

FOSE1025 — Scientific Computing

Week 9 Lecture 1: Summarising and Analysing Data

Diego Mollá

Department of Computer Science
Macquarie University

FOSE1025 2021H2

Programme

- 1 Excel's Pivot Tables
- 2 Processing Long Tables in MATLAB
- 3 Data Analysis in MATLAB

Reading

- These notes
- Related MATLAB scripts
 - <https://au.mathworks.com/help/releases/R2020a/matlab/ref/double.groupsummary.html>
 - <https://au.mathworks.com/help/releases/R2020a/matlab/ref/unstack.html>

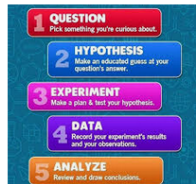
The Scientific Method



Steps of the Scientific Meth...
sciencebuddies.org



Scientific method & variables
slideshare.net



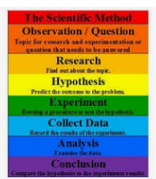
Essays on Scientific Method: exa...
studymoose.com



The scientific met...
khanacademy.org



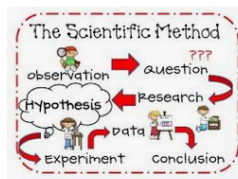
Why does the scientific ...



Formula for Using the Scient...



scientific process for ki...



The Scientific Method

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

Excel and MATLAB to Manage Data in Science

We are covering these aspects in FOSE1025:

- Represent data in Excel — Weeks 2 & 3.
- Represent data in MATLAB — Weeks 3 & 5.
- Explore data in Excel — Week 4.
- Visualise data in Excel — Week 5.
- Import data from external files (e.g. CSV) — Week 6.
- MATLAB scripts for reproducibility — Week 6.
- Clean the data (Excel, MATLAB) — Week 7.
- Preprocess, transform the data (Excel, MATLAB) — Week 8.
- (you are here)
- Analyse, summarise, interpret the data (MATLAB) — Week 9.
- Ethics of Data — Week 10.

Programme

- 1 Excel's Pivot Tables
 - Excel's Pivot Tables for Charts
- 2 Processing Long Tables in MATLAB
- 3 Data Analysis in MATLAB

Pivot Tables: A Motivational Example

(data from <https://www.linkedin.com/learning/excel-pivottables-for-beginners>)

- Find the total shopping in each category “Fuel”, etc, of file shopping.csv.
- Find the total shopping of each month.
- What shopping per month and per category??
- Pivot tables can help you generate data for all of above and more.

| Date | Buyer | Type | Amt |
|-------|-------|-----------|-------|
| 1-Jan | Mom | Fuel | \$50 |
| 2-Jan | Mom | Groceries | \$120 |
| 3-Jan | Dad | Cafes | \$10 |
| 4-Jan | Dad | Fuel | \$40 |
| 4-Jan | Kelly | Groceries | \$129 |
| 5-Jan | Mom | Cafes | \$12 |

A Simple Pivot Table

File: shopping.csv

| | A | B | C | D | E | F | G | H | I | J | K |
|----|-------------|-------|-------|---------------|------|-----------|-------|-------------|---------|-------------|---|
| 1 | Buyer | (All) | | | | | | | | | |
| 2 | | | | | | | | | | | |
| 3 | Sum of Amt | Type | | | | | | | | | |
| 4 | Month | Books | Cafes | Entertainment | Fuel | Groceries | Music | Restaurants | (blank) | Grand Total | |
| 5 | 1 | 169 | 36 | 271 | 209 | 2147 | 15 | | | 2847 | |
| 6 | 2 | 476 | 59 | 142 | 202 | 2820 | 15 | | | 3714 | |
| 7 | 3 | 160 | 48 | 51 | 329 | 2348 | 46 | 2519 | | 5501 | |
| 8 | 4 | 418 | 34 | 307 | 100 | 2985 | 9 | 3299 | | 7152 | |
| 9 | 5 | 96 | 63 | 240 | 288 | 2911 | 14 | 2136 | | 5748 | |
| 10 | 6 | 38 | 145 | 309 | 198 | 2905 | 86 | 3352 | | 7033 | |
| 11 | 7 | 60 | 33 | 722 | 228 | 2834 | 6 | 3419 | | 7302 | |
| 12 | 8 | 79 | 38 | 143 | 138 | 3120 | 17 | 3651 | | 7186 | |
| 13 | 9 | 61 | | | 163 | 2377 | 9 | 3783 | | 6393 | |
| 14 | 10 | 39 | | | 165 | 3063 | 13 | 3492 | | 6772 | |
| 15 | 11 | 67 | | | 927 | 117 | 2373 | 10 | 1030 | 4524 | |
| 16 | 12 | 328 | | | 2627 | 55 | 2786 | 9 | | 5805 | |
| 17 | (blank) | | | | | | | | | | |
| 18 | Grand Total | 1991 | 456 | 5739 | 2192 | 32669 | 249 | 26681 | | 69977 | |
| 19 | | | | | | | | | | | |
| 20 | | | | | | | | | | | |
| 21 | | | | | | | | | | | |
| 22 | | | | | | | | | | | |

PivotTable Fields

Choose fields:

- ☐ Day
- ☒ Month
- ☒ Buyer
- ☒ Type
- ☒ Amt

Drag fields between areas below:

FILTERS

Buyer

COLUMNS

Type

ROWS

Month

VALUES

Sum of Amt

Anatomy of a Pivot Table

Filters

- What column to use to filter values.
- Only for columns with categorical data.

Rows

- What column to use in the rows of the pivot table.
- Only for columns with categorical data.

Columns

- What column to use in the columns of the pivot table.
- Only for columns with categorical data.

Values

- What value we want to aggregate.
- Only for columns with numerical data.

Pivot Tables to Convert from Long to Wide

Exercise 1 (weather_data.csv)

What is the average precipitation in Antigo?

- Using AVERAGEIFS
- Using a pivot table

Exercise 2 (weather_data.csv)

What is the March-2013 average precipitation in Antigo?

- Using AVERAGEIFS
- Using a pivot table

| | A | B | C | D | E | F |
|---|---|------------|--------|---------------|------------|---|
| 1 | | data | date | param | siteid | |
| 2 | 1 | 0 | 1/1/03 | Precipitation | ACRE | |
| 3 | 2 | 0 | 2/1/03 | Precipitation | Albert Lea | |
| 4 | 3 | 11.3199997 | 3/1/03 | Precipitation | Ames | |
| 5 | 4 | 0 | 4/1/03 | Precipitation | Antigo | |

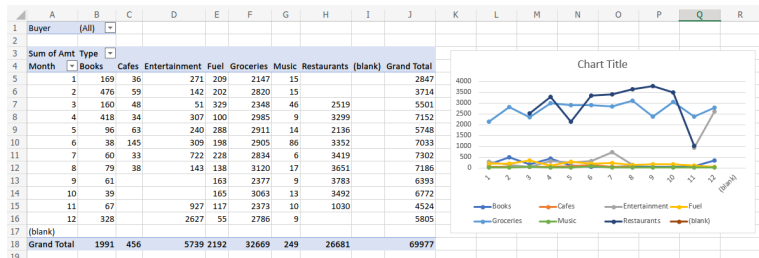
Programme

- 1 Excel's Pivot Tables
 - Excel's Pivot Tables for Charts
- 2 Processing Long Tables in MATLAB
- 3 Data Analysis in MATLAB

Pivot Tables for Charts

Use file shopping.csv

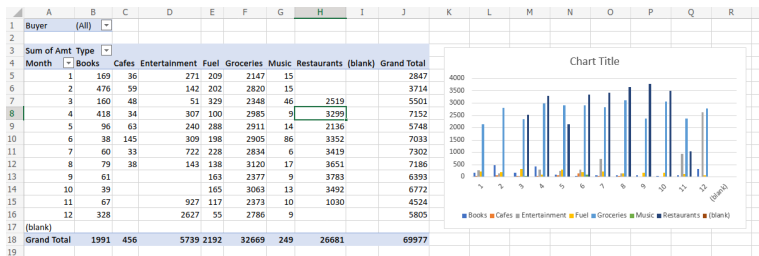
- Pivot tables facilitate the transformation of data for the creation of complex plots.
- In a **multiple chart**, each column of a table is plotted overlayed with the rest. Good for line charts.
- In a clustered chart, each row forms a cluster.
- In a stacked chart, the data of a table are plotted one on top of the other. Good for column charts.



Pivot Tables for Charts

Use file shopping.csv

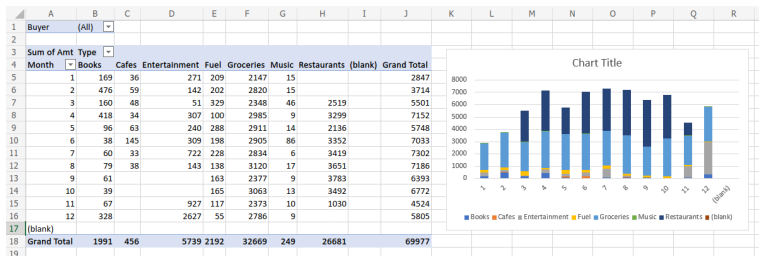
- Pivot tables facilitate the transformation of data for the creation of complex plots.
- In a multiple chart, each column of a table is plotted overlaid with the rest. Good for line charts.
- In a **clustered chart**, each row forms a cluster.
- In a stacked chart, the data of a table are plotted one on top of the other. Good for column charts.



Pivot Tables for Charts

Use file shopping.csv

- Pivot tables facilitate the transformation of data for the creation of complex plots.
- In a multiple chart, each column of a table is plotted overlayed with the rest. Good for line charts.
- In a clustered chart, each row forms a cluster.
- In a **stacked chart**, the data of a table are plotted one on top of the other. Good for column charts.

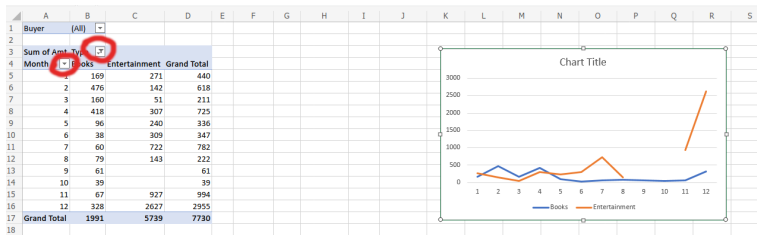


Exercise

Use file shopping.csv

Exercise: Can you plot (multiple line plot) the Books and Entertainment only?

- (hint: you can filter row labels and **column** labels.)



Programme

- 1 Excel's Pivot Tables
- 2 Processing Long Tables in MATLAB
- 3 Data Analysis in MATLAB

groupsummary

<https://au.mathworks.com/help/releases/R2020a/matlab/ref/double.groupsummary.html>

- groupsummary is one of the tools that MATLAB offers to obtain summaries from a long table.
- `groupsummary(T, groupvars, method, datavars)`
 - `T`: the table
 - `groupvars`: the variables to group
 - `method`: how to group them, e.g. `'sum'`, `'mean'`, etc. By default, if we don't say anything, it will count them.
 - `datavars`: what column to apply the method to. All other columns are ignored. By default, if we don't say anything, it will apply the method to all columns (except those specified in `'groupvars'`).

Demonstration

See file shopping.csv and script groupsummary_script.mlx

| | 1 | 2 | 3 | 4 |
|---|--------|-------|-----------|-----|
| | Date | Buyer | Type | Amt |
| 1 | 01-Jan | Mom | Fuel | 50 |
| 2 | 02-Jan | Mom | Groceries | 120 |
| 3 | 03-Jan | Dad | Cafes | 10 |
| 4 | 04-Jan | Dad | Fuel | 40 |
| 5 | 04-Jan | Kelly | Groceries | 129 |
| 6 | 05-Jan | Mom | Cafes | 12 |

- 1 How would you find the **total** shopping of each buyer?

```
groupsummary( shopping , ' Buyer ' , 'sum ' , 'Amt ' )
```

- 2 How would you find the **average** shopping of each buyer **per category**?

```
groupsummary( shopping , { ' Buyer ' , ' Type ' } , 'mean ' , 'Amt ' )
```

groupsummary with binning

See file shopping.csv and script groupsummary_script.mlx

<https://au.mathworks.com/help/releases/R2020a/matlab/ref/double.groupsummary.html>

- Sometimes we want to group by **parts of a date**. We can do this by specifying **group bins**.
- `groupsummary(T, groupvars, groupbins, method, datavars)`
- Possible types of group bins for dates:
 - **dayname**: the day of the week.
 - **monthname**: the month of the year.
 - **month**: by months.

(see lecture notes for more options)

- 1 How would you find the **total** shopping of **each month**?

```
groupsummary( shopping , 'Date' , 'monthname' , 'sum' , 'Amt'  
            ' )
```

unstack

Use file weather_data.csv

<https://au.mathworks.com/help/releases/R2020a/matlab/ref/unstack.html>

- unstack can be used to convert a long table into a wide table.
- `unstack(S,vars,ivar)`
 - `S` The table to unstack.
 - `vars` The values to fill in the new columns.
 - `ivar` The indicator variables. Different values in these variables will generate separate columns in the resulting table.

Example

```
S = readtable('weather_data.csv');
S2 = removevars(S,"Var1");
T = unstack(S2,'data','param')
;
```

218454 x 5 Table

| | date | sited | MaximumTemper... | MinimumTemper... | Precipitation |
|----|------------|---------------|------------------|------------------|---------------|
| 1 | 2003-01-01 | 'ACRE' | -3.7000 | -7.9400 | 0 |
| 2 | 2003-01-02 | 'Albert Lea' | -3.6500 | -5.9600 | 0 |
| 3 | 2003-01-03 | 'Ames' | -1.0900 | -12.3900 | 11.3200 |
| 4 | 2003-01-04 | 'Antigo' | -1.0400 | -12.1500 | 0 |
| 5 | 2003-01-05 | 'Appleton' | -1.1200 | -4.0300 | 3.0400 |
| 6 | 2003-01-06 | 'Arlington' | -0.1200 | -3.2400 | 0.4900 |
| 7 | 2003-01-07 | 'Beaumont' | -1.0300 | -5.2400 | 0 |
| 8 | 2003-01-08 | 'Brookings' | 9.1400 | -2.5000 | 0 |
| 9 | 2003-01-09 | 'Brownsville' | 10.7400 | -1.3100 | 0 |
| 10 | 2003-01-10 | 'Columbus' | 1.3600 | -10.1800 | 0 |
| 11 | 2003-01-11 | 'Crookston' | -9.2200 | -17.1700 | 0 |
| 12 | 2003-01-12 | 'DeKalb' | -9.3900 | -17.8800 | 0 |

Programme

- 1 Excel's Pivot Tables
- 2 Processing Long Tables in MATLAB
- 3 Data Analysis in MATLAB
 - Plotting in MATLAB
 - MATLAB: Finding Correlations

Analysing the Data

- Excel and MATLAB provide various tools for data analysis.
- Some of these tools are in Excel's **Data Analysis Tool Pack** plug-in.
 - <https://support.office.com/en-us/article/load-the-analysis-toolpak-in-excel-6a63e598-cd6d-42e3-9317-6b40ba1a66b4>
 - Available in the desktop version, sometimes in the online version (not available at Macquarie University).
 - Understanding most of these tools is beyond the scope of this unit.
- In this lecture we will look at how to do the following in MATLAB:
 - Plotting data.
 - Finding correlations.

Programme

- 1 Excel's Pivot Tables
- 2 Processing Long Tables in MATLAB
- 3 Data Analysis in MATLAB
 - Plotting in MATLAB
 - MATLAB: Finding Correlations

Programme

- 1 Excel's Pivot Tables
- 2 Processing Long Tables in MATLAB
- 3 Data Analysis in MATLAB
 - Plotting in MATLAB
 - MATLAB: Finding Correlations

Plotting with MATLAB

Demo using file trees.csv

MATLAB offers several options to display scatterplots (and other plots):

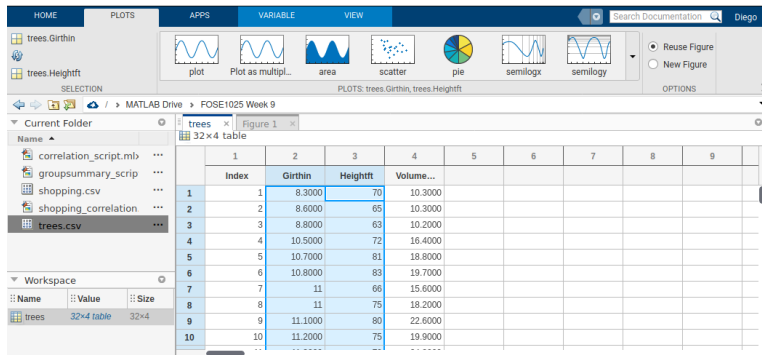
- 1 Executing the command (in the command window or in a script), e.g. for a scatterplot:

```
scatter(trees.Girthin , trees.Heightft )
```

- 2 Interacting graphically (more intuitive; see demo in the lecture)
 - This allows you to do more complex plots, e.g. multiple charts.
 - After interacting with MATLAB, you will see the resulting MATLAB command in the command window.

Steps to plot using the interactive interface

- 1 Double click on the variable that contains the table.
- 2 Select the columns to plot.
- 3 At the "Plots" tab, select the desired plot type.



Programme

- 1 Excel's Pivot Tables
- 2 Processing Long Tables in MATLAB
- 3 Data Analysis in MATLAB
 - Plotting in MATLAB
 - MATLAB: Finding Correlations

Programme

- 1 Excel's Pivot Tables
- 2 Processing Long Tables in MATLAB
- 3 Data Analysis in MATLAB
 - Plotting in MATLAB
 - MATLAB: Finding Correlations

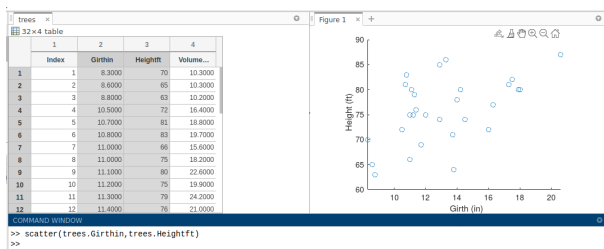
What is Correlation?

- Sometimes two separate sources of information are measuring the same property.
- You may detect this by observing that the values are the same.
- But sometimes this is not the case:
 - Each source may use different units of measure (e.g. metric vs. imperial).
 - Each source makes an independent measure that has some noise.
- In other cases, two variables are correlated but might not be identical.
 - For example, tree trunk height and girth are correlated.
 - Taller trees will normally have thicker trunks.
- MATLAB (and Excel) can detect the degree of **correlation** between two series of numbers.

Finding Correlations Graphically

Screenshot using file trees.csv

- A **scatterplot** can plot one variable against the other.
- If the two variables are not correlated, the scatterplots will look random.
- If the scatterplot has a distinct shape, the two variables are correlated.
- For example, if the shape looks like a line, then the two variables have a **linear correlation**.



Finding Correlations on Multiple Columns

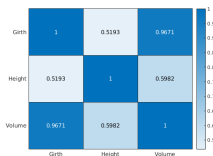
Examples and explanations in `correlation_script.mlx` using file `trees.csv`

- Scatterplots are intuitive but may be cumbersome if you want to check the correlations among many columns.
 - E.g. if there are 10 columns you will need to make a plot for each possible pair.
 - This means making $10 \times 9 = 90$ plots.
- MATLAB's `corr` computes **Pearson's Linear Correlation Coefficient** but you can specify others.
 - e.g. `corr(trees.Girthin, trees.Heightft)` computes the correlation between columns `Girthin` and `Heightft` of table `trees`.
 - `corr(trees.Girthin, trees.Heightft, "rows", "complete")` will ignore empty values.
- A number close to 1 (or -1) indicates positive (or negative) correlation; 0 means no correlation.

Correlation Matrix

Examples and explanations in `correlation_script.mlx`

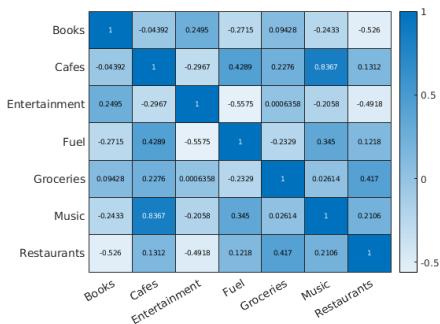
- MATLAB's **corrcoef** function returns a **correlation matrix**.
 - A correlation matrix returns the pairwise correlation between multiple columns.
- The input to **corrcoef** must be a matrix (not a table).
 - You can use the notation `mytable{rows,columns}` to extract rows and columns from a table and generate a matrix that can be fed to **corrcoef**
 - https://www.mathworks.com/help/matlab/matlab_prog/access-data-in-a-table.html
- This matrix can then be displayed using a **heatmap**.



Exercise

See detailed solution in script `shopping_correlation.mlx`

- File: `shopping.csv`
- Build the correlation matrix between all types of shopping.
- What are the two most correlated types of shopping?
- Show it clearly by creating a heatmap.



Take-home Messages

- EXCEL: You must be able to use pivot tables for a range of tasks.
- EXCEL: You must be able to create charts based on pivot tables.
- EXCEL and MATLAB: You must be able to plot data.
- MATLAB: You must be able to detect whether two variables are correlated.
- MATLAB: You should also be able to display correlation using heatmaps.

What's Next

- Test 3 in this week's SGTA.
- No classes Monday 4 October — Happy holiday!
- Week 10 lecture: Ethics related to Scientific Computing.
- Week 11:
 - Wed 20 October: Submit the project.
 - Fri 22 October: Submit Collaborator employability hurdle.