UNIVERSITÄT BIELEFELD
Faculty of Technology

Programming

Data Visualization & Numerical Data Analysis

Luna Pianesi

Faculty of Technology, Bielefeld University

Recap

File I/O and text mining

- File I/O: managing data in the form of files
- Reading, writing, and closing files
- File formats: plain text, XML, JSON, tables and matrices
- Text mining
- Information extraction with NLTK:
  - Lexical analysis: tokenization, stemming and lemmatization
  - Semantic analysis: parse trees
  - Domain analysis: anaphora resolution

Data Visualization

Numerical Data Analysis with NumPy

Modeling Experimental Data

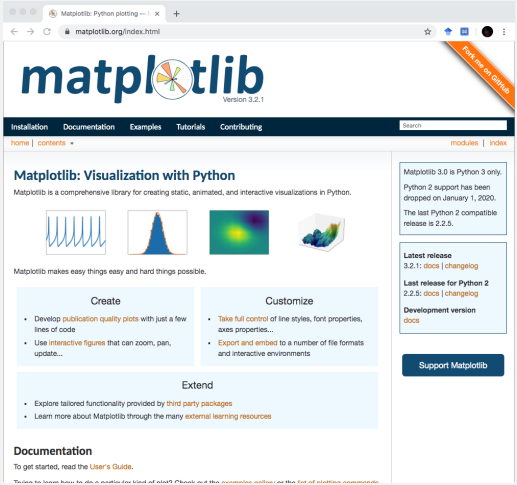
What is data visualization?

Also known as *dataviz*, data visualization is the practice of designing and creating ***easy-to-communicate*** and ***easy-to-understand*** images or other types of visual representations of complex data.

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

Matplotlib: dataviz with Python

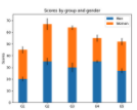
- de-facto standard library for scientific visualizations
- Many third party packages built on top of Matplotlib
- Comprehensive library for creating static, animated, and interactive visualizations



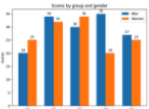
source: https://matplotlib.org/

What you can do with Matplotlib

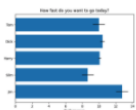
Lines, bars and markers



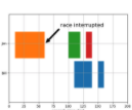
Stacked bar chart



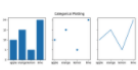
Grouped bar chart with labels



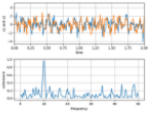
Horizontal bar chart



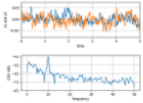
Broken Barh



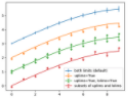
Plotting categorical variables



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

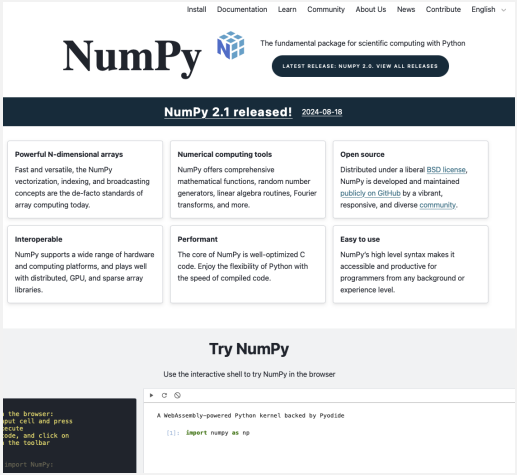
What is numerical data analysis?

Now we know how to plot data, but what data are we plotting? Numerical analysis is the study of the methods that find ***approximate*** solutions to problems. Our numbers will be anything that can be measured, and our analyses will focus on algorithms that *approximately* make sense of that data.

source: `https://en.wikipedia.org/wiki/Numerical_analysis`

NumPy: numerical analysis with Python

- Fundamental package for scientific computing in Python
- The library provides:
  - A *multidimensional array object*
  - Fast and easy operations on *arrays*



source: https://numpy.org

N-dimensional array: `numpy.ndarray`

Array data structure

- ***immutable***: can't be changed after creation
- ***n-dimensional***: very useful for multidimensional data
- ***storage efficient***: Python takes care of it
- can store only data of ***same type***: can't mix `int` and `float`, for example

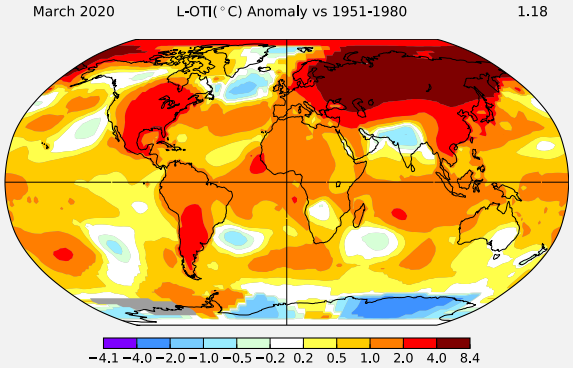
source: `https://numpy.org/doc/stable/user/absolute_beginners.html`

Data Visualization

Numerical Data Analysis with NumPy

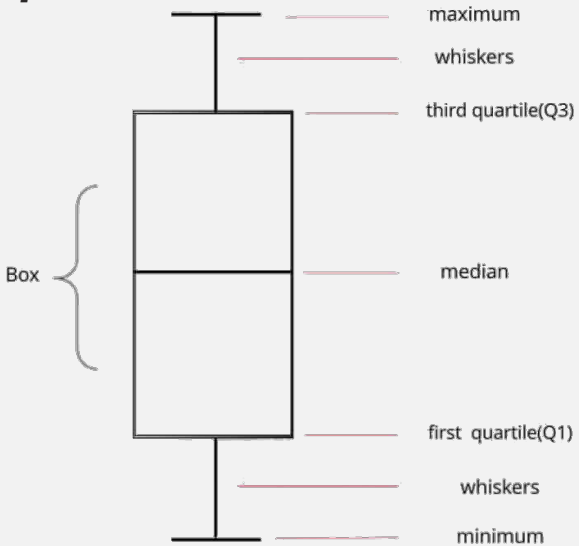
Modeling Experimental Data

NASA's GISS Surface Temperature Analysis



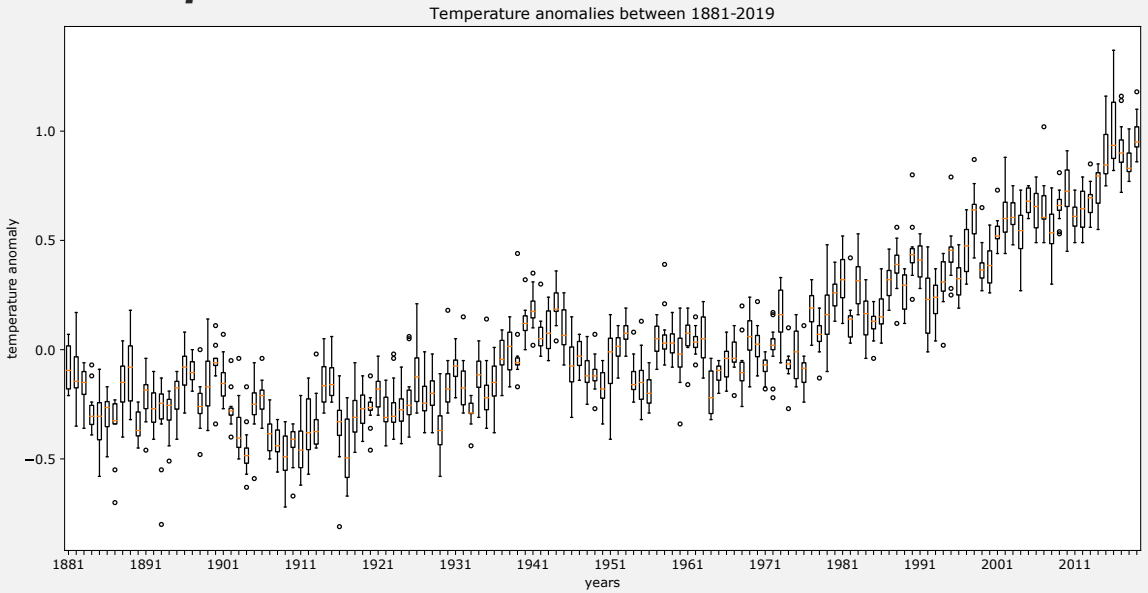
- `https://data.giss.nasa.gov/gistemp`
- Collection of temperature data from thousands of meteorological stations
- Data represents *anomalies*, i.e., deviations from mean temperature measured in 1951-1980

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:

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

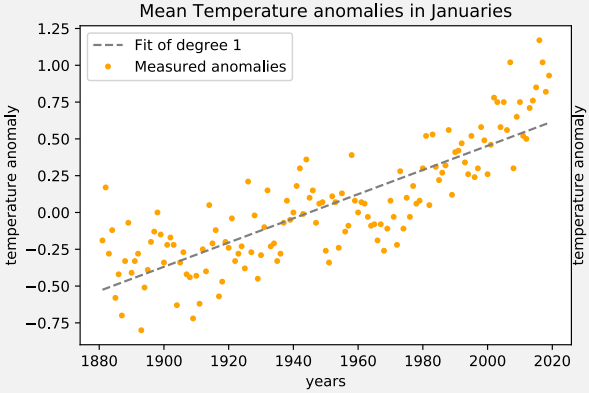
Estimator:

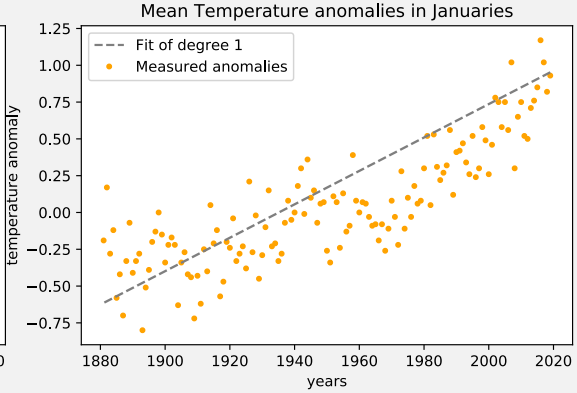
$\hat{Y} = \alpha_0 + \alpha_1 X + \alpha_2 + X^2 + \cdots + \alpha_{N-1} X^{N-1}$

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?

id est, ***Which line is better?***



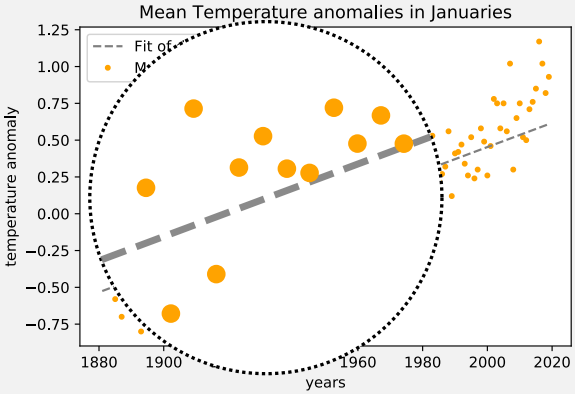


Optimization criteria

- 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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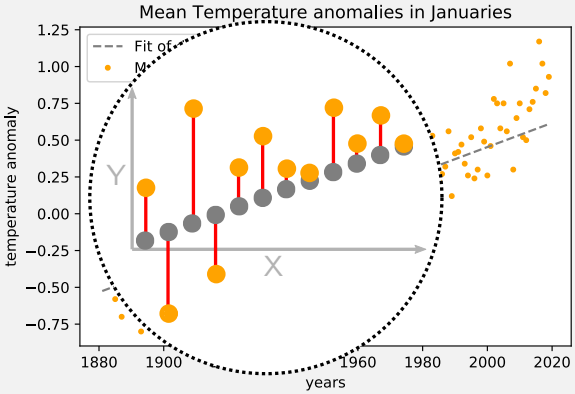


Why least squares?

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?

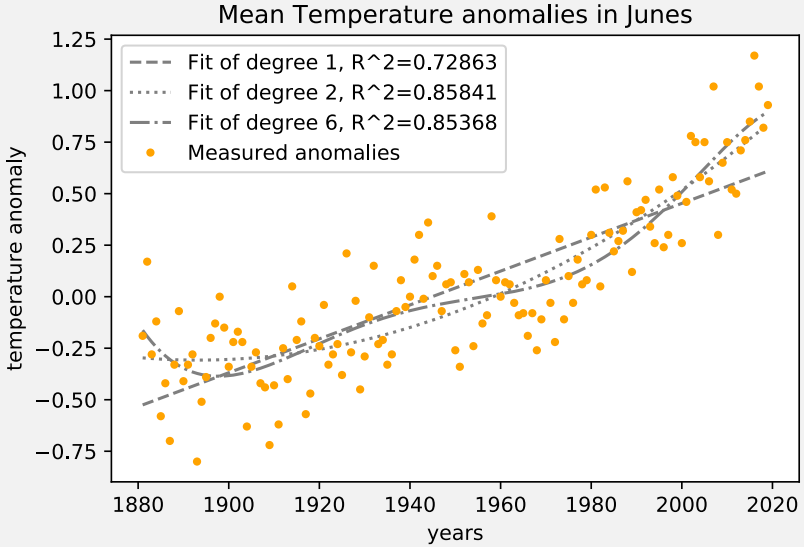
Recall: Ordinary Least squares optimization minimizes Var_{res}

R^2 is a normalized measure thereof:

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

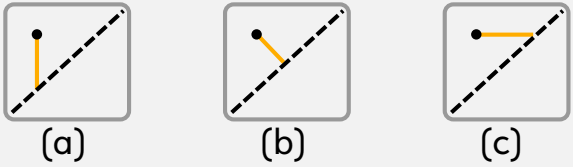
i.e, $R^2 \to 0$ bad fit, $R^2 \to 1$ good fit

Separated training from testing



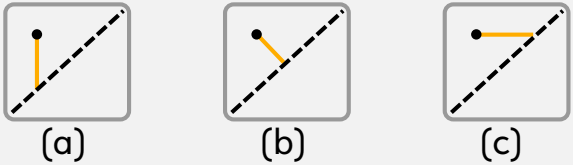
Quiz

- *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 11, 2pm, 2024***.

Next lecture: Pandas! …