

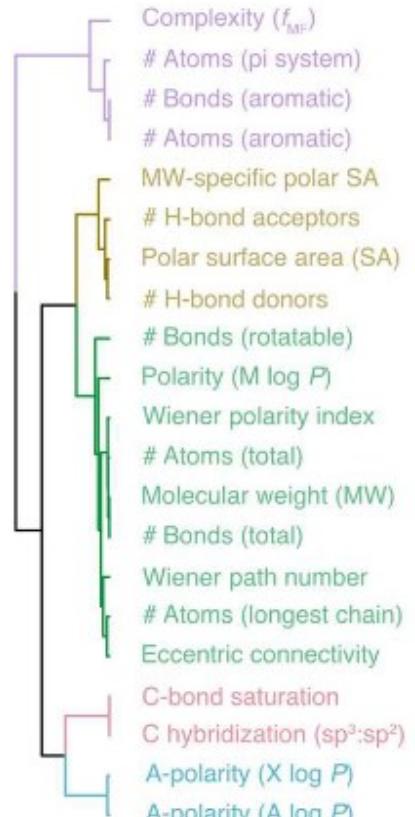


DSA103 Advanced Chemical Data Science

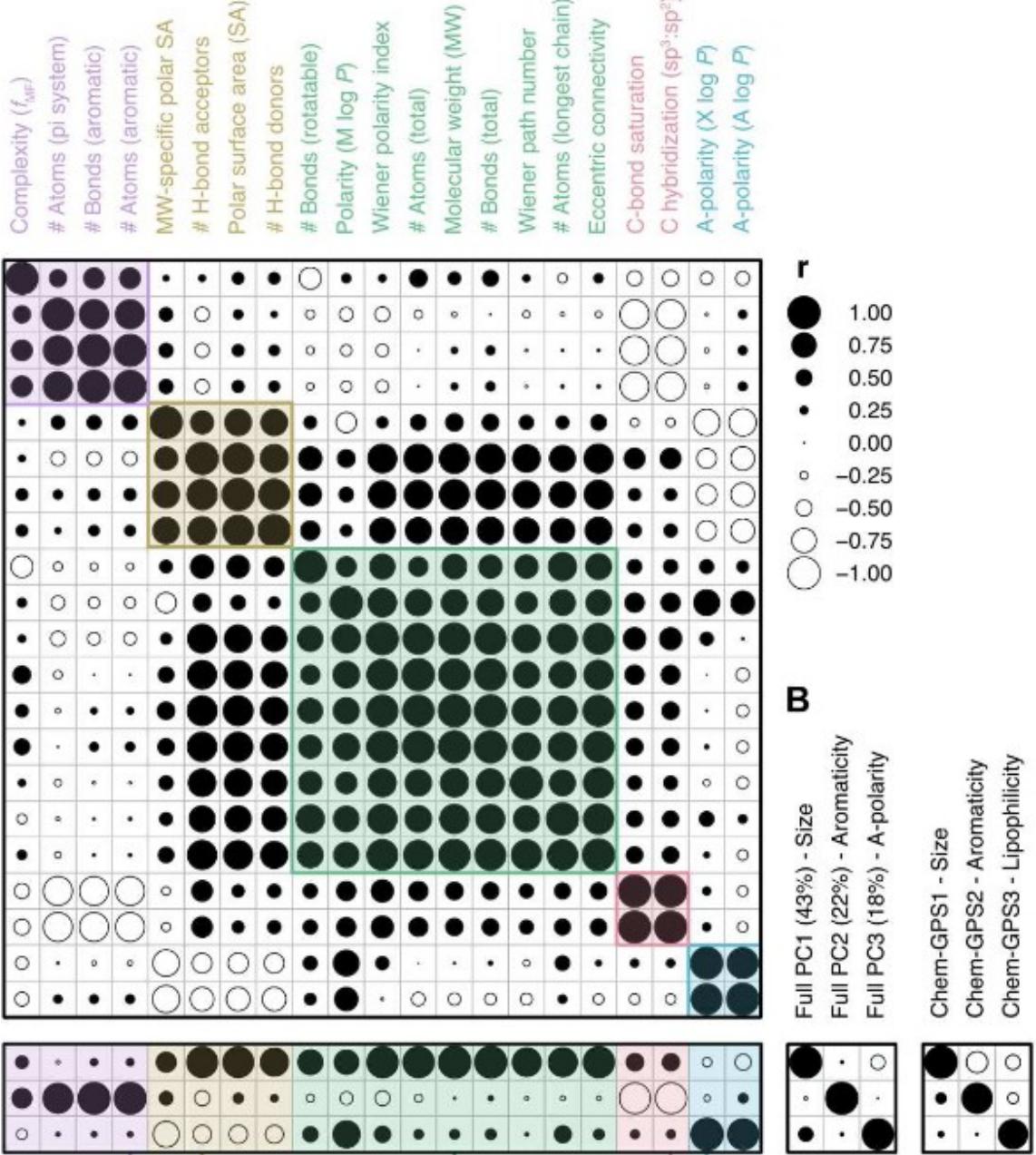
Lecture 21: Data Visualization Recap & Starting Projects

Prof. Meredith C. Schuman

meredithchristine.schuman@uzh.ch



Subset PC1 (38%) - Size
Subset PC2 (37%) - Aromaticity
Subset PC3 (22%) - A-polarity



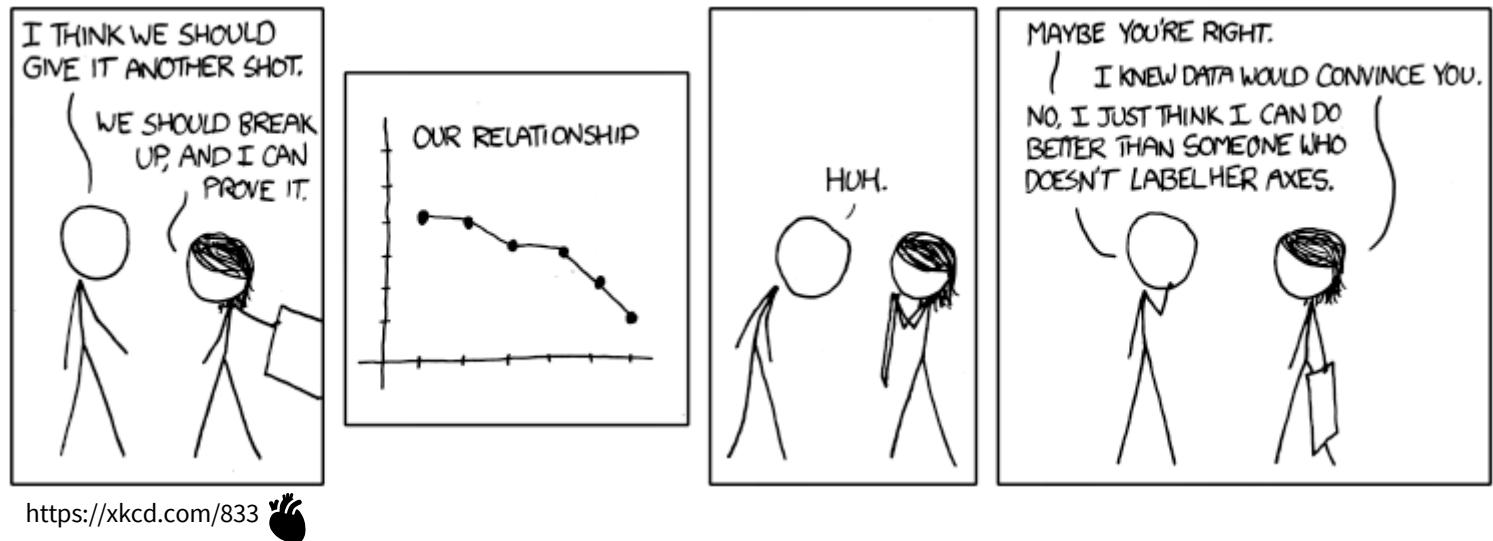
DSA103 revised overview

Block	Topic	Instructor(s)
17.-26.09. (sessions 1-4)	Computational thinking with Python: review and practice	Merry
01.-03.10. (sessions 5-6)	Version control: review and practice	Johannes
08.-10.10. (sessions 7-8)	Exploring data	
15.-17.10. (sessions 9-10)	Generating and reporting on data	
22.-29.10. (sessions 11-13)	Exploring life science data	
31.10. (session 14)	Recap / Q&A	Both
05.-07.11. (sessions 15-16)	Data wrangling	Johannes
12.11. (session 17)	Statistics (review)	
14.-19.11. (sessions 18-19)	Data visualization	
21.11. (session 20)	Recap / Q&A	
26.-28.11. (sessions 21-22)	Putting it together: small projects	Merry
03.12. (session 23)	Outlook: machine learning	
05.12. (session 24)	Free working time; projects due by end of day (23:59)	
10.12. (session 25)	Outlook: vibe coding	Both
12.12. (session 26)	Mock exam	
17.12. (session 27)	Recap / Q&A	
19.12. (session 28)	Exam	

Data visualization review

https://github.com/schoergj/DSA103/tree/main/exercises/lecture_18_visualisation

- Appropriate plot selection
- Units
- Color palette
- Uncertainty indication
- Exporting figures
- Labels, annotations, legends
- Scales
- Multiple axes
- Distributions
- Multi-panel figures
- (Executable publications)



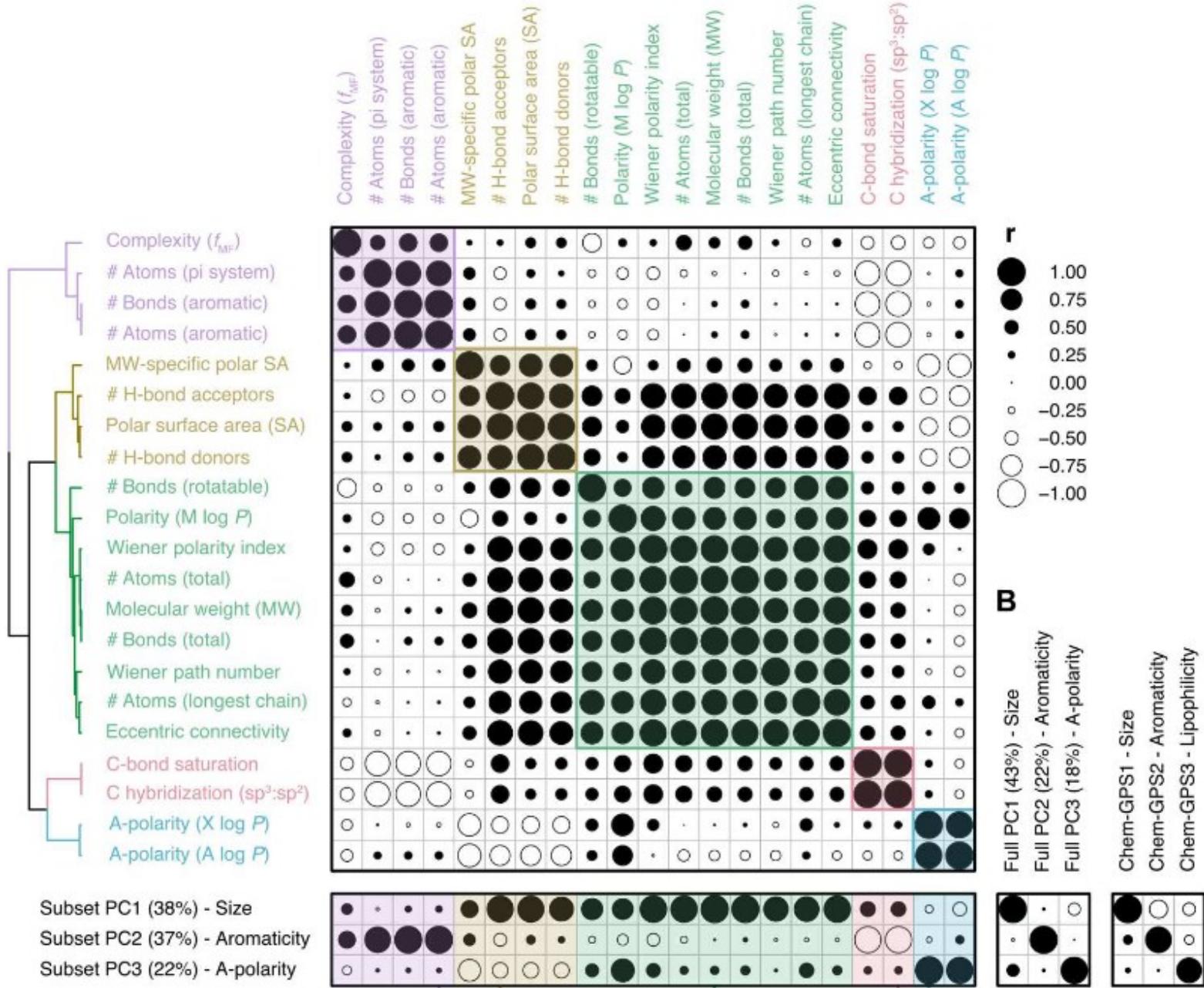
Starting on projects

Make a new repository for your project with the contents of the folder main/projects.

Then:

- Read the paper and summarize key points for yourself: fill in “ReadingScientificPapers”
- Make your documentation and data management plan: fill in “DocumentationDataManagementTemplate”

I'm here for questions. Bring filled-out documents on Friday! We'll discuss and start the next steps.



Project assignment

To hand in by 23:59 on Fri Dec 5 by sharing your repository:

- Filled-out sheets “ReadingScientificPapers” (for Walker et al. 2023) and “DocumentationDataManagementTemplate” (for your workflow)
- A one-page data story on your project (I’ll introduce this Friday Nov 28)
- Your code in Python*

*Note that Walker *et al.* has associated source data and code – have a look at it! Their code is in R, so you won’t be able to directly adopt it in Python, but it will help you see exactly what they did.