Introduction to Computational Social Science

(Week 13: "Other" CSS skills)

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Intro to CSS course outline and syllabus

Universität Rostock

- Week 1 – Introduction ... What is "Computational Social Science"? Inductive and deductive research; Big data revolution
- Week 2 – Open Science and Reproducibility ... Reproducibility crisis; Pre-registration; Version control, Git, GitHub, Accessing course materials
- Week 3 – Digital Trace Data ... Observational data; Available vs. designed data; APIs and web scrapping; Representativeness
- Week 4 – Mobility and Migration ... Computational approaches to migration research; The Scholarly Migration Database
- Week 5 – Network Analysis ... Migration networks; Tie formation mechanisms in social networks; Violence of independence of observations
- Week 6 – Science of Science ... Robert K. Merton; Sociology of scientific knowledge vs Bibliometrics/ Scientometrics
- Week 7 – Text as Data ... Natural Language Processing; Topic modelling; LDA; Structural Topic Models
- Week 8 – Ethics in Computational Social Science ... Informed consent; Personal data; GDPR
- Week 9 – Social Simulation ... Agent-based modelling for social scientists; Micro-Macro link and Coleman's boat
- Week 10 – Machine Learning ... Supervised and unsupervised use of observational data; Feature learning
- Week 11 – "Other" CSS Skills ... Parallelization; Functional vs Object-Oriented; Graph databases; DuckDB; SnakeMake Workflows
- Week 12 – Limitations of Computational Social Science ... Pitfalls of digital trace data and computational approaches; Representativeness
- Week 13 – Conclusions ... Thick vs Big data, Survey experiments; Linked data; Future of CSS + LIST OF FINAL ASSIGNMENTS
- Week 14 – Final semester evaluation ... 6 weeks to prepare a short essay and empirical analysis on one of the CSS topics/skills

Intro to CSS course outline and syllabus (2025's updated timing)

Universität Rostock

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- Week 4,5 — Digital Trace Data ... Observational data; Available vs. designed data; APIs and web scrapping; Representativeness
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DISCLAIMER:

I will only share leads, links, and show you “example” scripts in R, Python, and SQL in this introductory short session; you would need to extend them on your own.

"Other" useful skills to have as a Computational Social Scientist

- Parallelization of extract, transform, load (ETL) tasks in Python and R;

Variables/attributes

Respondents/ Observations

ID	Name	Age	Political view	Education
1	Tom	24	left	NA
2	Sara	22	right	BA
3	Bill	30	neutral	MA
4	Margaret	31	NA	PhD

Example variable by observation table. Rows are independent!

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An example of the NDJSON format.

ndjson-sample.json

```
{"url":"https://www.yelp.com/search?find_desc=Desserts&find_loc=San+Jose,
{"url":"https://www.yelp.com/search?find_desc=Desserts&find_loc=San+Jose,
{"url":"https://www.yelp.com/search?find_desc=Desserts&find_loc=San+Jose,
{"url":"https://www.yelp.com/search?find_desc=Desserts&find_loc=San+Jose,
{"url":"https://www.yelp.com/search?find_desc=Desserts&find_loc=San+Jose,
```

Example unstructured text data, ndjson (same as jsonl) from: https://gist.github.com/rfmcnally/0a5a16e09374da7dd478ffbe6ba52503 Lines are independent.

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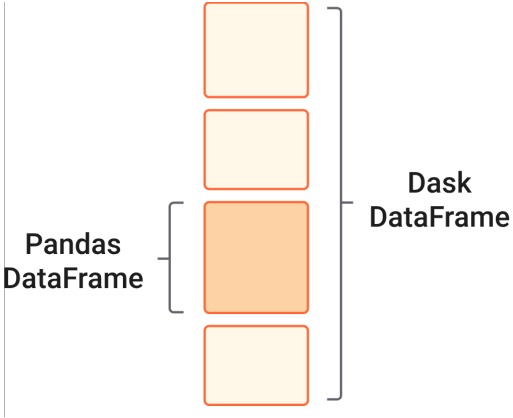

Example Dask data frame from:
https://docs.dask.org/en/stable/dataframe.html
to show independence of rows even in a table!

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Load Data | Data Processing | Machine Learning

Pandas and Dask have the same API, and so switching from one to the other is straightforward.

```
>>> import pandas as pd

>>> df = pd.read_parquet('s3://mybucket/myfile.parquet')
>>> df.head()
0  1  a
1  2  b
2  3  c
```

```
>>> import dask.dataframe as dd

>>> df = dd.read_parquet('s3://mybucket/myfile.*.parquet')
>>> df.head()
0  1  a
1  2  b
2  3  c
```

Example Dask data frame syntax vs Pandas from: https://docs.dask.org/en/stable/dataframe.html.

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towards data science

DATA SCIENCE

Saving Pandas DataFrames Efficiently and Quickly – Parquet vs Feather vs ORC vs CSV

Speed, RAM, size and convenience. Which storage method is best?

Mike Clayton
Nov 27, 2024 • 15 min read

Example comparison of parquet, CSV, feather etc.:
https://towardsdatascience.com/saving-pandas-dataframes-efficiently-and-quickly-parquet-vs-feather-vs-orc-v

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- Functional programming versus Object-Oriented Programming;

Example

Insert a function that prints a greeting, and execute it on the p1 object:

```
class Person:
  def __init__(self, name, age):
    self.name = name
    self.age = age

  def myfunc(self):
    print("Hello my name is " + self.name)

p1 = Person("John", 36)
p1.myfunc()
```

Example Python class and methods from: https://www.w3schools.com/python/python_classes.asp.

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Add Methods

Example

Add a method called `welcome` to the `Student` class:

```
class Student(Person):
  def __init__(self, fname, lname, year):
    super().__init__(fname, lname)
    self.graduationyear = year

  def welcome(self):
    print("Welcome", self.firstname, self.lastname, "to the
class of", self.graduationyear)
```

Try it Yourself »

Example Python class inheritance from: https://www.w3schools.com/python/python_inheritance.asp.

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Example violation of independence of observations, use a clustering framework or network graph/modeling?!

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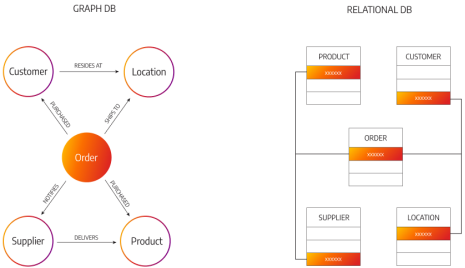

Example difference of tabular/relational versus graph DB from: https://memgraph.com/blog/graph-database-vs-relational-database.

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- In general, check DuckDB's community extensions https://duckdb.org/community_extensions/list_of_extensions
- If you want to run Graph analytics, see "duckpgq" https://duckdb.org/community_extensions/extensions/duckpgq.html

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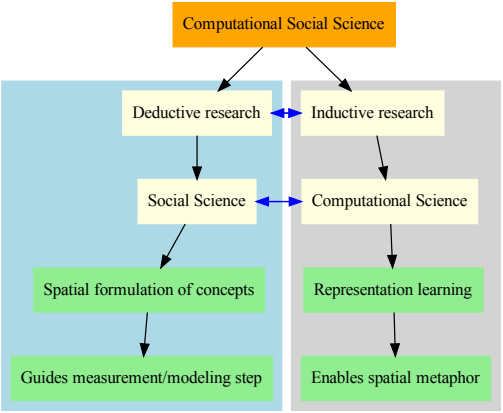

Check other discipline's skill sets, e.g., see more: Akbaritabar, 2024;

Parallelised analysis of large-scale bibliometric data w/ Dask
Using the example of ORCID 2019 XML files

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- Python users see: paralleliza-tion_with_dask_precompiled.html
- Video of a tutorial I gave on this, https://youtu.be/pYDVrBcluYI, including:
  - 00:00 - 02:45; Introduction
  - 2:45 - 11:04; Requirements and installation
  - 11:05 - 38:00; Steps in using Dask/Python and results

Parallelised analysis of large-scale bibliometric data with Dask in Python, DuckDB/DBeaver in SQL

Aliakbar Akbaritabar
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423 views Feb 21, 2022

Parallelised analysis of large-scale bibliometric data (with Dask in Python, DuckDB and DBeaver in SQL) Using example of ORCID 2019 XML files

Repository of codes/data: https://github.com/akbaritabar/dask-d...

30 minutes for the introduction and tutorial, 9 minutes for required installation that can be skipped if they followed tutorial's instructions provided on the repository (https://github.com/akbaritabar/dask-d....

- From the beginning up to 02:45 – Introduction

Parallelization saves you a lot of time!

Parallelization saves you a lot of time!

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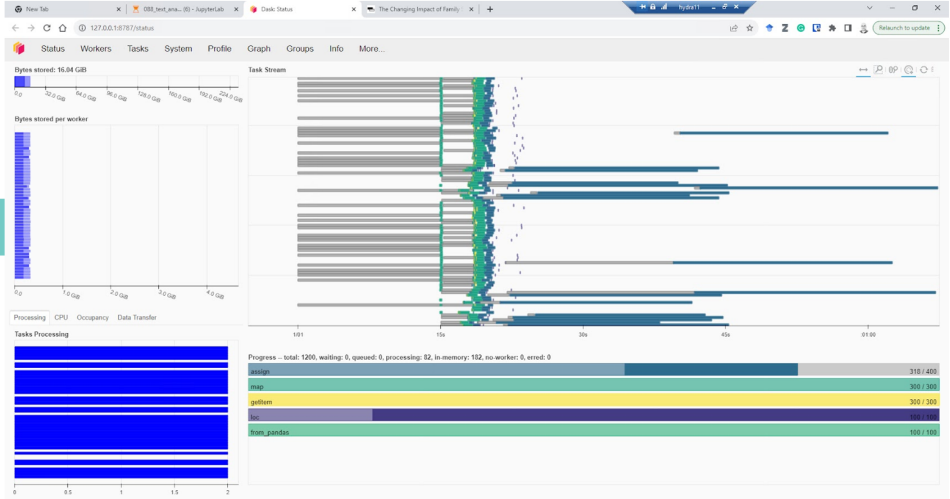
Dask dashboard



See more on Dask: Daniel, 2019

For R

- Purrr package to run map-like queries not sequentially (Wickham et al., 2023), see: https://purrr.tidyverse.org/reference/pmap.html
- If you liked Purrr's idea, then check out Furrr: https://furrr.futureverse.org/
- Or use "data.table": https://rdatatable.gitlab.io/data.table/

- Or leave I/O to DuckDB in R
- Do "install.packages("duckdb")" and see examples in hands-on scripts

For any platform (CLI)

- DuckDB Command Line Interface (CLI): https://duckdb.org/docs/installation/
- Or browser shell (note resource limitations, i.e., 4GB RAM, 1 core): https://shell.duckdb.org/
- Check their book Needham et al., 2024

For Python

- Leave I/O to DuckDB in Python
- Do “pip install duckdb” and see examples in hands-on scripts
- Check User-defined-functions (UDFs) for more advanced jobs: https://duckdb.org/docs/stable/clients/python/function.html
- Check Ibis: writing Python with DuckDB backend, no SQL needed (but possible): https://ibis-project.org/tutorials/basics
- "Workflow management using SnakeMake" (e.g., Targets in R): https://snakemake.readthedocs.io/en/stable/ (Mölder et al., 2021)

For Python

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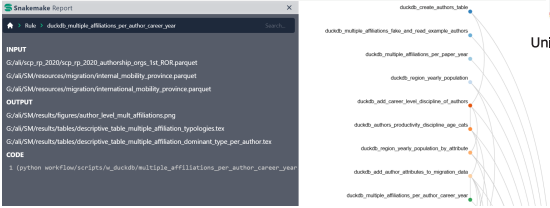

workflow > rules > snakefile_map_figures.smk

You, last month | 1 author (You)

```
## File name to use in search: snakefile_map_figures.smk ##

# ===========
## NMR and MEI MAPS for all time_span combinations ##
# ===========

rule plot_map_NMR_AND_MEI_MAPS:
    input:
        rules.prepare_data_for_mapping.output
    output:
        NMR_AND_MEI_MAPS
    log:
        NMR_AND_MEI_MAPS_LOG
    shell:
        "(python workflow/scripts/generic_src_mapping_figures.
        py --input {input} --MEASURE_MAPPED {wildcards.
        measure_mapped} --MIGRATION_SYSTEM {wildcards.
        migration_system} --GEO_REGION {wildcards.geo_region}
        --TIME_SPAN {wildcards.time_span} --output {output})
        2> {log}"
```

See: Akbaritabar and Dańko, 2025

Hands-on part

Needed installations (or checking requirements)

For the Hands-on part of this session, I used R, Python, and SQL with DuckDB. See the Readme file for this week.

Needed: Python (Vanilla or Miniforge), and virtualenv environments; R and Rstudio, DuckDB CLI

The example script shows 1) a toy example using these three languages, 2) a heavier example, and 3) a two for the price of one in Python, as I show how to use DuckDB inside SnakeMake workflows.

Where to learn basics of R and Python?

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To start with Python

Check this website first:
https://www.w3schools.com/python/python_intro.asp

Check this repository by Vincent Traag and others, for an introductory course and code:
https://github.com/vtraag/intro-python

Or this one by Data Carpentry:
https://datacarpentry.org/python-ecology-lesson/

To start with R

Check this website first:
https://www.w3schools.com/r/default.asp

This "very short introduction to R" is a good start:
https://cran.r-project.org/doc/contrib/Torfs+Brauer-Short-R-Intro.pdf

Or this course by Data Carpentry:
https://datacarpentry.org/R-genomics/index.html

Reading materials for today

Key reading material

- Mölder, F., Jablonski, K. P., Letcher, B., Hall, M. B., Tomkins-Tinch, C. H., Sochat, V., Forster, J., Lee, S., Twardziok, S. O., Kanitz, A., Wilm, A., Holtgrewe, M., Rahmann, S., Nahnsen, S., & Köster, J. (2021, April 19). Sustainable data analysis with Snakemake. 10:33. https://doi.org/10.12688/f1000research.29032.2

Additional reading materials

- Wickham, H., Çetinkaya-Rundel, M., & Grolemund, G. (2023, June). R for Data Science. "O'Reilly Media, Inc."
- Besta, M., Peter, E., Gerstenberger, R., Fischer, M., Podstawski, M., Barthels, C., Alonso, G., & Hoefler, T. (2021).Demystifying Graph Databases: Analysis and Taxonomy of Data Organization, System Designs, and Graph Queries. arXiv:1910.09017 [cs].
- Daniel, J. (2019, July). Data Science with Python and Dask. Manning Publications.
- Needham, M., Hunger, M., & Simons, M. (2024, August). Duckdb in Action. Manning Publications.

Thanks for your attention!

Questions and comments are welcome!

Aliakbar Akbaritabar

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To contact, please use Email: "aliakbar.akbaritabar@uni-rostock.de" and include in the subject line: "CSS-SoSe-2025"

LinkedIn/BlueSky/Twitter/Mastodon: @akbaritabar

References

- Akbaritabar, A. (2024).Thinking spatially in computational social science. EPJ Data Science, 13(1), 1–12. https://doi.org/10.1140/epjds/s13688-023-00443-0
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- Besta, M., Peter, E., Gerstenberger, R., Fischer, M., Podstawski, M., Barthels, C., Alonso, G., & Hoefler, T. (2021).Demystifying Graph Databases: Analysis and Taxonomy of Data Organization, System Designs, and Graph Queries. arXiv:1910.09017 [cs].
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- Needham, M., Hunger, M., & Simons, M. (2024, August). Duckdb in Action. Manning Publications.
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