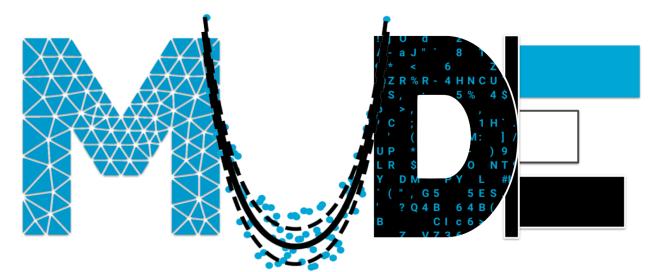
Welcome to...



Modelling, Uncertainty, and Data for Engineers

Sensing and Observation Theory part 2



Course evaluation

Please help us evaluate and improve MUDE with your feedback!





6. Observation theory \wedge 6.1. Introduction 6.2. Least-squares estimation ~ 6.3. Weighted least-squares V estimation 6.4. Best linear unbiased estimation 6.5. Precision and confidence \vee intervals 6.6. Maximum Likelihood **Estimation** 6.7. Non-linear least-squares V estimation 6.8. Model testing 6.9. Hypothesis testing for ~ Sensing and Monitoring 6.10. Notation and formulas

6.7. Non-linear least-squares estimation Notebook Gauss-Newton iteration for GNSS Trilateration 6.8. Model testing 6.9. Hypothesis testing for Sensing and Monitoring Notebook exercise: which melting model is better? Notebook exercises: is my null hypothesis good enough?

Review



Estimators - overview

Functional model: $\mathbb{E}(Y) = \mathrm{A} \cdot \mathrm{x}$

Stochastic model: $\mathbb{D}(Y) = \Sigma_Y$

Weighted Least-Squares estimation: minimizing weighted sum of squared errors
 allows to give different weights to observations

$$\hat{X} = (\mathbf{A}^T \mathbf{W} \mathbf{A})^{-1} \mathbf{A}^T \mathbf{W} \cdot Y$$

• Best Linear Unbiased estimation : $\min\left(trace(\Sigma_{\hat{X}})\right)$ (best), $\hat{X}=\mathbf{L}^T\cdot Y$ (linear), $\mathbb{E}(\hat{X})=\mathbf{x}$ (unbiased)

$$\hat{X} = \left(\mathbf{A}^T \Sigma_Y^{-1} \mathbf{A}\right)^{-1} \mathbf{A}^T \Sigma_Y^{-1} Y$$

Maximum Likelihood estimation : most likely x for given y,

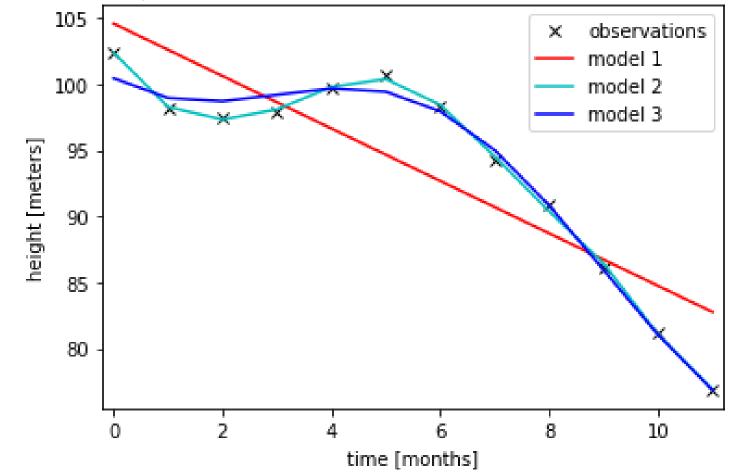
for normally distributed data same as BLUE

Maximum likelihood estimation is an important method, also for machine learning (Q2), and is included as reference material (will not be on exam or in assignments)



Results from notebooks

- Underfitting: model too simplistic, does not capture the real signal
- Overfitting: nearly perfect fit, but no physical interpretation



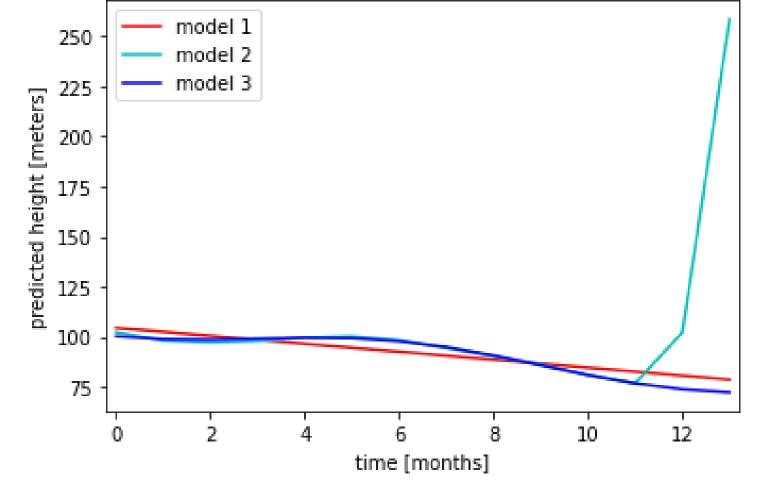


Results from notebooks

Underfitting: model too simplistic, does not capture the real signal

Overfitting: nearly perfect fit, but no physical interpretation → very risky if you use model for

prediction

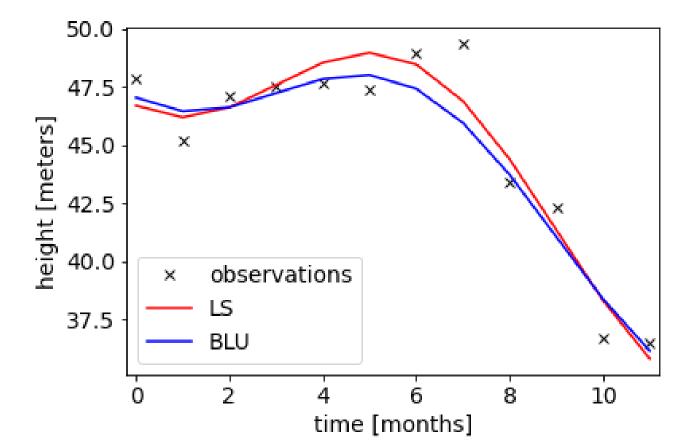




Best linear unbiased estimator = best weighted least squares estimator

Weight matrix is inverse covariance matrix:

Makes sense: high precision → small variance → large weight





.

$$Y = A \cdot x + \epsilon$$

$$\mathbb{D}(Y) = \Sigma_Y = \Sigma_\epsilon$$

Question that may have popped up:

Where does Σ_V come from?

- → Calibration:
 - > Repeated measurements
 - Calculate standard deviation

Usually observables are assumed to be independent, since the random errors are independent (error of observation Y_i does not depend on the error of observation Y_i

When would observable be dependent?

- due to signal processing in sensor (often when sampling rate is too high)
- if we use differential observables
- if we apply a common correction to our observations which is stochastic



Open questions

- (How to come up with a model?)
- What if my model is non-linear?
- Does my model really fit?
- Which models fits best?



What if my observation equations are non-linear?



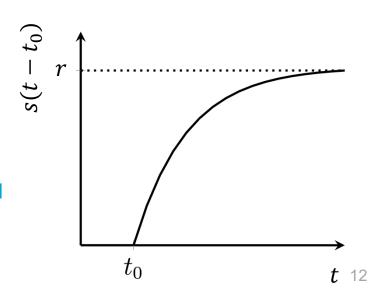
Observed: ground water level rise due to rainfal

$$E(Y_i) = p \cdot r \left(1 - \exp\left(-\frac{t - t_0}{a}\right) \right)$$

$$s(t - t_0)$$

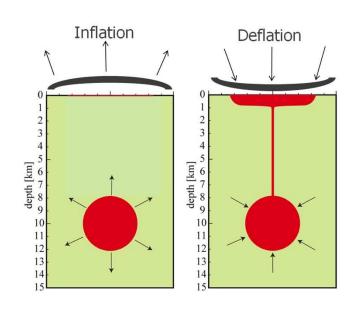
- Known parameter:
 - > p [m]: constant water inflow during rain event
- Unknown parameters:
 - \triangleright scaling parameter a [days] (memory of system),
 - \triangleright response r [m/m] of the aquifer depending on the amount of rainfall



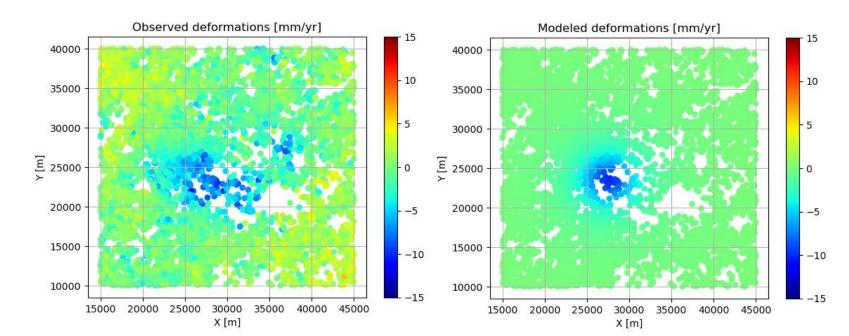


Volcano deformation rates at known locations (x_i, y_i)

$$\mathbb{E}(Y_i) = \frac{0.73\Delta V}{\pi d^2} \cdot (1 + \frac{1}{d^2}((x_i - x_s)^2 + (y_i - y_s)^2))^{-\frac{3}{2}}$$



Unknown parameters: volume change ΔV , depth of magma chamber d, (x_s, y_s) horizontal coordinates of centre



Linearized observation equation using 1st order Taylor approximation 1 observation 1 unknown

$$y = q(x) + \epsilon \approx q(x_{[0]}) + \partial_x q(x_{[0]})(x - x_{[0]}) + \epsilon$$

for now: omit ϵ from equations

initial guess

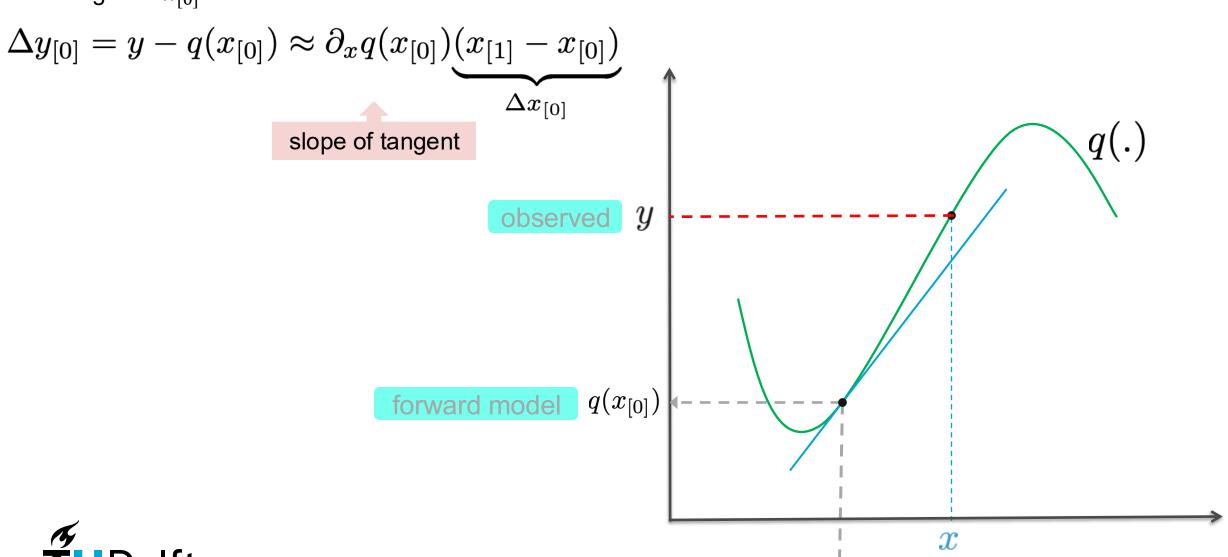
$$\Delta y = y - q(x_{[0]}) \approx \partial_x q(x_{[0]}) \underbrace{(x - x_{[0]})}_{\Delta x}$$

observed-minuscomputed



Input:

- observation *y*
- initial guess $x_{[0]}$



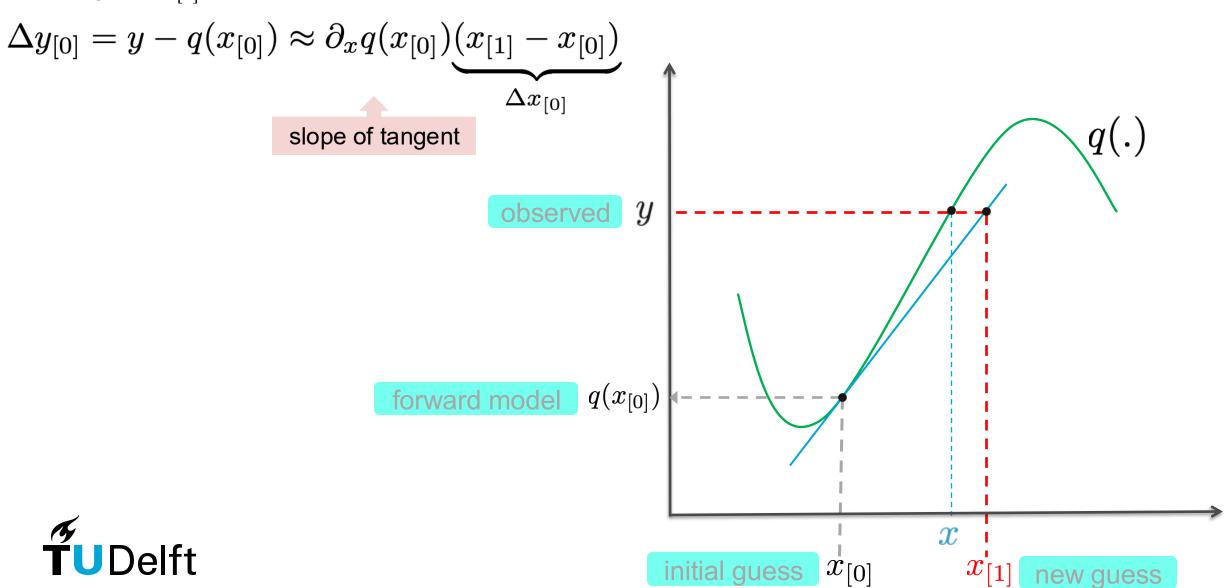
 $x_{[0]}$

initial guess



Input:

- observation *y*
- initial guess $x_{[0]}$



new guess

Input:

- observation *y*
- new guess $x_{[1]}$

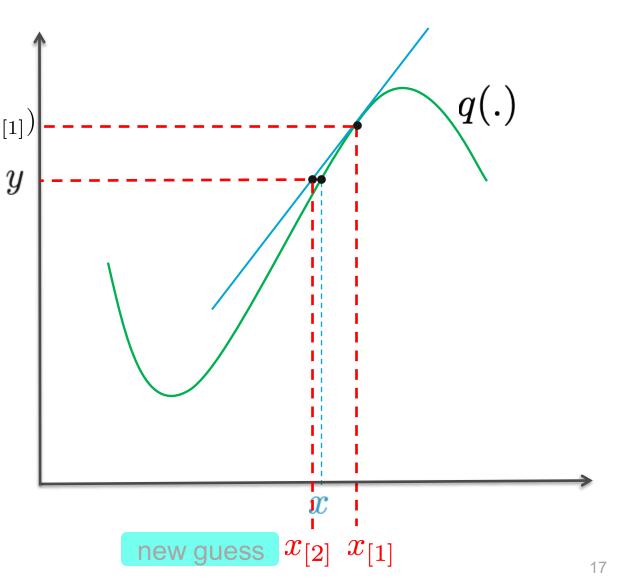
$$\Delta y_{[1]} = y - q(x_{[1]}) \approx \partial_x q(x_{[1]}) \underbrace{(x_{[2]} - x_{[1]})}_{}$$

 $c_{[2]}-x_{[1]}$ $\Delta x_{[1]}$ $q(x_{[1]})$ observed y

→ Gauss-Newton iteration

Continue until $\Delta x_{[i]}$ is very small





Linearized observation equation using 1st order Taylor approximation 1 observation n unknowns

$$\Delta y_{[i]} = y - q(\mathbf{x}_{[i]}) \approx \partial_{\mathbf{x}} q(\mathbf{x}_{[i]}) \underbrace{(\mathbf{x} - \mathbf{x}_{[i]})}_{\Delta \mathbf{x}_{[i]}}$$

$$= \begin{bmatrix} \partial_{x_1} q(\mathbf{x}_{[i]}) & \partial_{x_2} q(\mathbf{x}_{[i]}) & \cdots & \partial_{x_n} q(\mathbf{x}_{[i]}) \end{bmatrix} \begin{bmatrix} x_1 - x_{1,[i]} \\ x_2 - x_{2,[i]} \\ \vdots \\ x_n - x_{n,[i]} \end{bmatrix}$$

i is the iteration index



Non-linear functional model

$$\mathbb{E}(egin{bmatrix} Y_1 \ Y_2 \ dots \ Y_m \end{bmatrix}) = egin{bmatrix} q_1(\mathbf{x}) \ q_2(\mathbf{x}) \ dots \ q_m(\mathbf{x}) \end{bmatrix}$$

Linearized functional model

$$\mathbb{E}\begin{pmatrix}\begin{bmatrix}\Delta Y_1\\\Delta Y_2\\\vdots\\\Delta Y_m\end{bmatrix}_{[i]}\end{pmatrix} = \begin{bmatrix}\partial_{x_1}q_1(\mathbf{x}_{[i]}) & \partial_{x_2}q_1(\mathbf{x}_{[i]}) & \cdots & \partial_{x_n}q_1(\mathbf{x}_{[i]})\\\partial_{x_1}q_2(\mathbf{x}_{[i]}) & \partial_{x_2}q_2(\mathbf{x}_{[i]}) & \cdots & \partial_{x_n}q_2(\mathbf{x}_{[i]})\\\vdots\\\vdots\\\partial_{x_1}q_m(\mathbf{x}_{[i]}) & \partial_{x_2}q_m(\mathbf{x}_{[i]}) & \cdots & \partial_{x_n}q_m(\mathbf{x}_{[i]})\end{bmatrix}\begin{bmatrix}\Delta x_1\\\Delta x_2\\\vdots\\\Delta x_n\end{bmatrix}_{[i]}$$



Gauss-Newton iteration

Start with initial guess $x_{[0]}$, and start iteration with i = 0

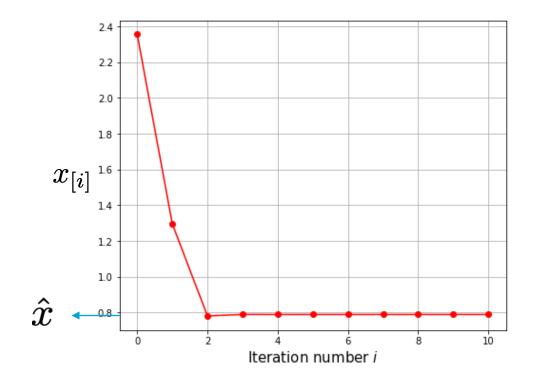
- 1. Calculate observed-minus-computed $\Delta y_{[i]}$
- 2. Determine the Jacobian
- 3. Estimate $\Delta \hat{x}_{[i]}$ by applying BLUE
- 4. New guess $x_{[i+1]} = \Delta \hat{x}_{[i]} + x_{[i]}$

WHEN TO STOP?

$$\mathbb{E}\begin{pmatrix}\begin{bmatrix} \Delta Y_1 \\ \Delta Y_2 \\ \vdots \\ \Delta Y_m \end{bmatrix}_{[i]} = \begin{bmatrix} \partial_{x_1} q_1(\mathbf{x}_{[i]}) & \partial_{x_2} q_1(\mathbf{x}_{[i]}) & \cdots & \partial_{x_n} q_1(\mathbf{x}_{[i]}) \\ \partial_{x_1} q_2(\mathbf{x}_{[i]}) & \partial_{x_2} q_2(\mathbf{x}_{[i]}) & \cdots & \partial_{x_n} q_2(\mathbf{x}_{[i]}) \\ \vdots & \vdots & & \vdots \\ \partial_{x_1} q_m(\mathbf{x}_{[i]}) & \partial_{x_2} q_m(\mathbf{x}_{[i]}) & \cdots & \partial_{x_n} q_m(\mathbf{x}_{[i]}) \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \vdots \\ \Delta x_n \end{bmatrix}_{[i]}$$



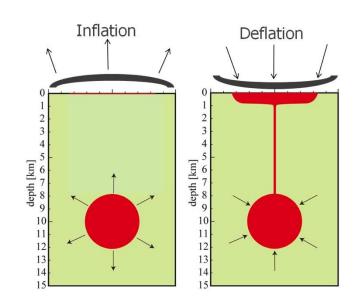
Convergence





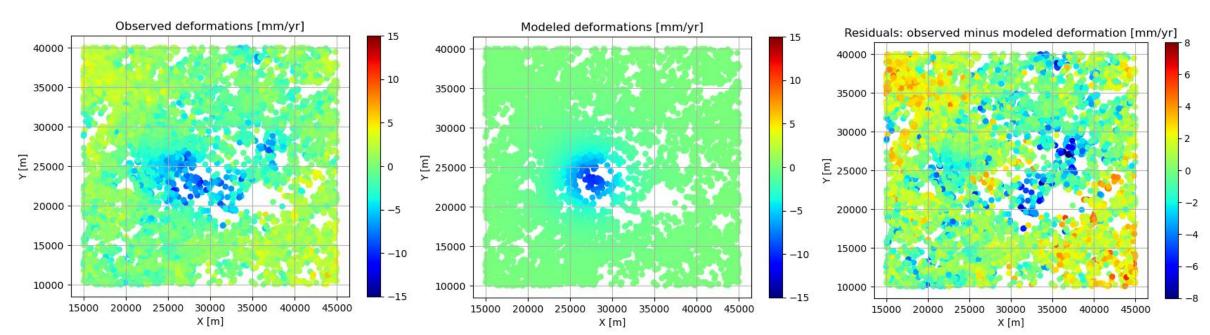
Volcano deformation rates at known locations (x_i, y_i)

$$\mathbb{E}(Y_i) = \frac{0.73\Delta V}{\pi d^2} \cdot \left(1 + \frac{1}{d^2} \left((x_i - x_s)^2 + (y_i - y_s)^2 \right) \right)^{-\frac{3}{2}}$$



Unknown parameters: volume change ΔV , depth of magma chamber d,

 (x_s, y_s) horizontal coordinates of centre



Volcano deformation – precision of estimated parameters

observed deformations at (x_i, y_i) as function of volume change, depth, horiz. position of centre

$$\mathbb{E}(Y_i) = \frac{0.73\Delta V}{\pi d^2} \cdot \left(1 + \frac{1}{d^2} \left((x_i - x_s)^2 + (y_i - y_s)^2 \right) \right)^{-\frac{3}{2}}$$

$$\begin{bmatrix} \hat{\Delta V} \\ \hat{d} \\ \hat{x}_s \\ \hat{y}_s \end{bmatrix} = \begin{bmatrix} -552352.169 \ m^3 \\ 3562.319 \ m \\ 27528.535 \ m \\ 23540.619 \ m \end{bmatrix}$$

$$\begin{bmatrix} \sigma_{\hat{\Delta V}} \\ \sigma_{\hat{d}} \\ \sigma_{\hat{x}_s} \\ \sigma_{\hat{y}_s} \end{bmatrix} = \begin{bmatrix} 1582.769 \ m^3 \\ 8.986 \ m \\ 8.238 \ m \\ 7.239 \ m \end{bmatrix}$$

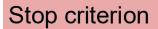
seems large, but look at units, and look at size compared to estimate!



Gauss-Newton iteration

Start with initial guess $x_{[0]}$, and start iteration with i = 0

- 1. Calculate observed-minus-computed $\Delta y_{[i]}$
- 2. Determine the Jacobian
- 3. Estimate $\Delta \hat{x}_{[i]}$ by applying BLUE
- 4. New guess $x_{[i+1]} = \Delta \hat{x}_{[i]} + x_{[i]}$
- 5. If stop criterion is met: set $\hat{x} = x_{[i+1]}$ and break, otherwise set i := i+1 and go to step 1



$$\Delta \hat{\mathbf{x}}_{[i]}^T \cdot \Sigma_{\hat{\mathbf{x}}}^{-1} \cdot \Delta \hat{\mathbf{x}}_{[i]} < \text{small value}$$

an estimated parameter with small variance should have a relatively small deviation compared to a parameter with large variance



$$\mathbb{E}(\begin{bmatrix} \Delta Y_1 \\ \Delta Y_2 \\ \vdots \\ \Delta Y_m \end{bmatrix}) = \begin{bmatrix} \partial_{x_1} q_1(\mathbf{x}_{[i]}) & \partial_{x_2} q_1(\mathbf{x}_{[i]}) & \cdots & \partial_{x_n} q_1(\mathbf{x}_{[i]}) \\ \partial_{x_1} q_2(\mathbf{x}_{[i]}) & \partial_{x_2} q_2(\mathbf{x}_{[i]}) & \cdots & \partial_{x_n} q_2(\mathbf{x}_{[i]}) \\ \vdots & \vdots & & \vdots \\ \partial_{x_1} q_m(\mathbf{x}_{[i]}) & \partial_{x_2} q_m(\mathbf{x}_{[i]}) & \cdots & \partial_{x_n} q_m(\mathbf{x}_{[i]}) \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \vdots \\ \Delta x_n \end{bmatrix}_{[i]}$$

Is it a good fit?



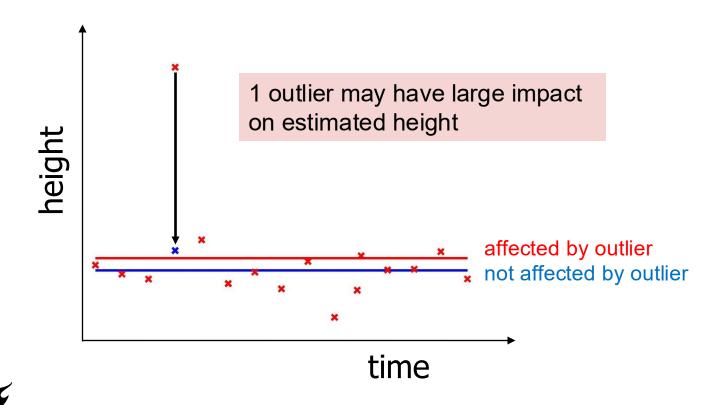
Sensing and observation theory - why

Needed for monitoring and prediction e.g., natural processes, human-induced deformations, structural health, climate & environment, geoenergy and geo-resources, ...

- Process measurements (= observations) to estimate parameters of interest
- In order to use estimation results for further analysis and interpretations (eventually to make decisions)
 - = uncertainty quantification
 - = detection of errors in data (outliers, systematic biases)
 - + correction / adaption for these errors
 - = model validation
 - detect model misspecifications
 - multiple candidate models → decide which one is best



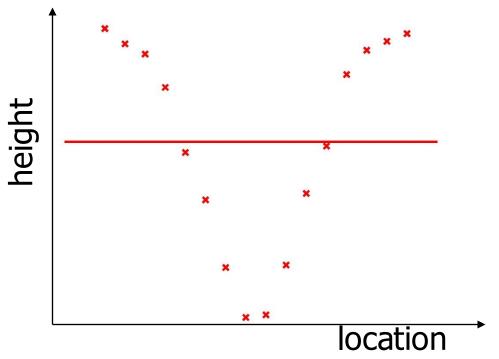
Example: outlier

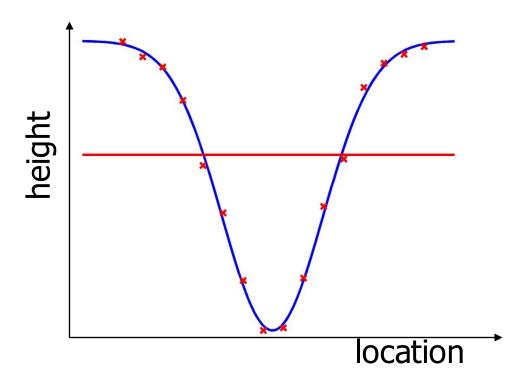




Example: model misspecification

Wrong model → large residuals (difference observations and fitted model)







Statistical hypothesis testing

→ test for compliance of model and data

Two competing hypothesis:

- Null hypothesis (nominal model): \mathcal{H}_0

- Alternative hypothesis:

 \mathcal{H}_a^0

Null hypothesis presumed to be 'true' until data provide convincing evidence against it

equivalent to:

" the defendant is presumed to be innocent until proven guilty"





Group assignment

$${\cal H}_0 \hspace{0.5cm} d=d_0+vt+A\sin(rac{2\pi t}{365}-\phi),$$

$$\mathcal{H}_a \qquad d = d_0 + v \ (1 - \exp\left(rac{-t}{a}
ight)) + A \sin(rac{2\pi t}{365} - \phi),$$

Apply non-linear least-squares
How to decide between the two models?



Enjoy...

