Advanced topics

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Unit 5: Advanced topics

- Basic analysis of algorithms: The Big O
- Visualizations for Data Science:
    - Picking the "right" visualization
    - Tooling primer: matplotlib, pandas
- (Library support):
    - High-level libraries: pandas (cont'd)
    - Low-level libraries: numpy, scipy
    - Plotting (cont'd): seaborn, bokeh
    - Parsing

Slides: This unit is also available in a PDF format and as a single HTML Page

Readings:

- Grus, J. (2015) Data Science from Scratch, O'Reilley, **Chapter 3** (available via the WU library, EBSCO)

Analysis of algorithms (1)

- We encountered many different computational procedures (algorithms) for different purposes in data processing throughout Units 1 to 5, e.g.:
    - Data filtering
    - Data sorting
    - Data sampling
    - Deduplication (blocking, windowing)
- Why do we want to describe the complexity of these procedures (or, the underlying algorithms)?
- How can we describe the their complexity: space vs. time complexity?

Analysis of algorithms (2)

- Studying the complexity of a computation (procedure, algorithm) involves quantifying and describing ...
    - ... the difficulty of solving a computational problem (e.g., sorting)
    - ... in terms of the required computational resources:
        - running time of a computation
        - memory ("space") consumed by a computation
    - Note: There can be a fundamental trade-off between running time

  and memory consumption.
- Our take: *Time complexity* of basic opterations in (Python) data processing.

Analysis of algorithms (3)

- How fast does the (running/ execution) time required by an operation grow as the size of the problem increases in the **worst case**?
- "Size of a problem" (n), eg.: number of elements in a list or array, number of rows in a table or DataFrame.
- "time required" (f): a function of N, i.e., $f(n)$
- When this function $f(n)$ grows rapidly, an operation (algorithm) will become unusable the larger n.
- When this function $f(n)$ grows "slowly, an operation (algorithm) will remain usable even at larger n.

Question.
What would you consider "rapidly", "slowly"?

Analysis of algorithms (4): Types of growth

Commonly found types of time growth for some input n:

- $f(n) = 1$: Time required is **constant**, independent of n (e.g., hash searching).

- $f(n) = log(n)$: increasing n by a factor c, e.g., doubling n

increases the required time by a constant amount, i.e. **logarithmic** (example: binary search).

- $f(n) = n$: Required time grows **linearly** with problem size (linear search in n-element list)

- $f(n) = n * log(n)$: Doubling n increases the required time by more than a double (merge sort, Python's timsort).

- $f(n) = n^2, f(n) = n^3$: **quadratic**, **cubic**, etc. Doubling n results in a four-/ eight-fold increase in the required time (simple sorting, matrix multiplication)

- $f(n) = c^n$: Doubling the problem size **squares** the time required, a.k.a. **exponential** growth).

Analysis of algorithms (5): Big O(rder) notation

- Often, when planning data-processing steps, we want to compare two or available operations (e.g., search strategies).
- Objective: Comparison based on their relative time complexities or growth rates: $f(n)$ vs. $g(n)$.
- "Strictness" of comparison, e.g., "equal or less than", "same as".
- Big O(rder): $g \in O(f)$ iff $|g(x)|$ is smaller than some constant multiple of $|f(x)|$ (i.e., f is of smaller or equal order than g).
- Example: n^2 vs. $(n^2 + 2n + 3)$ vs. $2n$

Analysis of algorithms (6): Big O(rder) notation

Analysis of algorithms (7): Urban Audit example

Question.
How could we sort it by a different column? e.g., how could we sort countries by population?

Let's look at the excerpts from the following notebook

```
haystack = [('BE', 10839905),
 ('BG', 7563710),
 ('CZ', 10532770),
 ('DE', 81802257),
 ('EE', 1365275),
 ('ES', 47021031),
 ('FR', 64611814),
 ('IT', 60340328),
 ('CY', 819100),
 ('HU', 10014324),
 ('NL', 16574989),
 ('PL', 38529866),
 ('PT', 10573479),
 ('RO', 22480599),
 ('SK', 5435273),
 ('FI', 5351427),
 ('SE', 9415570),
 ('NO', 4858199),
 ('CH', 7877571)]
haystack.sort() # by country code
haystack.sort(key=lambda x:x[1]) # by population count
```

Analysis of algorithms (8): Urban Audit (cont'd)

Note: if you know that a file is sorted, then **searching** in that file becomes easier/cheaper!

Question.

- "Find me a country with a population above 5000000 people?",

Analysis of algorithms (8): Urban Audit (cont'd)

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Question.

- "Find me a country with a population above 5000000 people?",
- What is the growth rate of the quickest searching algorithm you can think of?

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Question.

- "Find me a country with a population above 5000000 people?",
- What is the growth rate of the quickest searching algorithm you can think of?
- What if you have the cities and populations already in a sorted list?

Analysis of algorithms (8): Urban Audit (cont'd)

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Question.

- "Find me a country with a population above 5000000 people?",
- What is the growth rate of the quickest searching algorithm you can think of?
- What if you have the cities and populations already in a sorted list?

- Answer: $O(\log n)$

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- Answer: $O(\log n)$
- Why?

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- Answer: $O(\log n)$
- Why?
- Answer: Binary Search!

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- Answer: $O(\log n)$
- Why?
- Answer: Binary Search!

Bottomline: (pre-)sorting can be costly, but might speed up other operations... another example: grouping!

Analysis of algorithms (9): Urban Audit example

```python
# Search for first entry bigger than number in a sorted
# list of lists of length 2:
def binary_search(number, array, lo, hi):

    if hi < lo: return array[lo]       # no more numbers
    mid = (lo + hi) // 2               # midpoint in array
    if number == array[mid][0]:
        return array[mid]              # number found here
    elif number < array[mid][0]:
        # try left of here
        return binary_search(number, array, lo, mid - 1)
    else:
        # try above here
        return binary_search(number, array, mid + 1, hi)

# Sample call: Find me a country with a pop. > 5m people?
binary_search(5000000, haystack, 0, len(haystack))
```

Analysis of algorithms (10): Outlook

- Python's `sort` applies **Timsort**: $O(n \log n)$ (worst case).
- Custom algorithmic recipes for Python 3 (incl. sorting algorithms): `http://python3.codes/.`
- Sampling: probability-based sampling (pandas)
- Deduplication: total complexity of naive algorithm: $O(n^2)$ (pairwise comparison). Possible improvements:
  - Blocking: $O(n(n/b + \log n))$ with block size $b < n$
  - Windowing: $O(n(w + \log n))$ with window size $w < n$
  - Sorting+Scan: $O(n * \log n + n)$

Visualization (1)

- Visualizations
  - can support a number of data-processing activities (before analysis!);
  - can be used to deliver analysis results;
- See Chapter 3 of "Data Science from Scratch":
  - matplotlib
  - pandas wrapper around matplotlib
  - Notebook
- Corresponding code examples:
  - matplotlib: GitHub.
  - pandas: "Visualization tutorial":""
- Advanced use of visualizations, such as graphical inference, beyond the scope of this course.

Visualization (2)

- Tasks supported by visualisations:
  - Anomaly detection: data outliers;
  - Grouping: Forming and characterising aggregates of similar data points;
  - Finding association (correlation) between pairs of variables;
  - Computing derivatives (e.g., sums) of data points;
  - Finding extremes, ranges, and orders (rankings) in data points;
  - Filtering data points (e.g., for ranges);
  - Retrieval of selected data points;
  - (Describing data distributions;)

Visualization (3)

- Which visualization type is most effective for a given task?
  - Accuracy
  - Performance time
  - Personal preferences
- No One Size Fits All!

Visualization (4a): Scatterplot

Visualization (4b): Scatterplot

Visualization (5a): Lineplot

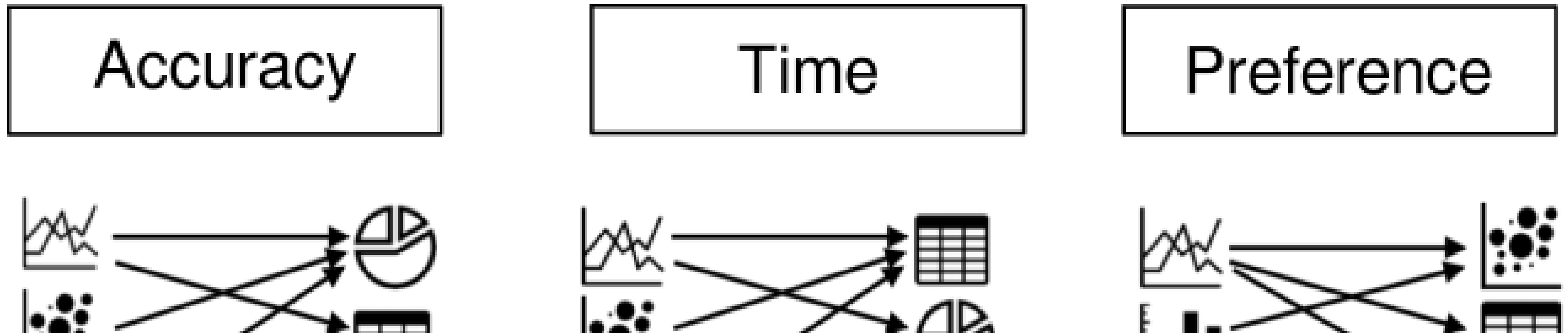
Visualization (5b): Lineplot

Visualization (6a): Barplot

Visualization (6b): Barplot

Visualization (7): Boxplot

Visualization (8): Task-based effectiveness



Visualization (9)

- Dos:
  - Finding groups: Use bar charts (preference bias towards pie charts!)
  - Finding associations and trends: Use line plots and scatterplots (preference bias towards line plots!)
  - Finding anomalies: Use scatterplots
- Donts:
  - Finding groups: Avoid line charts;
  - Compute derivatives: Avoid line charts;
  - Finding associations and trends: Avoid tables and pie charts;

High-level libraries

- Agate: agate is a Python data analysis library that is optimized **for humans instead of machines**. It is an alternative to numpy and pandas that solves real-world problems with readable code.

- Pandas: pandas is an open source, BSD-licensed library providing high-performance, easy-to-use data structures and data analysis tools for the Python programming language.

Pandas

```python
import pandas as pd
```

contains high-level data structures and tools designed to make data analysis fast and easy. Pandas are built on top of NumPy, and makes it easy to use in NumPy-centric applications.

Pandas is well suited for many different kinds of data:

- Tabular data with heterogeneously-typed columns
- Ordered and unordered (not necessarily fixed-frequency) time series data.
- Arbitrary matrix data (homogeneously typed or heterogeneous) with row and column labels
- Any other form of observational / statistical data sets. The data actually need not be labeled at all to be placed into a pandas data structure

Pandas features (1/2)

Here are just a few of the things that pandas does well:

- Handling of **missing data**
- **Adding and deleting** columns_ on the fly
- **data alignment**: objects can be explicitly aligned to a set of labels/columns
- **Group by functionality** and apply split-apply-combine operations on data sets to aggregate and transform data
- **label-based slicing**, no need for indices
- **Merging and joining**

Pandas features (2/2)

- **Reshaping**
- Hierarchical labels
- Loading data from flat files (CSV and delimited), Excel files, databases, and saving / loading data from the ultrafast HDF5 format
- **Time series-specific functionality**: date range generation and frequency conversion, moving window statistics, moving window linear regressions, date shifting and lagging, etc.
- **plotting support**. e.g. see the official tutorial

Pandas: Some more words

It takes a while to get used to pandas. The documentation is exhaustive and there exists hundreds of tutorials and use cases

- Pandas Cookbooks
- Datacamp tutorial
- Dataquest.io tutorial

Some hands on

Checkout the notebook **pandas.ipynb**

Low-level libraries

- Chardet: Character encoding auto-detection in Python. As smart as your browser. Open source.
- dateutils: The dateutil module provides powerful extensions to the standard datetime module, available in Python.
- Csvkit: csvkit is a suite of command-line tools for converting to and working with CSV, the king of tabular file formats
- Numpy the fundamental package for scientific computing with Python
- SciPy is open-source software for mathematics, science, and engineering

Numpy

```
import numpy as np
```

Numpy the fundamental package for scientific computing with Python. It contains among other things:

- a powerful N-dimensional array object
- sophisticated (broadcasting) functions
- tools for integrating C/C++ and Fortran code
- useful linear algebra, Fourier transform, and random number capabilities

Check out this tutorial or this one (includes also scipy and matplotlib)

NumPy does not provide high-level data analysis functionality, having an understanding of NumPy arrays and array-oriented computing will help you use tools like Pandas much more effectively.

SciPy

SciPy is open-source software for mathematics, science, and engineering

The SciPy library depends on NumPy, which provides convenient and fast N-dimensional array manipulation. The SciPy library is built to work with NumPy arrays, and provides many user-friendly and efficient numerical routines , such as routines for numerical integration and optimization.

SciPy subpackages (1/2)

- cluster: Clustering algorithms
- constants: Physical and mathematical constants
- fftpack Fast Fourier Transform routines
- integrate Integration and ordinary differential equation solvers
- interpolate Interpolation and smoothing splines
- linalg Linear algebra
- ndimage N-dimensional image processing

SciPy subpackages (2/2)

- odr Orthogonal distance regression
- optimize Optimization and root-finding routines
- signal Signal processing
- sparse Sparse matrices and associated routines
- spatial Spatial data structures and algorithms
- special Special functions
- stats Statistical distributions and functions

```
from scipy import linalg, optimize
```

SciPy

Again, check out the official tutorials

Some examples:

- Interpolation
- Solving linear system, Eigenvalues and eigenvectors
- Signal processing
- Statistics, random variables, fitting distributions, ..

Plotting

Plotting

There exists many libraries for plotting:

- matplotlib: Python's most popular and comprehensive plotting library that is especially useful in combination with NumPy/SciPy.
- seaborn: extension for matplotlib with enchanced visual styles and additional plots
- qqplot (like qqplot2 in R)
- bokeh: Bokeh is a plottling library for interactive plots typically viewed in Web applications
- folium leaflets

Machine learning?

Machine learning

- scikit-learn builds on NumPy and SciPy, including clustering, regression, and classification, well documented, many tutorials and examplesUsed by data-heavy startups, including Evernote, OKCupid, Spotify, and Birchbox.
- Theano Theano is a Python library that allows you to define, optimize, and evaluate mathematical expressions involving multi-dimensional arrays efficiently. Theano features:
- TensorFlow developed by Google, is an open source software library for numerical computation using data flow graphs. It can be used for deep learning scenarios. Check out their Python API
- Keras: Keras is a high-level neural networks API, written in Python and capable of running on top of either TensorFlow or Theano. It was developed with a focus on enabling fast experimentation. Being able to go from idea to result with the least possible delay is key to doing good research.

Data Mining & NLP

Data Mining & NLP

- Scrapy an open source and collaborative framework for extracting the data you need from websites. In a fast, simple, yet extensible way.

- NLTK NLTK is a leading platform for building Python programs to work with human language data. It provides easy-to-use interfaces to over 50 corpora and lexical resources such as WordNet, along with a suite of text processing libraries for classification, tokenization, stemming, tagging, parsing, and semantic reasoning and wrappers for industrial-strength NLP libraries.

References

- Chapter 3, Data Science from Scatch
- Reingold (2014): "Basic Techniques for Design and Analysis of Algorithms", Chapter 4, In: Computing Handbook, CRC Press.
- B. Saket, A. Endert and Ç. Demiralp (2019), "Task-Based Effectiveness of Basic Visualizations," in IEEE Transactions on Visualization and Computer Graphics, vol. 25, no. 7, pp. 2505-2512, DOI: 10.1109/TVCG.2018.2829750