

FOSE1025 — Scientific Computing

Week 6 Lecture 1: Towards Using Scripts for Reproducibility

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FOSE1025 2020H2

Abstract

In this lecture we will have a very brief introduction to the use of scripts to store and manipulate data. We move away from Excel and enter the area of programming. The emphasis will be on how to use scripts for reproducibility, and we will focus in a particular environment: MATLAB.

Update August 25, 2020

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Reading

- These notes
- <https://au.mathworks.com/help/matlab/getting-started-with-matlab.html>
- <https://au.mathworks.com/videos/getting-started-with-matlab-1564521672719.html>
-

FOSE1025's public github page

FOSE1025/S2_2020

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dmollalid Copy of 2020S1 for weeks 1 to 5 cc988b 35 minutes ago 2 commits

lectureNotes	Copy of 2020S1 for weeks 1 to 5	35 minutes ago
practicals	Copy of 2020S1 for weeks 1 to 5	35 minutes ago
LICENSE	Initial commit	1 hour ago
README.md	Copy of 2020S1 for weeks 1 to 5	35 minutes ago

README.md

Public resources for FOSE125 & FOSX1025 - Scientific Computing; 2020 Semester 2

Some of the unit's public resources will be available in this github repository. Feel free to clone or fork it! But make sure to make your copy private if you decide to store your assignment solutions.

- [FOSE1025 unit guide at Macquarie University](#)
- [FOSX1025 unit guide at Macquarie University](#)

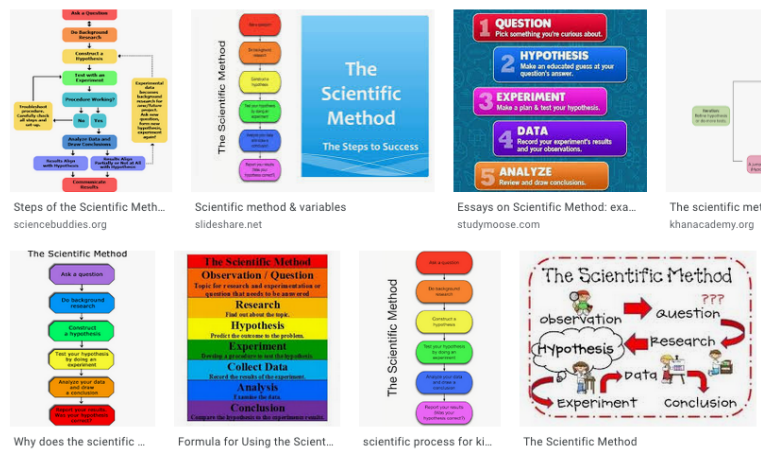
About: Resources for FOSE1025 Scientific Computing, Readme, MIT License

Releases: No releases published, Create a new release

Packages: No packages published, Publish your first package

1 Review: Excel for Science

The Scientific Method



Some results of a Google image search with the words "scientific" and "method" — 1 April 2020.

Excel to Manage Data in Science

We are covering these aspects in FOSE1025:

- Import data from external files (e.g. CSV) — Week 3.
- Explore the data — Week 4, Week 5.
- *(you are here)*
- Clean the data — Week 7.
- Preprocess, transform the data — Week 8.
- Analyse, summarise, interpret the data — Week 5, Week 9.

Importing Data

CSV — Comma Separated Values

- In practice, the file could use other delimiters: tab, semicolon (;), blank space, ...
- Some times, the data fields are determined by the width.

Data Types

- Numbers
- Text
- Dates
- Currency
- ...

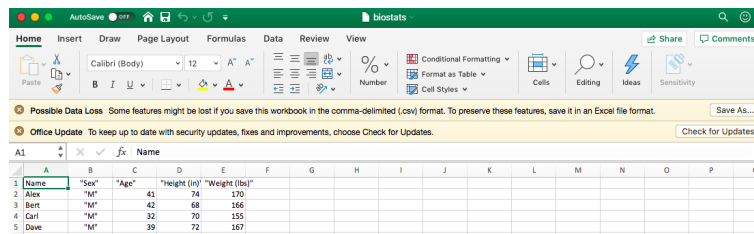
Example CSV File

(The lecturer will demo how to import this)

biostats.csv from <https://people.sc.fsu.edu/~jburkardt/data/csv/csv.html>

"Name"	"Sex"	"Age"	"Height (in)"	"Weight (lbs)"
"Alex"	"M"	41	74	170
"Bert"	"M"	42	68	166
"Carl"	"M"	32	70	155
"Dave"	"M"	39	72	167
"Elly"	"F"	30	66	124
"Fran"	"F"	33	66	115
"Gwen"	"F"	26	64	121
"Hank"	"M"	30	71	158
"Ivan"	"M"	53	72	175
"Jake"	"M"	32	69	143
"Kate"	"F"	47	69	139
"Luke"	"M"	34	72	163
"Myra"	"F"	23	62	98
"Neil"	"M"	36	75	160
"Omar"	"M"	38	70	145
"Page"	"F"	31	67	135
"Quin"	"M"	29	71	176
"Ruth"	"F"	28	65	131

Careful if you double-click on a CSV file!



- If you double-click on a CSV file, Excel will open the file.
- But the file opened is a CSV file, not an Excel (.xlsx) file!
 - Read the warning that you get if you double-click on the CSV file.
- There are many things that you cannot save in a CSV file.
 - Formulas, formatting, charts, etc.

Tables in Excel

- Tables are the fundamental data structure.
- Each row indicates a data sample.
- Each column indicates a type of data.
 - Number, string, date, etc.

- Categorical data: when there is a pre-determined set of values.

	A	B	C	D	E	F
1	Name	"Sex"	"Age"	"Height (i	"Weight (lbs)"	
2	Alex	"M"	41	74	170	
3	Bert	"M"	42	68	166	
4	Carl	"M"	32	70	155	
5	Dave	"M"	39	72	167	
6	Elly	"F"	30	66	124	
7	Fran	"F"	33	66	115	
8	Gwen	"F"	26	64	121	
9	Hank	"M"	30	71	158	
10	Ivan	"M"	53	72	175	
11	Jake	"M"	32	69	143	
12	Kate	"F"	47	69	139	
13	Luke	"M"	34	72	163	
14	Myra	"F"	23	62	98	
15	Neil	"M"	36	75	160	
16	Omar	"M"	38	70	145	
17	Page	"F"	31	67	135	
18	Quin	"M"	29	71	176	
19	Ruth	"F"	28	65	131	

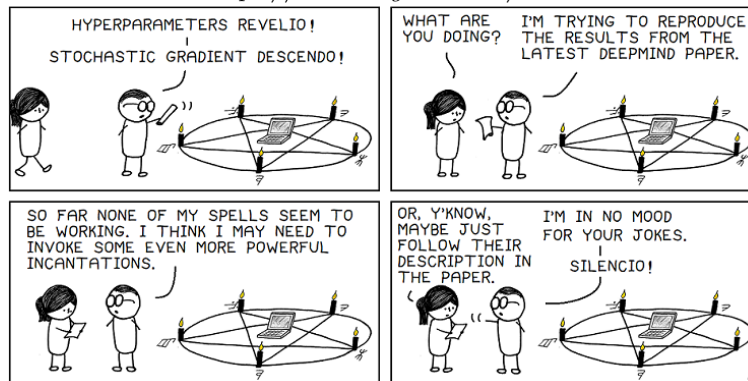
Question: What are the data types of each column?

2 Scripts for Reproducibility

The Problem with Reproducibility

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

<https://abstrusegoose.com/588>



Reproducibility in Science

- When you conduct science, you need to make sure that others can reproduce what you did.
 - If others can reproduce what you did, then your claims are more likely to be taken as valid.
- Reproducibility means that someone else should be able to do the same as you did by following your instructions.
- When the experiments are performed with computers, there is some discussion/disagreement about what does “following your instructions” means:
 1. I can re-implement what you did after I read your report.
 2. I can run the code you wrote.
- The employability modules (“Achiever” and “Communicator”) touch item 1.
- Here we will touch item 2.

Scripting Languages

- Scripting languages are programming languages designed for *rapid prototyping*.
⇒ These languages make it easy to quickly write and execute a program.
- Scripting languages are normally *interpreted languages*.
⇒ 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 unit)*
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.

MATLAB Online

- <https://au.mathworks.com/academia/tah-portal/macquarie-university-916052.html>
- Create an account with your student email address
- Do not use your student password (create a new one)

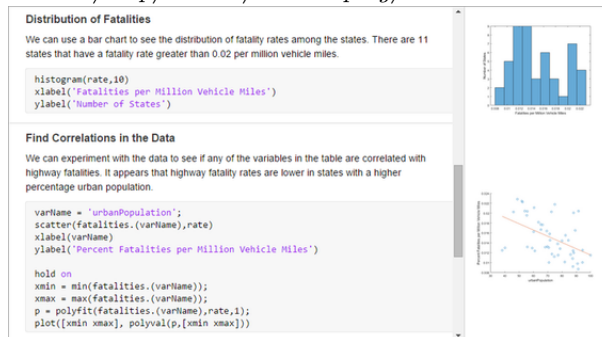
Scripting Languages and Reproducibility

- 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
 - ⇒ and then we cannot tell if they are correct.
 - *Portability*: Scripts running in a computer might not run in another computer.
 - ⇒ 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

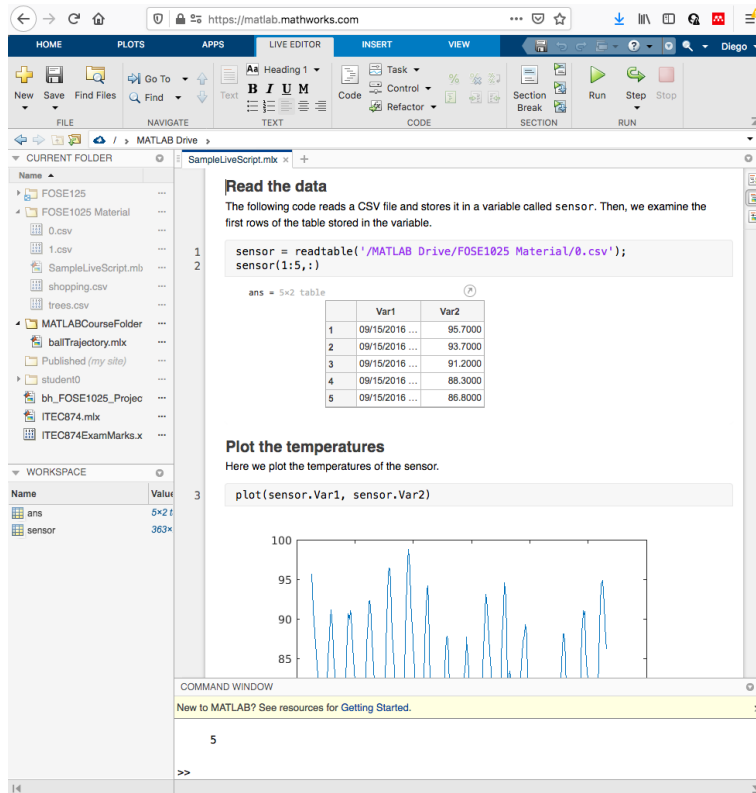
- Some run time environments allow the creation of notebooks.
 - Called *live scripts* in MATLAB.
- These notebooks are the digital equivalent of lab notebooks.
- Notebooks contain sections that can be executed.
- The results of execution appear in the notebook.
- Notebooks also contain formatted text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



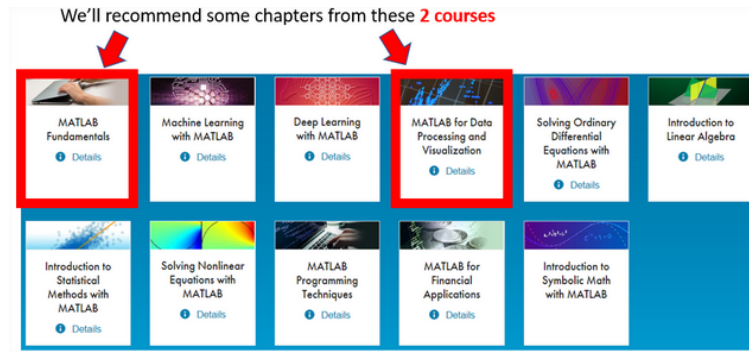
3 MATLAB

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

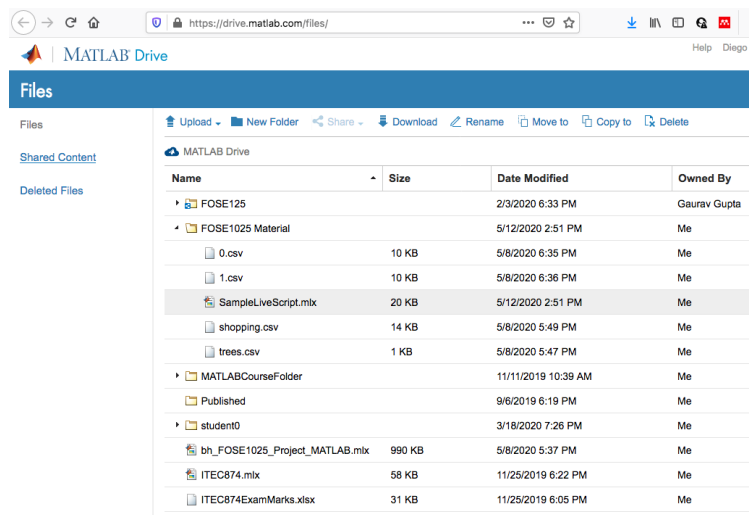
Accessing MATLAB and MATLAB Online

- 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:

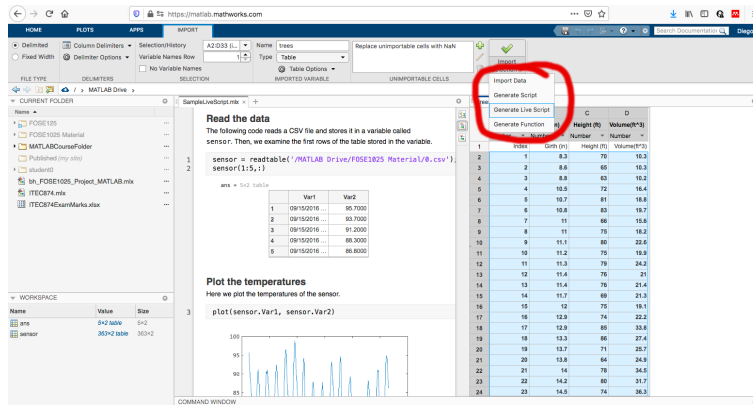
```
table0 = readtable("0.csv");  
table1 = readtable("1.csv");  
table = [table0; table1];
```

Participation Activity – MATLAB Grader

1. Access course FOSE1025 and FOSX1025 2020 S2 at MATLAB Grader
 - You should have received an invitation by email — check your student email.
2. Complete Lecture Participation Week 6
 - Read a CSV file
 - Extract a column
 - Extract a row

Creating and Reusing MATLAB Scripts

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



Saving a MATLAB table as a CSV file

- MATLAB's writetable will write a table into a CSV file.
- https://au.mathworks.com/help/releases/R2019b/matlab/matlab_prog/create-a-table.html
- <https://au.mathworks.com/help/matlab/ref/writetable.html>
- writetable(table, 'table.csv') will save the table into file table.csv
- writetable(table, 'table.csv', 'WriteRowNames', true) will also write the column names.

Take-home Messages

- Excel as a tool to manage data in science.
- Excel tables.
- 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.
- Importing data in MATLAB.
- Accessing table rows and columns in MATLAB.

What's Next

- Week 7 lecture: Cleaning data
- Week 7, Friday 11 September: Communicator hurdle