FOSE1025 — Scientific Computing

Week 10 Lecture 1: Towards Using Scripts for Reproducibility

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Programme

1. Scripts
2. MATLAB

Reading

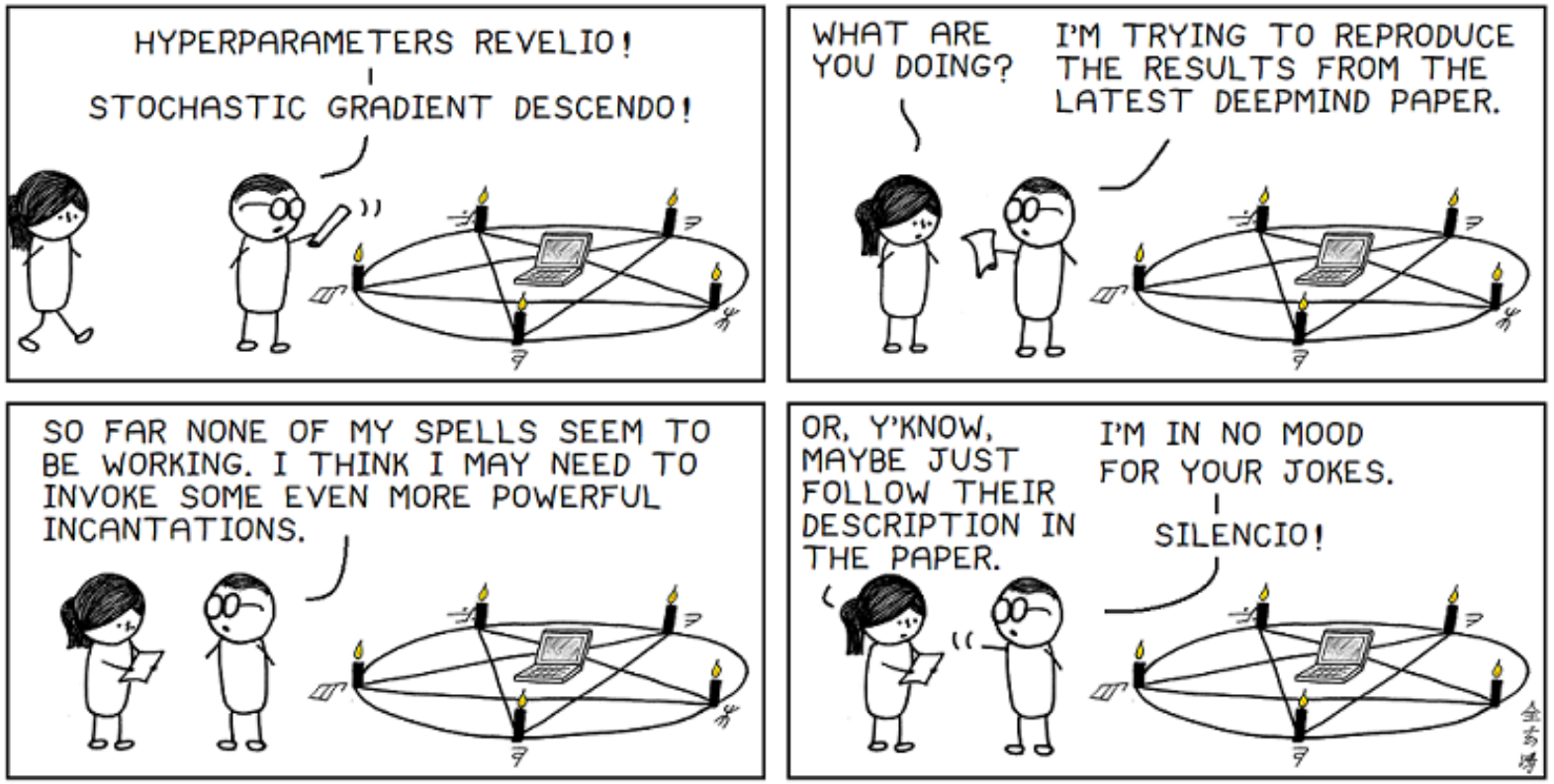
- Lecture notes

Programme

The Problem with Reproducibility

It can be difficult to write clearly enough to allow reproducibility.

https://abstrusegoose.com/588



Scripting Languages

- Scripting languages are programming languages designed for rapid prototyping.
  - $\Rightarrow$ These languages make it easy to quickly write and execute a program.
- Scripting languages are normally interpreted languages.
  - $\Rightarrow$ This means that you can execute instructions one by one using a run time environment.

Example of Steps

1. Start the run time environment (e.g. MATLAB).
2. Type instructions (or load instructions stored in a file).
3. Run the instructions in the run time environment.

Top 10 Programming Languages for Data Science

https://www.analyticsinsight.net/top-10-data-science-programming-languages-for-2020/

1. Python (popular among programmers and web developers)
2. R (popular among statisticians)
3. SQL (designed for querying relational databases)
4. C (C++)
5. Java
6. JavaScript (originally designed to run in a browser)
7. MATLAB (the focus of this lecture)
8. Scala
9. Swift
10. Julia

Demonstration Using MATLAB Online

- In this demonstration, the runtime runs in the cloud.
- We use a web browser to interact with the runtime.
- Can be done with any computer as long as it has:
  - An internet connection.
  - A modern browser.
- There is no need to install additional software in your computer.

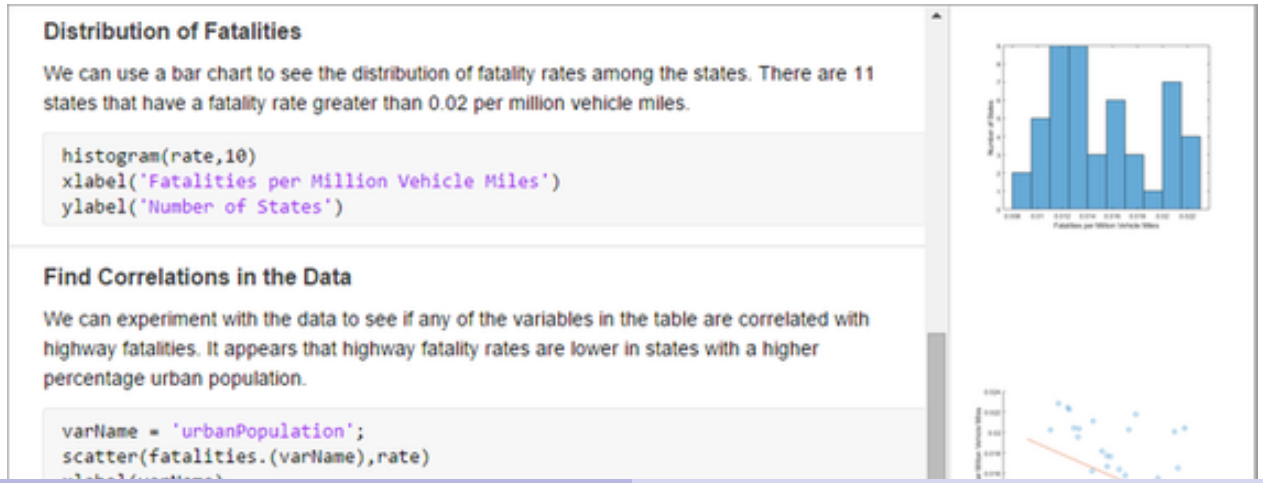
Scripting Languages and Reproducibility

- Instructions written in a scripting language ensure reproducibility . . . or does it not?
- While instructions written in a scripting language can be executed by a computer . . .
  - . . . instructions may not do what we intended them to do (e.g. because there are errors in the instructions).
  - Poorly-written scripts may not be understandable by people
    $\Rightarrow$ and then we cannot tell if they are correct.
  - Portability: Scripts running in a computer might not run in another computer.
    $\Rightarrow$ often you need to provide instructions for installation of necessary software dependencies.
- Normally we want to supplement the instructions with comments and explanations.

Notebooks for Reproducibility

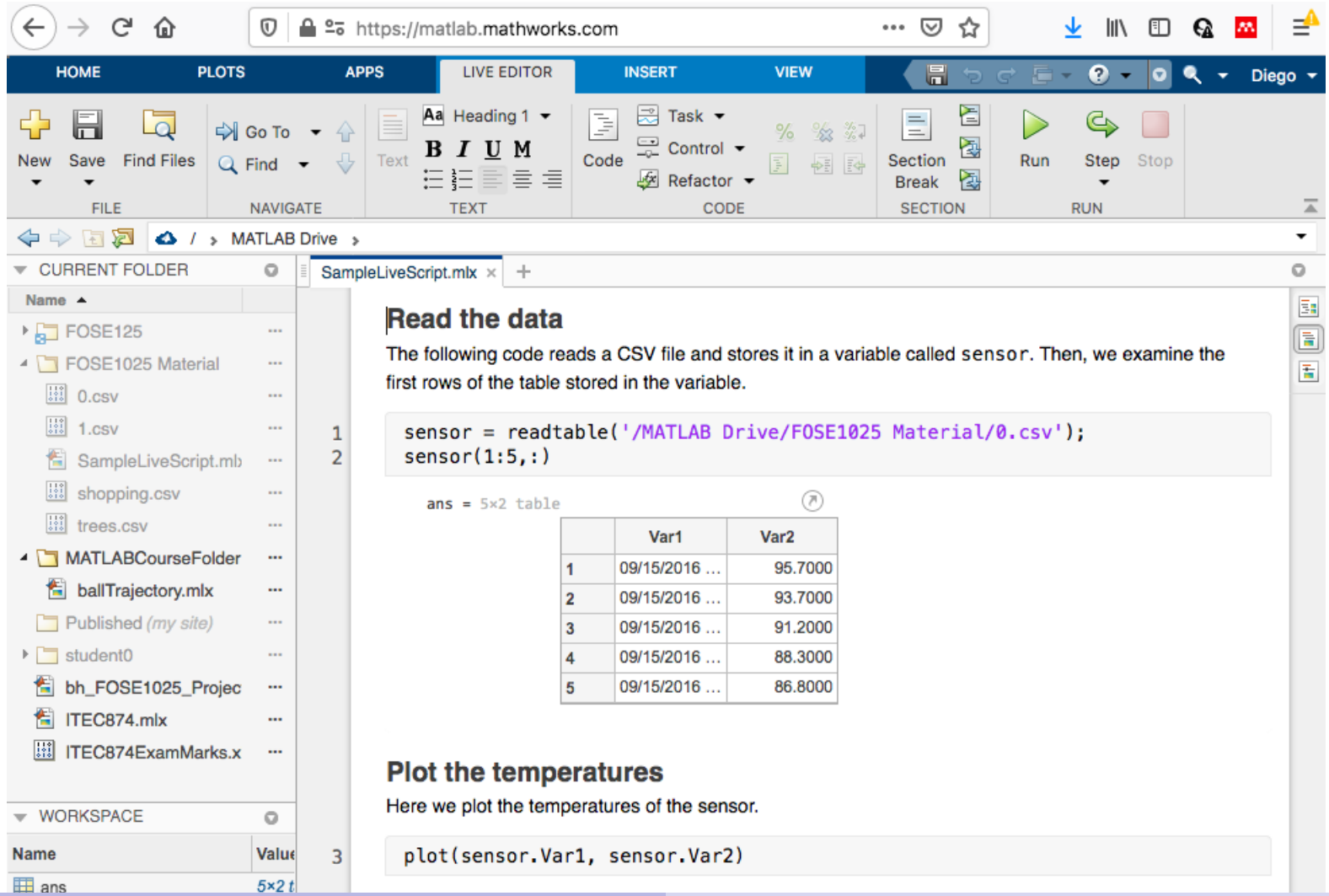
- Some run time environments allow the creation of notebooks.
  - Called live scripts in MATLAB.
- These notebooks are the digital equivalent of lab notebooks.
- Notebooks contain sections that can be executed.
- The results of execution appear in the notebook.
- Notebooks also contain formatted text for documentation and explanations.

https://au.mathworks.com/help/matlab/matlab_prog/what-is-a-live-script-or-function.html



Demonstration of a Live Script

SampleLiveScript.mlx



Programme

What is MATLAB?

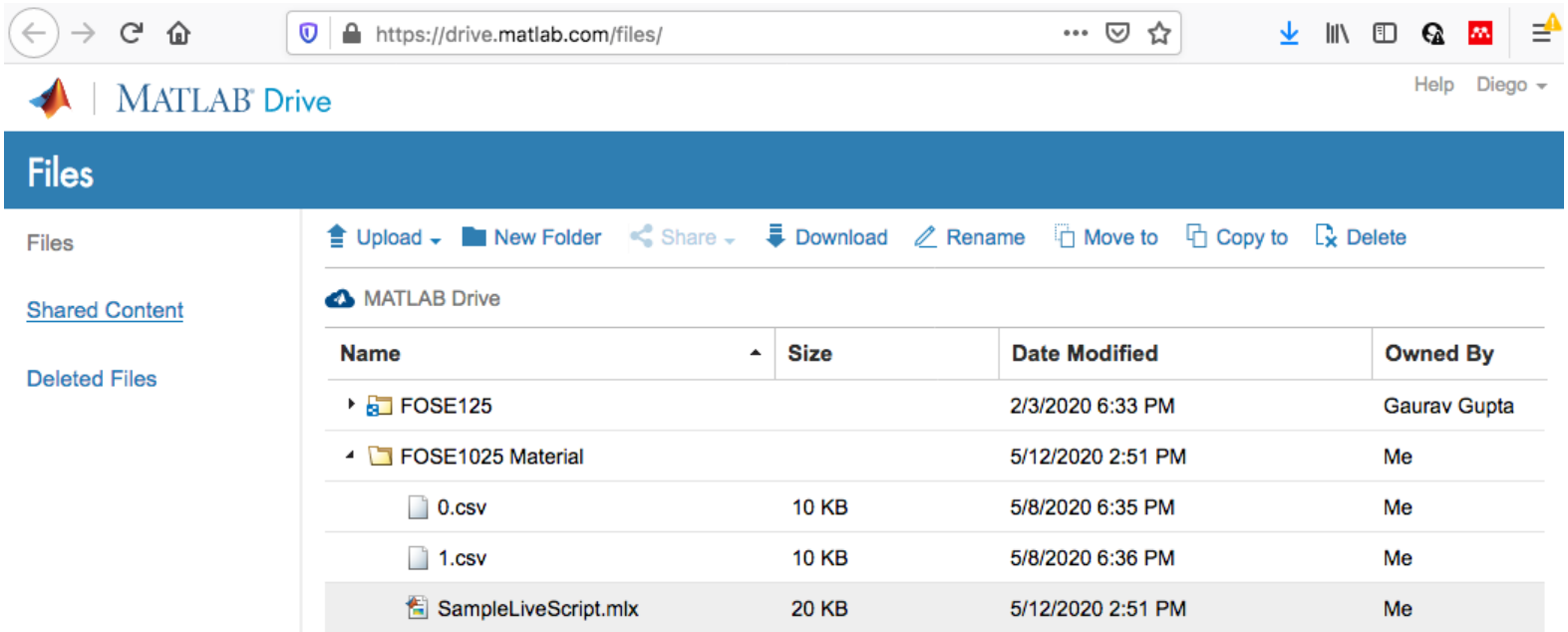
- MATLAB is a scripting language.
- Includes types designed to store and manipulate data.
  - Matrices (MATLAB = MATrix LABoratory)
  - Tables
- Includes a large library of functions for data analysis, manipulation, and visualisation.
- Has extensive documentation and on-line courses.
- Easy to use
- Others programming languages have attempted to integrate some of MATLAB's features.
  - Matrices, tables
  - Plots
  - Interactive notebooks

Accessing MATLAB and MATLAB Online

- Macquarie University has a license for students: https://au.mathworks.com/academia/tah-portal/macquarie-university-916052.html
- MATLAB Online here: https://matlab.mathworks.com/
- Getting started: https://au.mathworks.com/help/matlab/getting-started-with-matlab.html
- Self-paced courses: https://matlabacademy.mathworks.com/

MATLAB Online and MATLAB Drive

- MATLAB Online runs in the cloud.
- To upload files to the cloud you can use MATLAB Drive.
- You can use a browser to upload and download files.
- Or you can install software that integrates with your computer file system.
  - It looks and feels like MATLAB drive is a folder in your computer.



Loading data in MATLAB

- MATLAB Fundamentals, Chapter 10, "Tables of Data"
- https://au.mathworks.com/help/releases/R2019b/matlab/matlab_prog/create-a-table.html
- MATLAB can store tables into variables.
- You can use the MATLAB "Import Data" wizard.
  - Looks like a more sophisticated version of Excel's Import tools.
- Or you can use the readtable instruction.
  - `trees = readtable("trees.csv");`

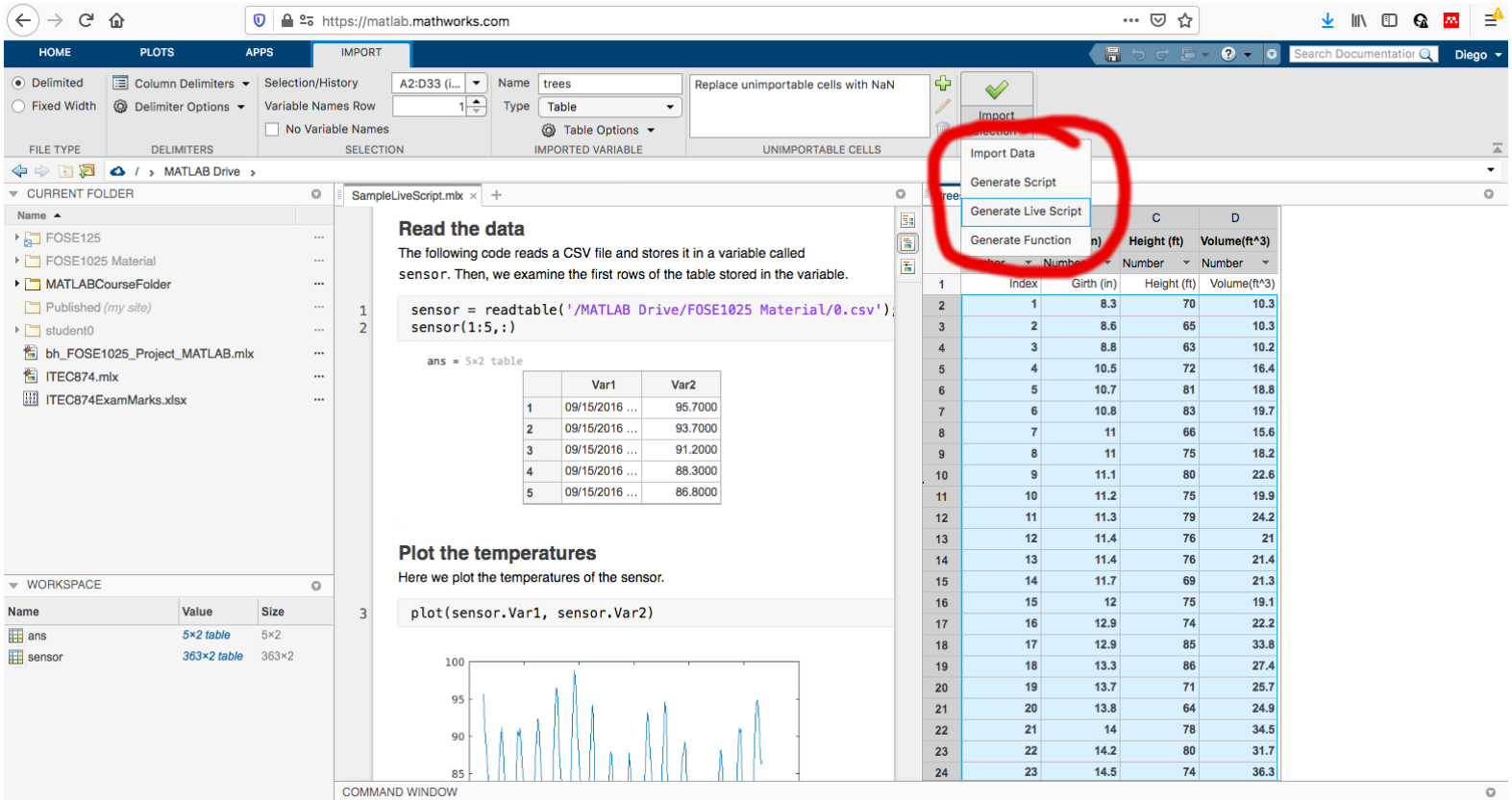
Processing data in MATLAB

- https://au.mathworks.com/help/releases/R2019b/matlab/matlab_prog/access-data-in-a-table.html
- Accessing a column: `girth = trees.("Girth (in)")`
- Accessing a full row: `sample = trees(5,:)`
- Adding a column:
  `trees.("Girth (cm)") = trees.("Girth (in)") * 2.54`
- Concatenating tables:

```
table0 = readtable("0.csv");
table1 = readtable("1.csv");
table = [table0; table1];
```

Creating and Reusing MATLAB Scripts

- Many MATLAB wizards can generate scripts.
- You can write your own script.
- Then you can run it again later.



Take-home Messages

- Scripting languages are powerful means to allow reproducibility.
- Scripting languages can be executed by a computer.
- Some environments allow the use of interactive notebooks for better reproducibility.
- MATLAB is a powerful scripting language designed for data analysis.

What's Next

- Monday 18 May: Submit your report for reproducibility.
- Wednesday 20 May, 10am: In-class quiz 4.
- Friday 22 May: Submit Collaborator Module (hurdle, Turnitin).
- Friday 29 May: Complete peer review of report for reproducibility.
- Friday 29 May: Submit Professional Module (hurdle, Quiz).
- Friday 5 June: Problem Solver Module (hurdle, Quiz).