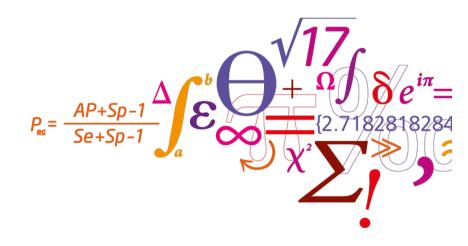
How to organize a project

The most important talk you never heard!

DTU Bioinformatics hackinar February 8th 2018

Leon Eyrich Jessen Postdoc Immunoinformatics and Machine Learning Department of Bio and Health Informatics Technical University of Denmark

Immunoinformatics and Machine Learning Department of Bio and Health Informatics



The most important talk you never heard!

- Think about it...
 - How many courses have you attended?
 - How many classes have you taken?
 - How many talks have you been to?
 - Etc.
- Has anyone ever talked to you about the underlying machinery?
- Has anyone ever presented you to or with a project organisation plan?
- How were the results you are being presented to produced?
- I know there are supposed to be a materials and methods section in papers Have you ever been tasked with deciphering and repeating such a section?

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The Corner Stone of Research

- In essence What is that we do?
 - We produce knowledge!
 - We disseminate knowledge!

• But...

- You cannot simply say I found 'Z'
- You HAVE to be able to account for how you got from 'A' to 'Z'
- Reproducible Research!
 - Being able to (easily) reproduce every single result from a paper
- Why?
 - Basically, we need to be able to see if you are cheating
 - Others need to stand on your shoulders

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So, how are we doing?

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NATURE | NEWS FEATURE

1,500 scientists lift the lid on reproducibility

Survey sheds light on the 'crisis' rocking research.

Monya Baker

25 May 2016 | Corrected: 28 July 2016

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Hackinars in Bioinformatics 08 February 2018

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So, how are we doing?



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So, how are we doing?

- "More than 70% of researchers have tried and failed to reproduce another scientist's experiments"
- "More than half have failed to reproduce their own experiments"

So, what can we do?

- Granted, some of the reasons for the reproducibility crisis is beyond our control
 - Biology is notoriously messy
 - False positives
 - Etc.
- However, a step in the right direction is to think about organising and documenting your research
- I have seen many times people revisiting old projects only to find that they cannot figure the project out or even reproduce it or understanding the project is so time consuming, that repeating it is more time efficient
- Why does this happen?
 - Admitted, we're all storm chasers Always on the hunt for the next publication
 - Many see documentation as a waste of valuable time

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Familiar?

A STORY TOLD IN FILE NAMES			_ 🗆 🗙
Location: 😂 C:\user\research\data			~
Filename 🔺	Date Modified	Size	Туре
🚦 data_2010.05.28_test.dat	3:37 PM 5/28/2010	420 KB	DAT file
🚦 data_2010.05.28_re-test.dat	4:29 PM 5/28/2010	421 KB	DAT file
🚦 data_2010.05.28_re-re-test.dat	5:43 PM 5/28/2010	420 KB	DAT file
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🔞 data_2010.05.29_crap.dat	3:22 AM 5/29/2010	437 KB	DAT file
関 data_2010.05.29_notbad.dat	4:16 AM 5/29/2010	670 KB	DAT file
🚦 data_2010.05.29_woohoo!!.dat	4:47 AM 5/29/2010	1,349 KB	DAT file
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🗈 Notes_Meeting_with_ProfSmith.txt	11:38 AM 5/29/2010	1,673 KB	TXT file
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🚦 data_2010.05.30_startingover.dat	8:37 AM 5/30/2010	420 KB	DAT file
٢			>
Type: Ph.D Thesis Modified: too many times	Copyright: Jorge Cham	www.phdo	omics.com

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Who has taught you to organise a project?

• "In practice, the principles behind organizing and documenting ... are often learned on the fly"

PLoS Comput Biol. 2009 Jul; 5(7): e1000424. Published online 2009 Jul 31. doi: <u>10.1371/journal.pcbi.1000424</u> PMCID: PMC2709440

A Quick Guide to Organizing Computational Biology Projects

William Stafford Noble 1, 2, *

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Let's dive in...

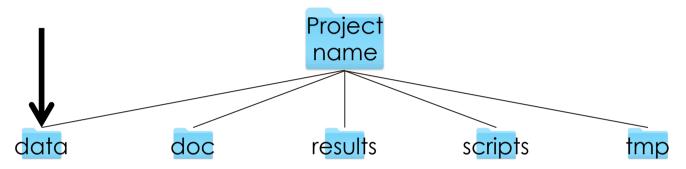
• The following is inspired by this paper

PLoS Comput Biol. 2009 Jul; 5(7): e1000424. Published online 2009 Jul 31. doi: <u>10.1371/journal.pcbi.1000424</u> PMCID: PMC2709440

A Quick Guide to Organizing Computational Biology Projects

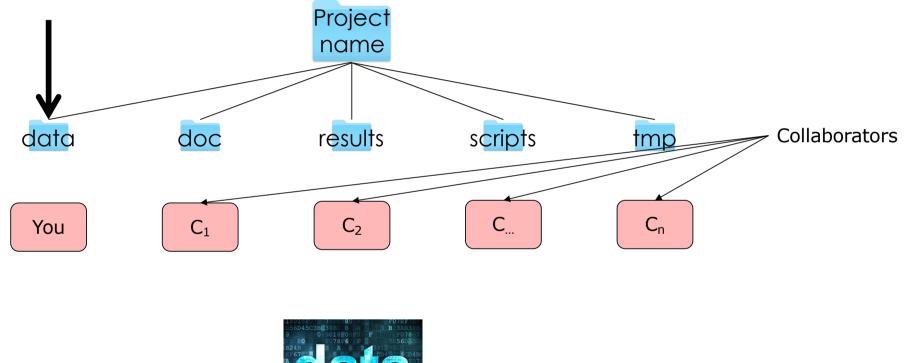
William Stafford Noble 1, 2, *

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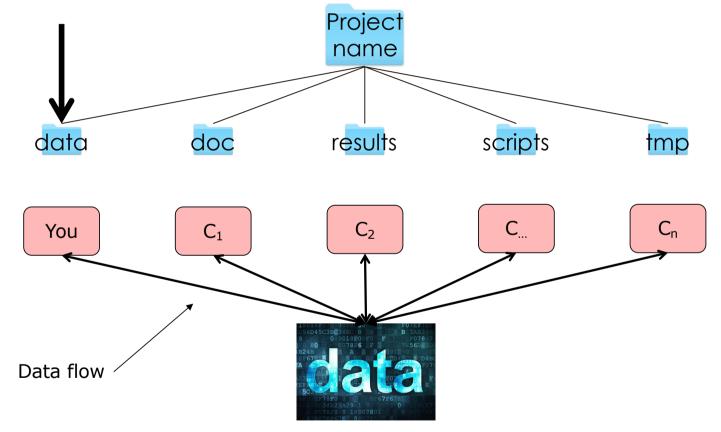
- Raw Data should always be pulled from central source, <u>never</u> from an excel sheet someone sent to you
- You are not allowed to touch or alter the original raw data
- Make sure that every step from the raw data, to the data you use for analysis can be repeated
- Save the cleaned data and proceed from that
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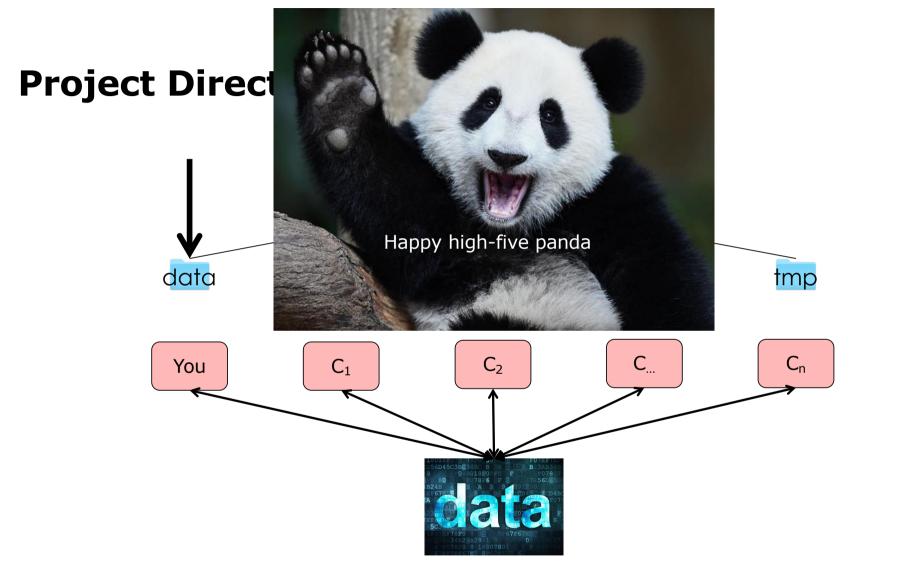




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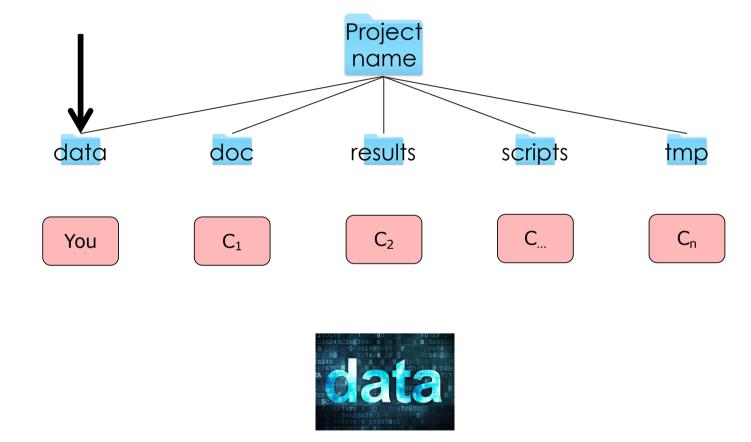
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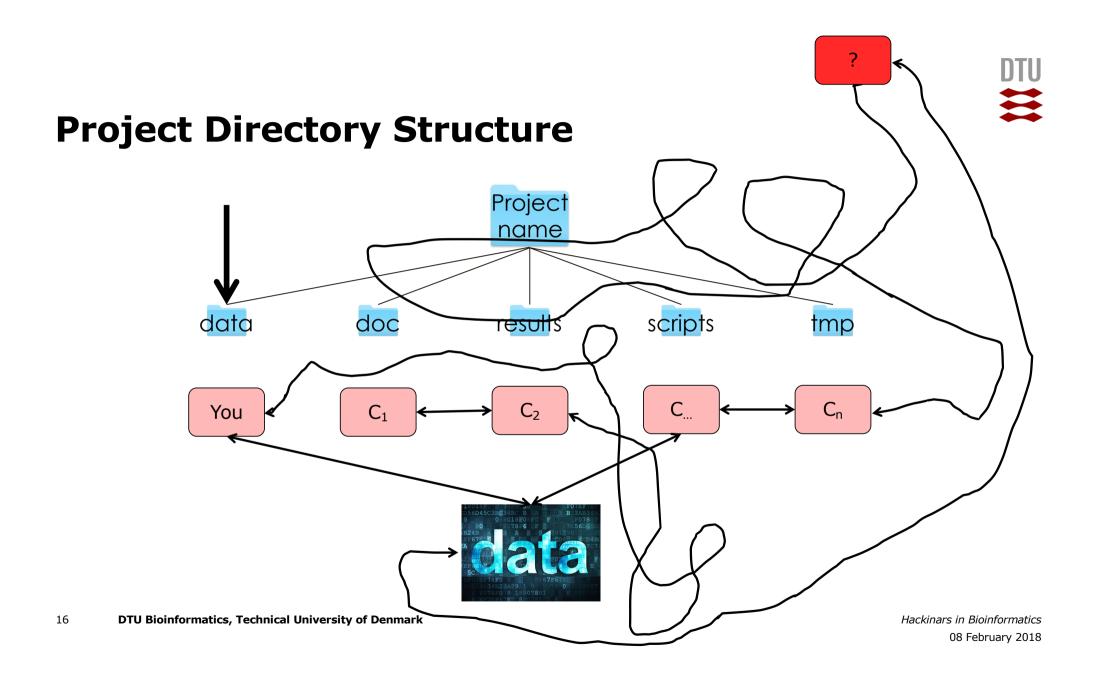
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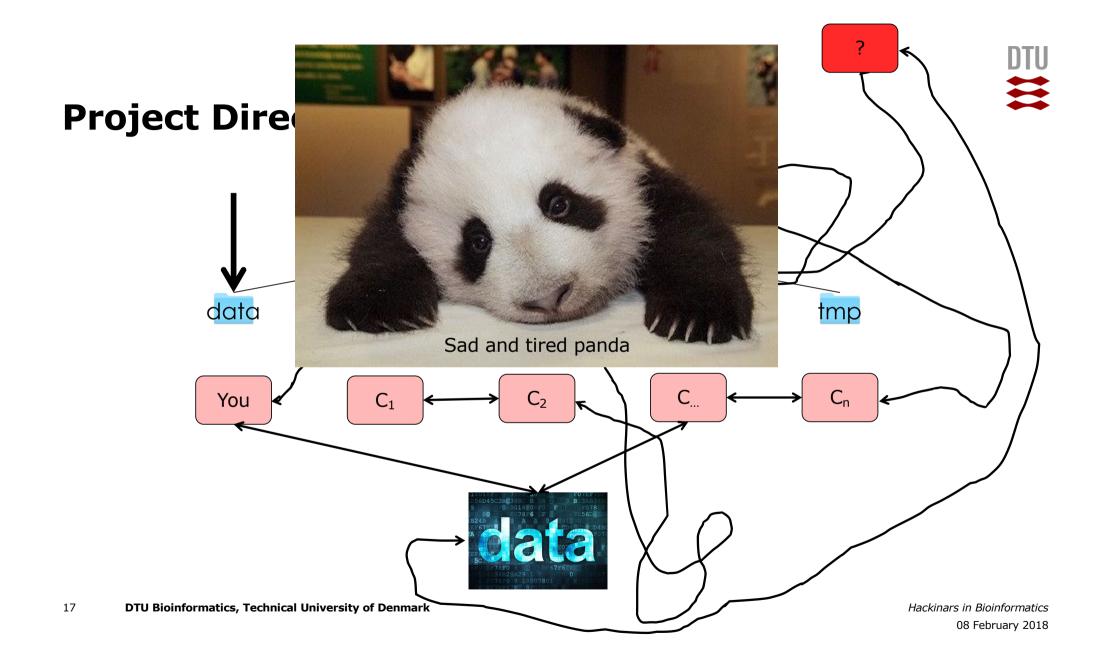
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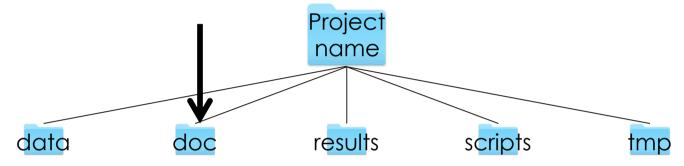
DTU



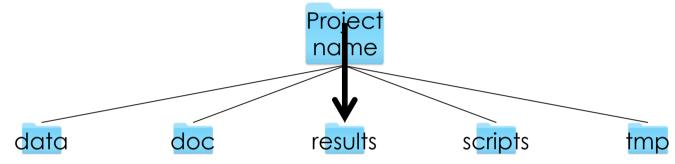
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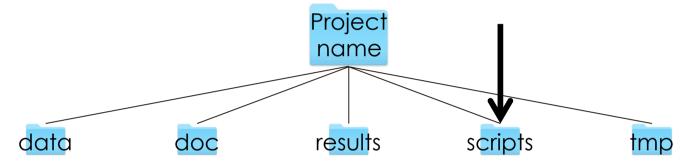


- This is where your manuscript lives
- Notes, presentations, pdfs and alike pertaining to the project
- Etc.

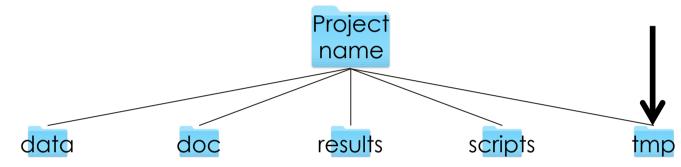


- Anything considered a results
- Plots
- Text file with p-value tables
- Etc.

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- This is where your analysis scripts are places
- All scripts shall be able to run from start-to-end



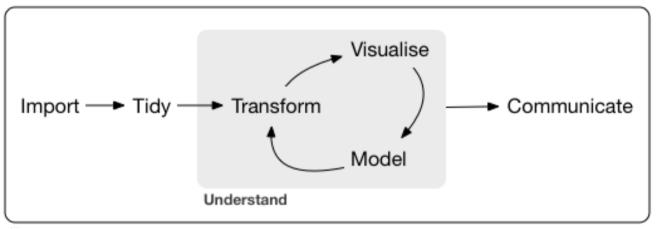
- Anything you can delete without thinking about it
 - Tests
 - Stuff you want to check
 - Temporary exploratory files
 - Etc...

Building your 'scripts' directory

- Load-clean-func-do philosophy
- First scripts takes your raw data from raw to analysis-ready
 - Raw data is loaded and cleaned
 - Clean data and versions hereof are saved for subsequent use
- Project specific functions are put in a separate file
- A single do file is defined capable of running the ENTIRE project and produce ALL results
- Collect the results in a markdown file
- Use GitHub for sharing, version control and backup

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The essence of data science

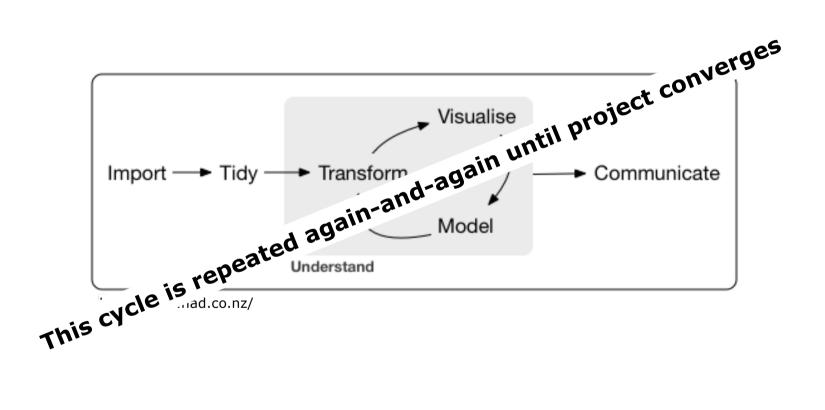


http://r4ds.had.co.nz/

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The essence of data science



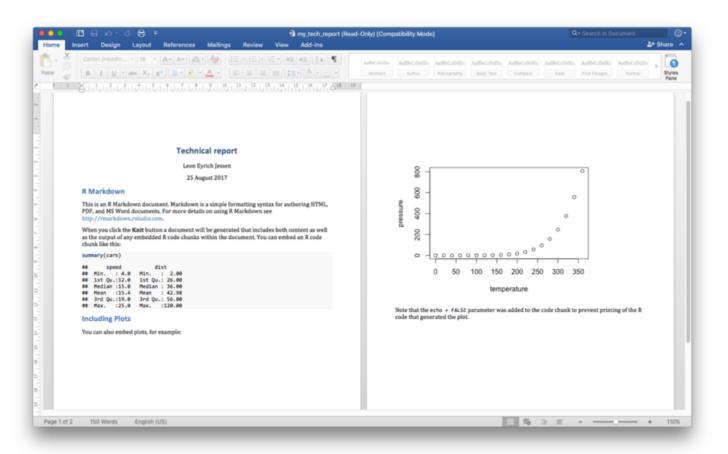
Project finalisation

- Ideally,
 - Once analysis has converged, a technical report should be created using markdown
 - Once the paper is published the project directory should be frozen as read-only
 - The directory should contain everything needed to recreate all the exact figures and tables in the paper

Briefly on markdown

- Dynamic generation of technical documents
- All numbers, pictures, tables etc. are dynamic
- If input changes, so does output
- Can be generated to output word, pdf and html

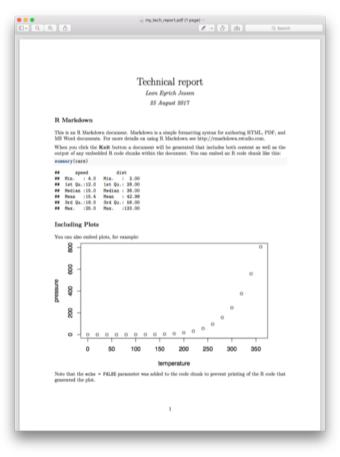
Markdown - Word



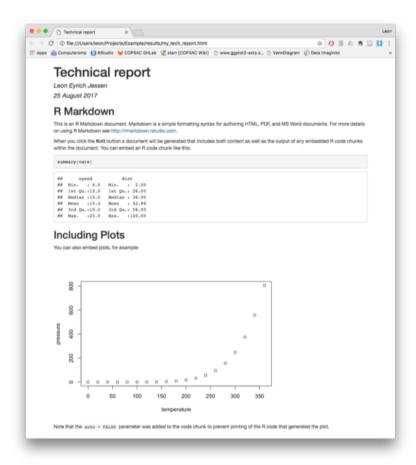
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Markdown - PDF



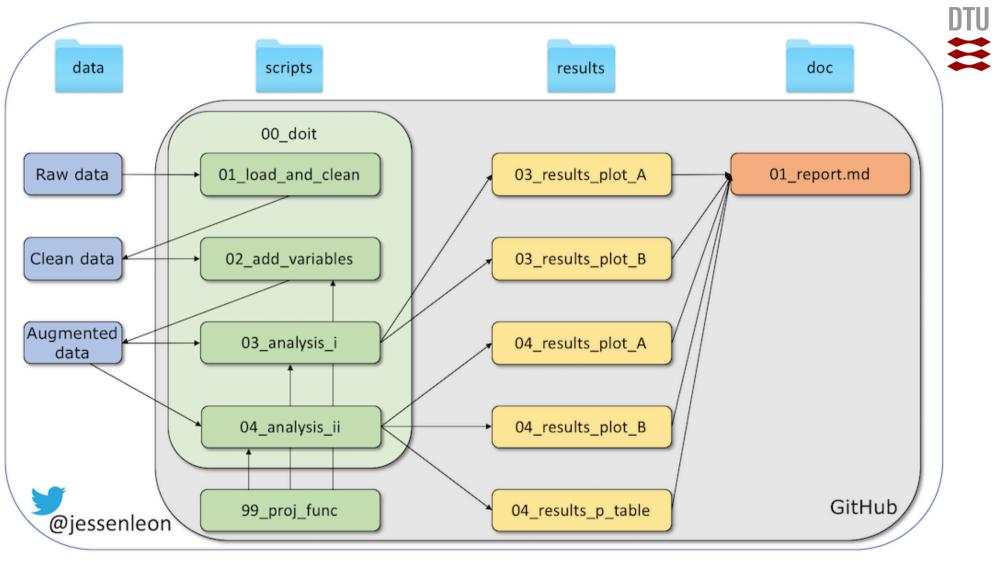
Markdown - HTML



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In conclusion

- This is not the absolute truth
- This is my current take on a how-to data science
- Structure takes time in order to save time
- Am I adhering 100% to this always and forever? No, but...
- I strongly believe that striving for structure is better than abandoning it
- A picture speaks a thousand words Let's try to visualise it!



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Think about readability of your code. Every project you work on is fundamentally collaborative. Even if you are not working with any other person, you are always working with future you and you really do not want to be in a situation where future you has no idea what past you was thinking, because past you will not respond to any emails! - Hadley Wickham