UNIVERSITÄT BIELEFELD
Faculty of Technology

Programming

Numerical Data Analysis & Visualization

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Recap

Reading from file

Dynamic: read from file with name requested by prompt

```
1 fName = input('Input␣file:␣')
2 lines = list()
3 f = open(fName)
4 for line in f:
5     lines.append(line)
```

File formats

Unstructured data

- Text

Structured data

- XML
- JSON
- Tables
- Matrices

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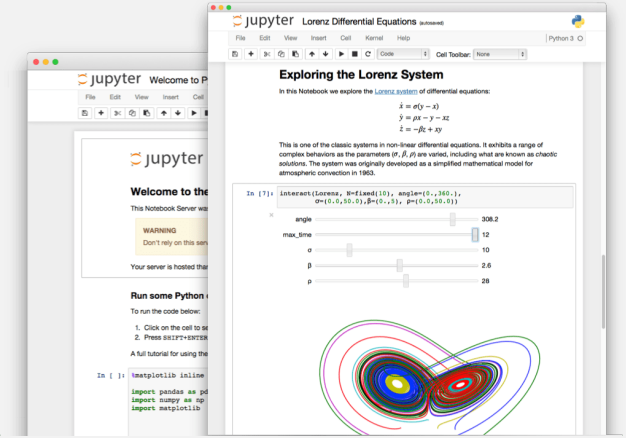
Jupyter Notebook

Why use Jupyter Notebook in Data Science?

- Simultaneous documentation & analysis
- Step-by-step processing
- Ensures reproducability

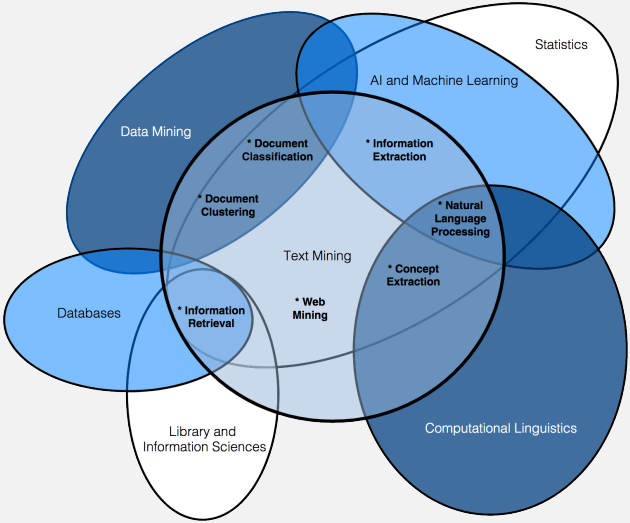


Text mining

Relies on *Natural Language Processing* (NLP)

Main (constitutive) tasks:

- Document summarization, clustering & classification
- Information extraction
- Information discovery



source: Miner, Gary. Practical Text Mining and Statistical Analysis for Non-structured Text Data Applications. 1st ed. Amsterdam: Academic Press, 2012.

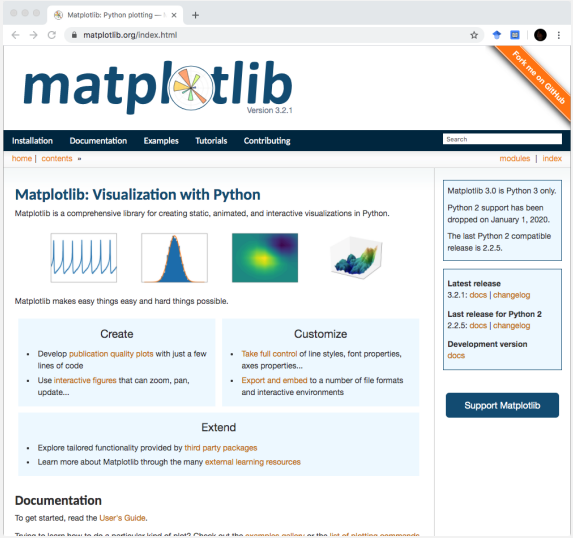
Data Visualization

Numerical Data Analysis with NumPy

Modeling Experimental Data

Matplotlib: Visualization with Python

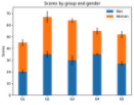
- de-facto standard library for scientific visualizations
- many third party packages built on top of Matplotlib
- comprehensive library for creating static, animated, and interactive visualizations



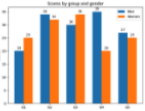
source: https://matplotlib.org/

Matplotlib: Visualization with Python

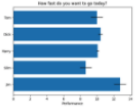
Lines, bars and markers



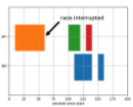
Stacked bar chart



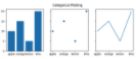
Grouped bar chart with labels



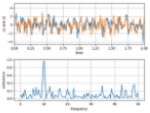
Horizontal bar chart



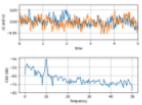
Broken Barh



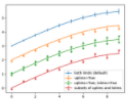
Plotting categorical variables



Plotting the coherence of two signals



CSD Demo



Errorbar limit selection

source: https://matplotlib.org/gallery/index.html

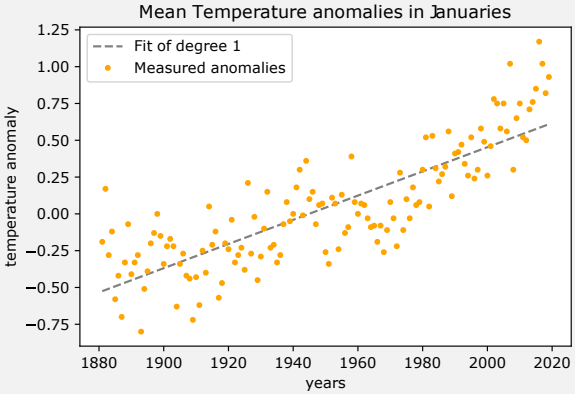
Data Visualization

Numerical Data Analysis with NumPy

Modeling Experimental Data

Numerical analysis

- Numerical data: anything measurable
- Methods:
  - Interpolation and regression
  - Solving differential equations
  - Optimization
  - …



N-dimensional array: `numpy.ndarray`

Array data structure

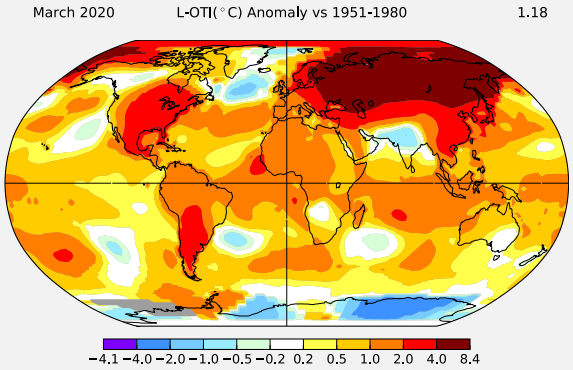
- immutable
- n-dimensional
- very storage efficient
- can store only data of same type

Data Visualization

Numerical Data Analysis with NumPy

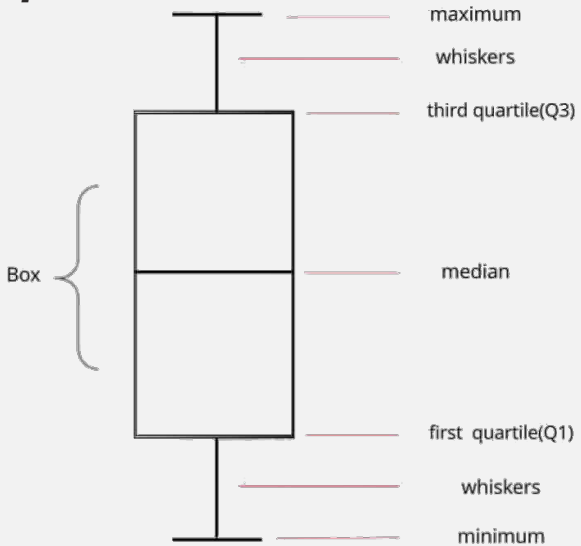
Modeling Experimental Data

NASA's GISS Surface Temperature Analysis



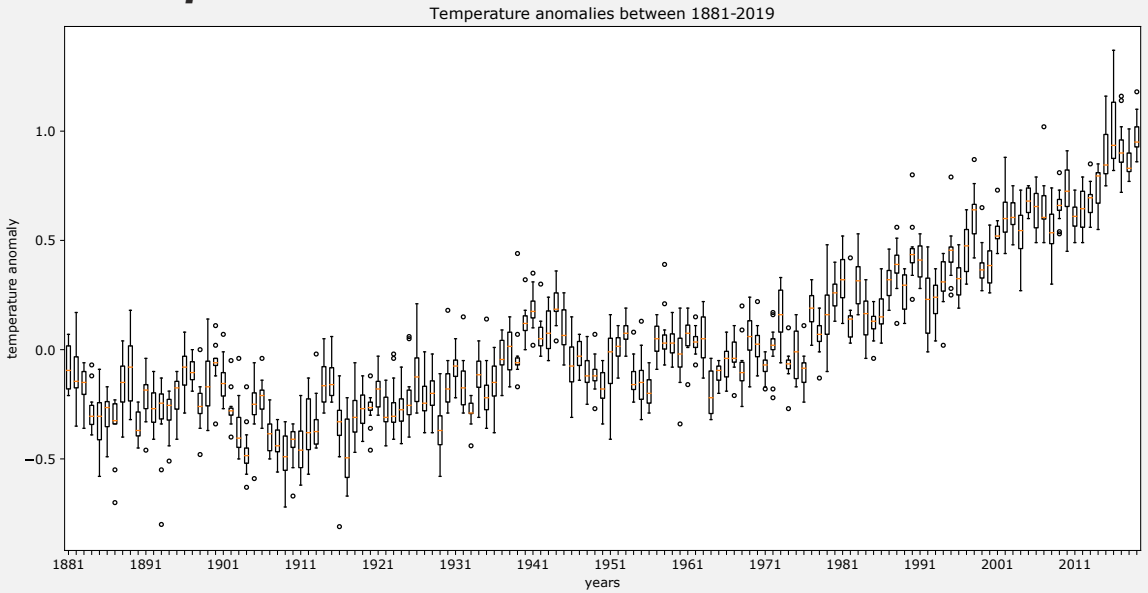
- `https://data.giss.nasa.gov/gistemp`
- Collection of temperature data from thousands of meteorological stations
- Data represents *anomalies*, i.e., deviations from mean temperature measured in 1951-1980

Box (whisker) plot



source: https://en.wikipedia.org/wiki/Box_plot

Whisker plot of GISS data



Further material on methods in Data Science

MIT Course 6.0002, Lectures on Understanding Experimental Data:

- `https://www.youtube.com/v/vIFKGFl1Cn8`
- `https://www.youtube.com/v/fQvg-hh9dUw`

Linear regression

Linear regression is a *linear* approach for modelling a predictive relationship between some parameters and a given input:

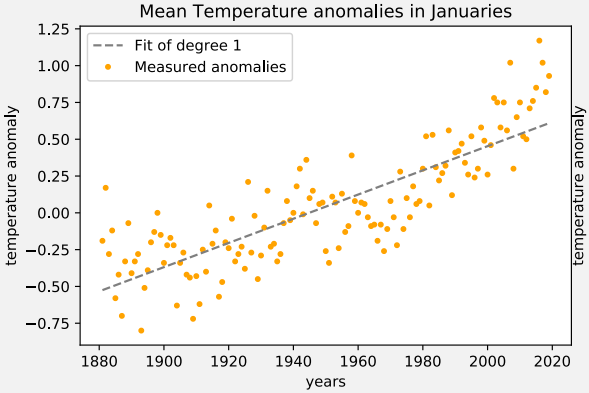
$$X = \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_{N-1} \end{pmatrix}, Y = \begin{pmatrix} Y_0 \\ Y_1 \\ \vdots \\ Y_{N-1} \end{pmatrix} \rightarrow \alpha = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{N-1} \end{pmatrix}$$

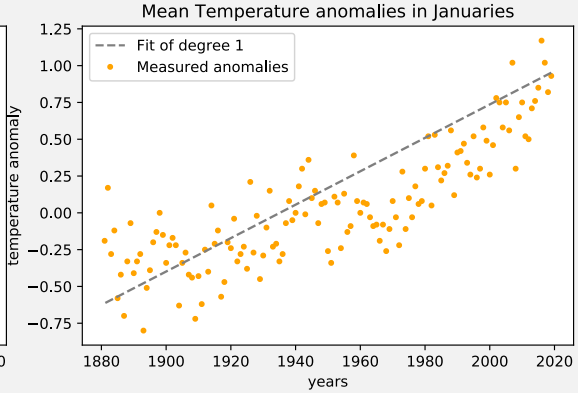
Estimator:

$\hat{Y} = \alpha_0 + \alpha_1 X + \alpha_2 + X^2 + \cdots + \alpha_{N-1} X^{N-1}$

Simple linear regression: Estimate line, i.e, estimate α_0, α_1 and set $\alpha_2 = \cdots = \alpha_{N-1} = 0$

What criterion to optimize? (->Which line is better?)



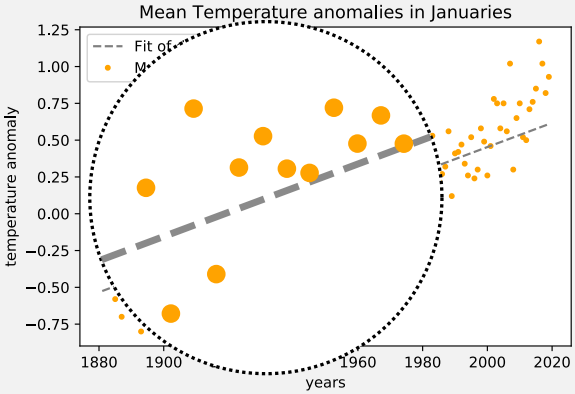


Optimization criteria

- Residual: difference predicted/observed $|Y_i - \hat{Y}_i|$
- Possible minimization criteria:
  - Sum of residuals
  - Maximum
  - Variance of residuals

$$Var_{res} := \frac{1}{N} \sum_i (Y_i - \hat{Y}_i)^2 = E[(Y - \hat{Y})^2]$$

- Minimize Var_{res} = ordinary least squares optimization



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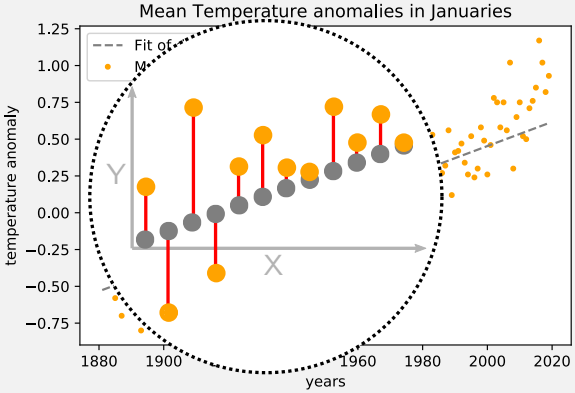


Why least squares?

Three advantages:

1. Penalizes large deviations from the observed data very strongly and sums over all data points;
2. Finding the polynomial that minimizes the variance can be done efficiently via least squares optimization methods;
3. Minimizing the variance guarantees that there is one and only one solution.

Coefficient of determination R^2

How to measure quality of fit?

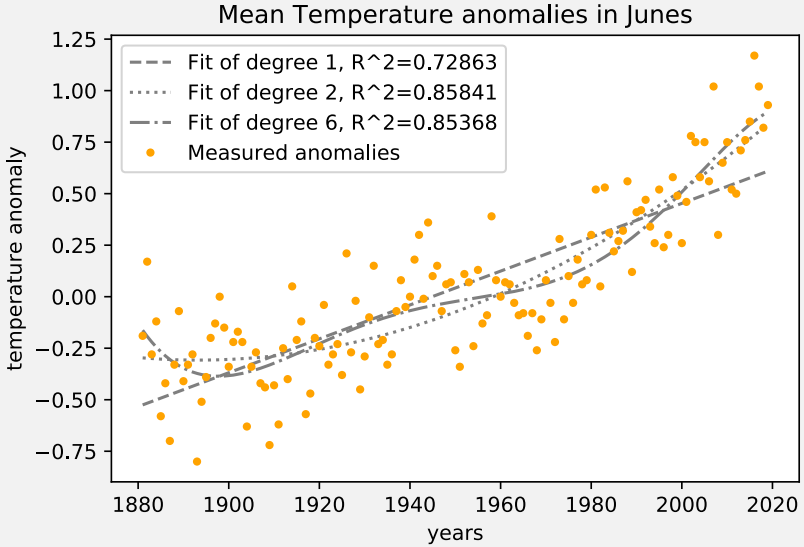
Recall: Ordinary Least squares optimization minimizes Var_{res}

R^2 is a normalized measure thereof:

$$R^2 := 1 - \frac{Var_{res}}{Var(Y)}$$

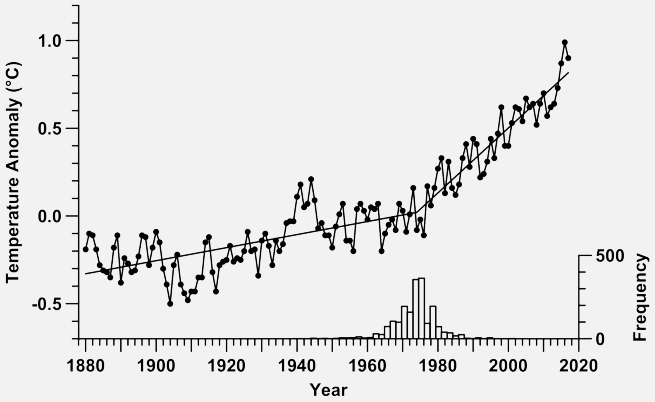
i.e, $R^2 \to 0$ bad fit, $R^2 \to 1$ good fit

Separated training from testing



The “break” model

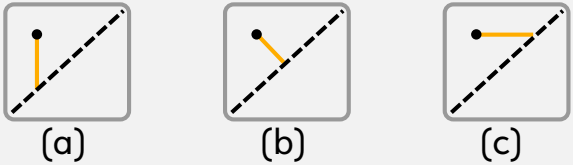
- Combination of two linear functions
- Estimated break around year 1974 ± 5.9



source: Mudelsee, M. (2019). Trend analysis of climate time series: A review of methods. Earth Science Reviews, 190, 310–322.

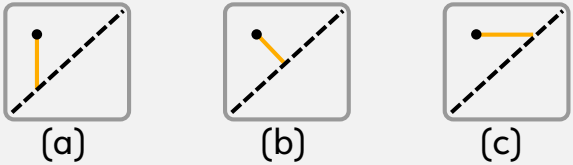
Quiz

- *True* or *false*?
  - The residual is the distance between an observed and its predicted data point
  - Linear regression always minimizes the variance of residuals
  - Linear regression is the task of fitting a line to a set of data points
  - Ordinary least squares always minimizes the variance of residuals
- How does linear regression measure the distance between an observed and its predicted data point?



Quiz

- *True* or *false*?
  - The residual is the distance between an observed and its predicted data point — true
  - Linear regression always minimizes the variance of residuals — false
  - Linear regression is the task of fitting a line to a set of data points — false
  - Ordinary least squares always minimizes the variance of residuals — true
- How does linear regression measure the distance between an observed and its predicted data point? (a)



Recap

Summary

- Plots with `matplotlib`:
  - Line- and scatter plot
  - Histogram
  - Whisker (box) plot
- Numpy
  - `ndarray` data type
  - Vectorized operations, broadcasting
  - Curve fitting: `polyfit()`
- Realistic data analysis: climate trends

What comes next?

- Draw your first plots with `matplotlib`
- Further reading about NumPy: Chapter 2 of the “Python Data Science Handbook”:
  `https://jakevdp.github.io/PythonDataScienceHandbook/`
- Due date for this week’s exercises is ***Wednesday, December 20, 2pm, 2023***.

Next lecture: Pandas, applied machine learning, etc. …