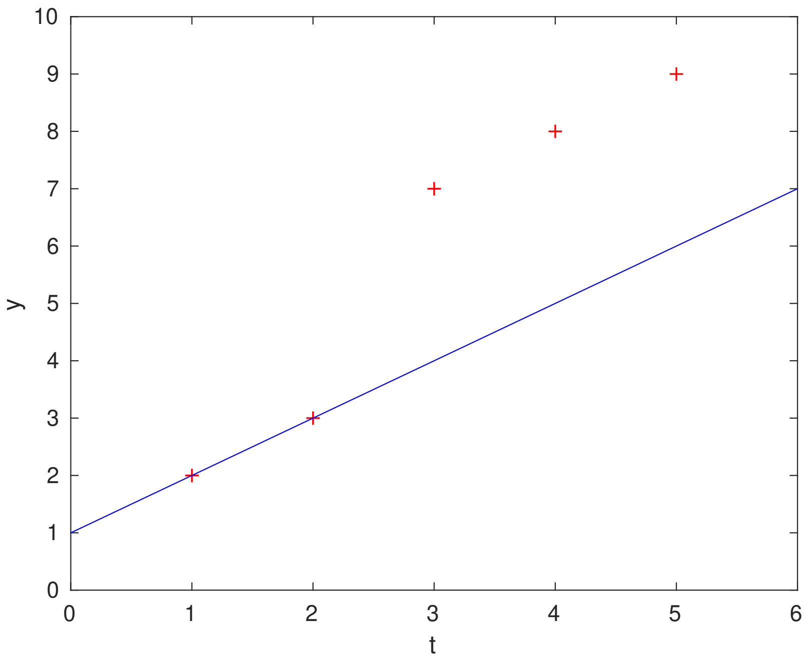
Linear Regression - 1st Try

Theory: $y(t) = 1 + t$

Data: (t_i, y_i)

Error (residuum): $r_i = y_i - y(t_i) = y_i - 1 - t_i$

i	t_i	y_i	$y(t_i)$	r_i	r_i^2
1	1	2	2	0	0
2	2	3	3	0	0
3	3	7	4	3	9
4	4	8	5	3	9
5	5	9	6	3	9
				$\Sigma_{i=1}^5 r_i^2$	$= 27$



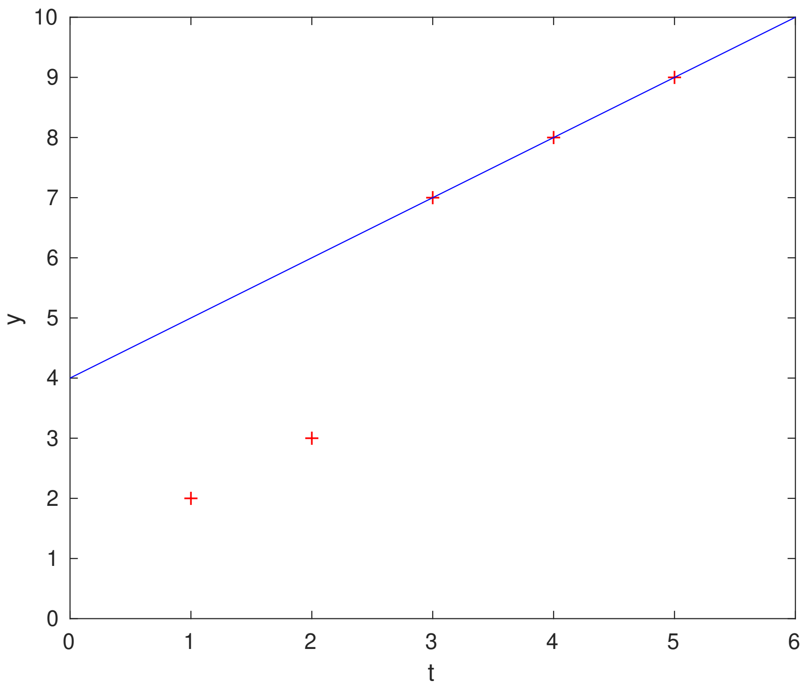
Linear Regression - 2nd Try

Theory: $y(t) = 4 + t$

Data: (t_i, y_i)

Error (residuum): $r_i = y_i - y(t_i) = y_i - 4 - t_i$

i	t_i	y_i	$y(t_i)$	r_i	r_i^2
1	1	2	5	-3	9
2	2	3	6	-3	9
3	3	7	7	0	0
4	4	8	8	0	0
5	5	9	9	0	0
				$\Sigma_{i=1}^5 r_i^2$	$= 18$



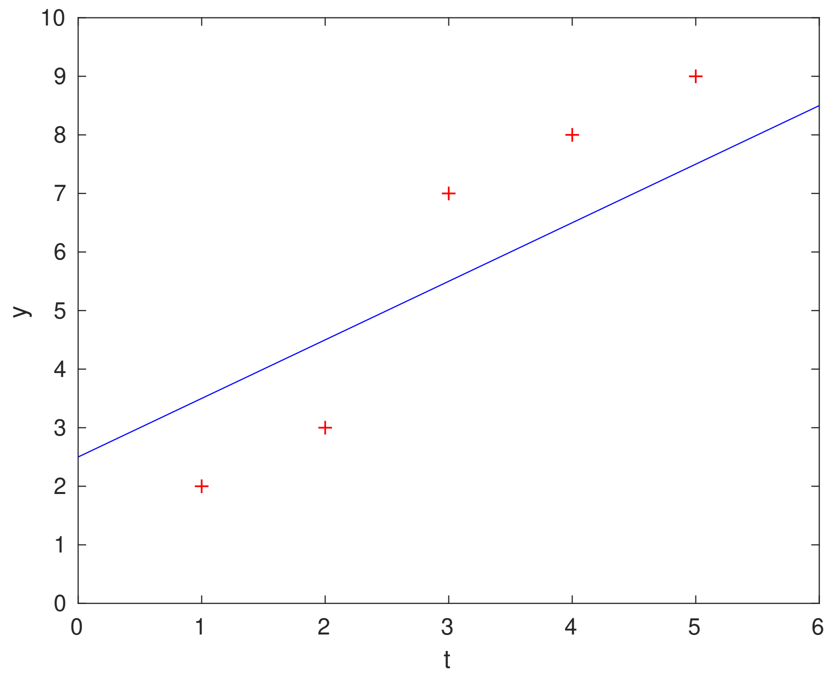
Linear Regression - 3rd Try

Theory: $y(t) = 2.5 + t$

Data: (t_i, y_i)

Error (residuum): $r_i = y_i - y(t_i) = y_i - 2.5 - t_i$

i	t_i	y_i	$y(t_i)$	r_i	r_i^2
1	1	2	3.5	−1.5	2.25
2	2	3	4.5	−1.5	2.25
3	3	7	5.5	1.5	2.25
4	4	8	6.5	1.5	2.25
5	5	9	7.5	1.5	2.25
				$\Sigma_{i=1}^{5} r_i^2 = 11.25$	



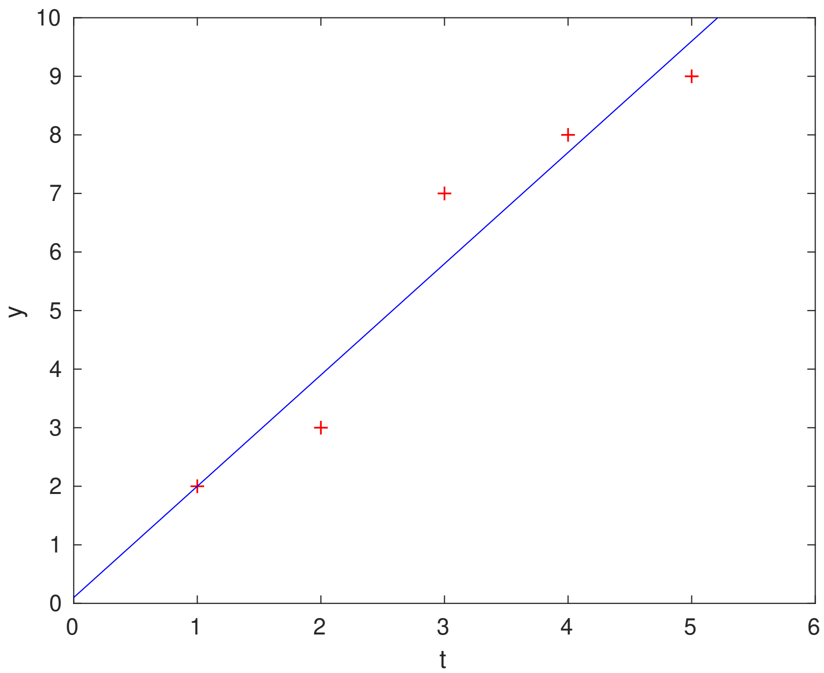
Linear Regression - Solved

Theory: $y(t) = 0.1 + 1.9\,t$

Data: (t_i, y_i)

Error (residuum): $r_i = y_i - y(t_i) = y_i - 0.1 - 1.9\,t_i$

i	t_i	y_i	$y(t_i)$	r_i	r_i^2
1	1	2	2	0	0
2	2	3	3.9	-0.9	0.81
3	3	7	5.8	1.2	1.44
4	4	8	7.7	0.3	0.09
5	5	9	9.6	-0.6	0.36
				$\Sigma_{i=1}^5 r_i^2 = 2.7$	



Linear Regression: Normal Equations $(n=2)$

Motivation normal equations $\rightsquigarrow$ see blackboard

In general (m arbitrary):

$$A^\top A = \begin{pmatrix} m & \sum_{i=1}^m t_i \\ \sum_{i=1}^m t_i & \sum_{i=1}^m t_i^2 \end{pmatrix}, \quad A^\top \mathbf{y} = \begin{pmatrix} \sum_{i=1}^m y_i \\ \sum_{i=1}^m t_i y_i \end{pmatrix}$$

$$x_1 = \frac{\sum_{i=1}^m t_i^2 \sum_{j=1}^m y_j - \sum_{i=1}^m t_i \sum_{j=1}^m t_j y_j}{m \sum_{i=1}^m t_i^2 - \left(\sum_{i=1}^m t_i\right)^2}$$

$$x_2 = \frac{m \sum_{i=1}^m t_i y_i - \sum_{i=1}^m t_i \sum_{j=1}^m y_j}{m \sum_{i=1}^m t_i^2 - \left(\sum_{i=1}^m t_i\right)^2}$$

Case $m=5$:

$$A^T A = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ t_1 & t_2 & t_3 & t_4 & t_5 \end{pmatrix} \begin{pmatrix} 1 & t_1 \\ 1 & t_2 \\ 1 & t_3 \\ 1 & t_4 \\ 1 & t_5 \end{pmatrix} = \begin{pmatrix} 5, & \sum_{i=1}^5 t_i \\ \sum_{i=1}^5 t_i, & \sum_{i=1}^5 t_i^2 \end{pmatrix}$$

Linear Regression: Motivation & Aims

We conclude:

- In general more data points y_i (here 5) as parameters x_i (here 2)
- Measurement of process/data collection afflicted with uncertainties (w/o systematical errors)
- Overdetermined LES $\rightsquigarrow$ in general no solution exists

Aims:

- Determine $\mathbf{x} = (x_1, \ldots, x_n)^\top$ "optimally" from data
- General method to do that

We call this **regression** (in particular in stochastics) or **curve fitting**.

Special case of a mathematical optimization method

Linear Regression: Stochastic Uncertainties

Problem (Linear Regression)

Assume: linear relation (e.g. from physics)

$$y(t) = x_1 + x_2 t$$

Given: data points (t_i, y_i), $i = 1, \dots, m$, afflicted with uncertainties (errors) ε_i. The uncertainties are random variables and 0 in average.

Searched for: $x_1, x_2 \in \mathbb{R}$, such that

$$\begin{pmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_i \\ \vdots & \vdots \\ 1 & t_m \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_m \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_i \\ \vdots \\ \varepsilon_m \end{pmatrix}$$

We write

$$A\mathbf{x} = \mathbf{y} + \boldsymbol{\varepsilon}$$

with $A \in \mathbb{R}^{m \times 2}$, $\mathbf{x} \in \mathbb{R}^2$, $\mathbf{y}, \boldsymbol{\varepsilon} \in \mathbb{R}^m$.

Minimization Problem

General situation: $A \in \mathbb{R}^{m\times n}$, $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$

Idea: determine $\mathbf{x} = (x_1, \dots, x_n)^\top$, such that the error in the LES

$$\|A\mathbf{x} - \mathbf{y}\|_2 = \sqrt{\sum_{i=1}^{m}\left(\sum_{j=1}^{n} A_{ij}x_j - y_i\right)^2} \quad \text{bzw.} \quad \frac{1}{2}\|A\mathbf{x} - \mathbf{y}\|_2^2$$

is minimized.

The minimum is denoted by $\hat{\mathbf{x}}$.

This minimization problem is called a **linear regression problem** or **least-squares problem**.

Method of least squares, better **method of least residual sum of squares**
By C. F. Gauß and A.-M. Legendre (1805)

General problem

Problem ($\star$) (Lin. regression as minimization problem)

Let be given a matrix $A \in \mathbb{R}^{m \times n}$ and a vector $\mathbf{y} \in \mathbb{R}^m$ with $m, n \in \mathbb{N}$.

We search for the solution $\hat{\mathbf{x}} \in \mathbb{R}^n$ of the minimization problem

$$\frac{1}{2}\|A\hat{\mathbf{x}} - \mathbf{y}\|_2^2 = \min_{x \in \mathbb{R}^n} \frac{1}{2}\|A\mathbf{x} - \mathbf{y}\|_2^2.$$

- If $m = n$ and A invertible, then $A\mathbf{x} = \mathbf{y}$ has a unique solution.
- The case $m > n$ is of uttermost importance in applications.
- In the case $m < n$ the LES $A\mathbf{x} = \mathbf{y}$ is underdetermined. It may be unsolvable, if $\cancel{R}ank(A) \neq \cancel{R}ank(A \mid \mathbf{y})$.

Moreover, other norms as $\|\cdot\|_2$ could be considered. Then the determination of solutions is harder in general, since differentiability might not be given.

Gaussian normal equations

Theorem (Gaussian normal equations)

$\hat{x}$ solves Problem $(\star)$ if and only iff the **normal equations**

$$A^\top A \hat{\mathbf{x}} = A^\top \mathbf{y}.$$

hold true.

$A^\top A \in \mathbb{R}^{n \times n}$ is symmetric and positive semi-definite.

Theorem (Uniqueness)

Let $m \geq n$. Suppose $A \in \mathbb{R}^{m \times n}$ has maximal rank,
d.h. $rank(A) = n$.
Exactly then the minimization problem $(\star)$ or the normal equations, resp., are uniquely solvable.

Then $A^\top A \in \mathbb{R}^{n \times n}$ is invertible and positive definite.

(Non-)Linear Regression: TTF under Temperature Stress

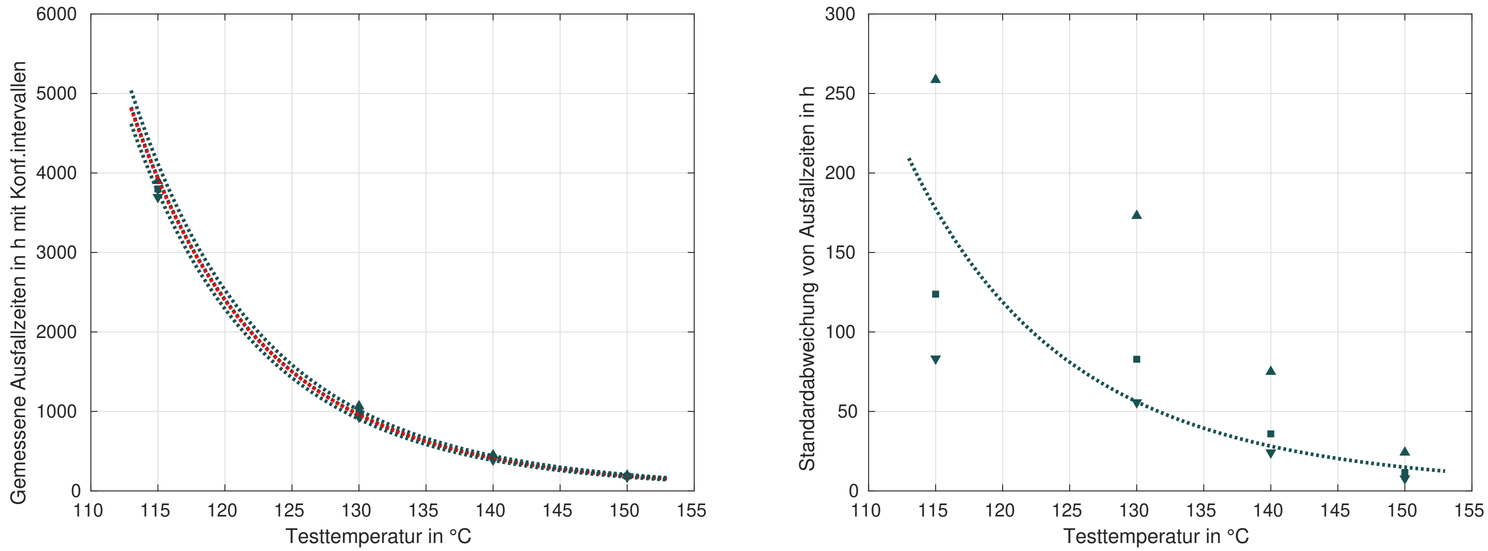


Figure: Curve fitting over different temperatures T compared with measured data points (squares) with confidence intervals for $q = 90\%$ (triangles). Left-hand side for $\mu_{krit}(T) \pm \sigma_{krit}(T)$, in red the fitted curve, right-hand side $\sigma_{krit}(T)$. [K., Dvorsky, Ließ, Avenhaus 2019]

Model based approach

$$f_{krit}(T) = t_{\ominus} + t_0 \exp\left(\left(\frac{T_a}{T - T_\infty}\right)^d\right)$$

Lin. Regression: Transformation

Example (Measurement of TTF (Time-To-Failure) of Electrical Automotive Components)

T	[°C]	115	130	140	155
μ_{krit}	$[h]$	3791.62	987.74	439.66	189.94

Conjecture (model based): Arrhenius law

$$\mu_{krit}(T) = t_0 \exp\left(\frac{T_a}{T - T_\infty}\right)$$

(μ_{krit} TTF in h, t_0 reaction-kinetic period in h, T temperature in K, T_a activation temperature in K, $T_\infty = 173.15$ consolidation temperature in K)

We may transform this into an affine-linear relation

$$ln(\mu_{krit}(T)) = ln(t_0) + \frac{T_a}{T - T_\infty} \qquad \Longleftrightarrow \qquad y(t) = x_1 + x_2 t$$

By insertion of measured data we obtain a linear equation system (LES)

$$y_i = x_1 + x_2 t_i, \quad i = 1, \ldots, 4.$$

Linear Regression: Example - Result

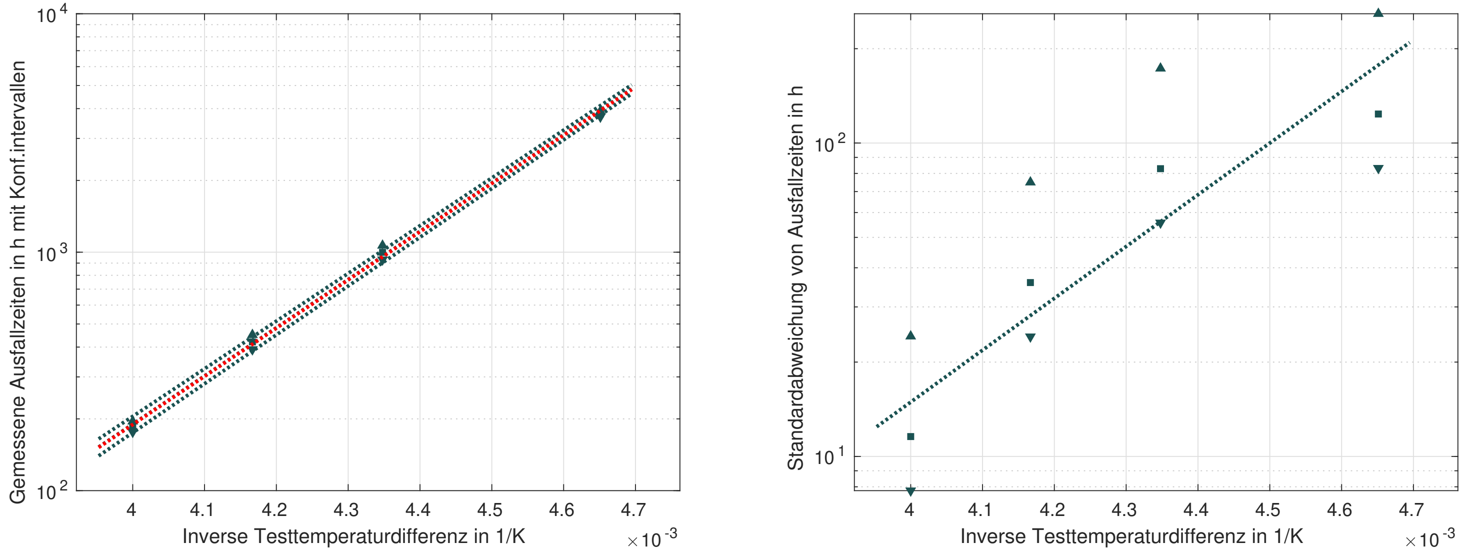


Figure: Curve fitting over different inverse temperature differences t, in semi-logarithmic representation and compared with measured data points (squares) together with confidence intervals for $q = 90\%$ (triangles). Left-hand side for $t_{krit}(1/t) \pm \sigma_{krit}(1/t)$, in red the fitted curve. Right-hand side $\sigma_{krit}(T)$. [K., Dvorsky, Ließ, Avenhaus 2019]

Linear Regression: Example - Re-transformed Result

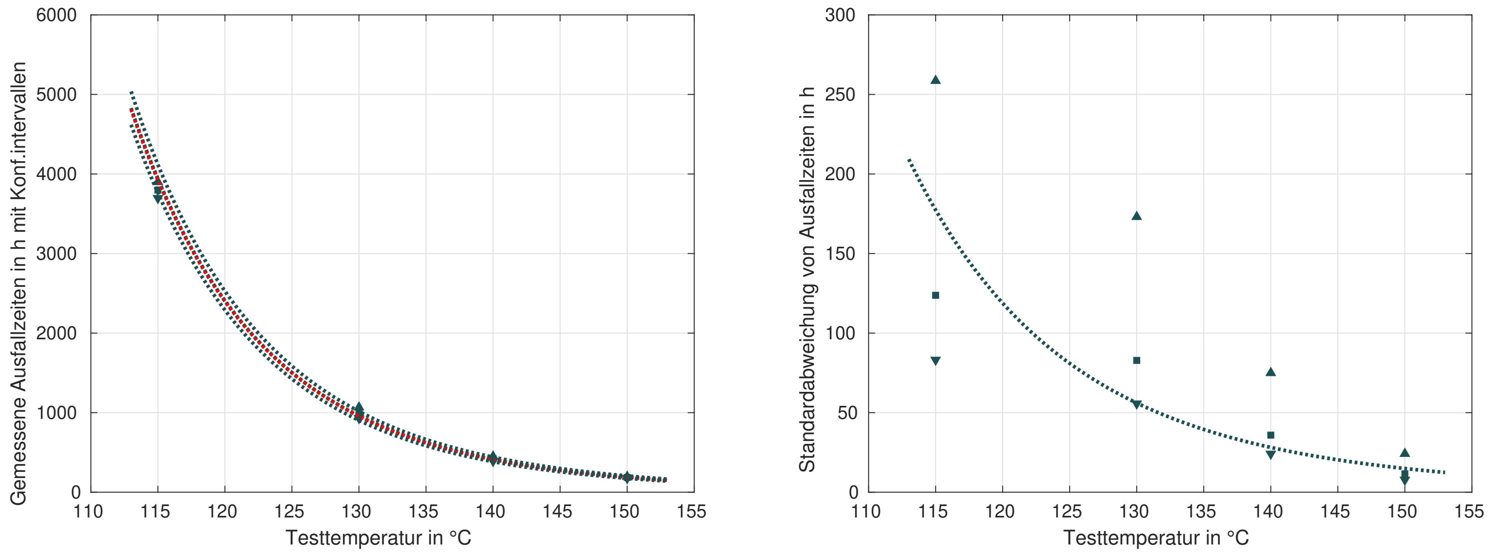


Figure: Curve fitting over different temperatures T, re-transformed in exponential representation and compared with measured data points (squares) together with confidence intervals for $q = 90\%$ (triangles). Left-hand side for $t_{krit}(T) \pm \sigma_{krit}(T)$, in red the fitted curve. Right-hand side $\sigma_{krit}(T)$. [K., Dvorsky, Ließ, Avenhaus 2019]