

# COMP1730/COMP6730

## Programming for Scientists

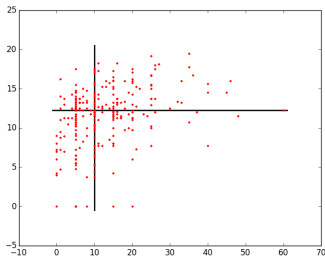
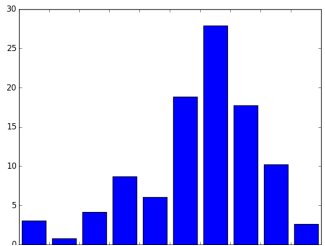
Data science

# Lecture outline

- \* Analysing data: an example
- \* Advanced modules

# Data analysis

- \* Reading data files
- \* Representing tables
- \* Working with data:  
selecting, visualising,  
counting
- \* Interpretation



# Reading data files

- \* Many data file formats (e.g., excel, csv, json, binary).
- \* Use a python module that helps with reading the file format:

```
import csv
with open("filename.csv") as csvfile:
    reader = csv.reader(csvfile)
    data = [ row for row in reader ]
```

- \* More about (reading and writing) files later in the course.

# Representing tables

- \* Lists are 1-dimensional, but a list can contain values of any type, including lists.
- \* A table can be stored as a list of lists, by row, for example:

```
data[i] # i:th row
```

```
data[i][j] # j:th column of i:th row
```

- \* Indexing (and slicing) are *operators*
- \* Indexing (and slicing) associate to the left:  

```
data[i][j] == (data[i])[j].
```

- ★ *A list comprehension* creates a list by evaluating an expression for each value in an iterable collection (e.g., a sequence).

```
first_col = [ row[0] for row in data ]  
last_two_cols = [ row[-2:]  
                  for row in data ]
```

- ★ Can also have a filtering condition:

```
sel_rows = [ row for row in data  
             if row[0] > 1 ]
```

- \* `sorted(seq)` returns a list with values in `seq` sorted in default order ( $<$ ).
  - We can sort the rows in a table.
  - Reminder: comparison of sequences is lexicographic.
- \* `sorted(seq, key=fun)` sorts value `x` by `fun(x)`.

```
def new_order(row):  
    return -row[-1] # decreasing  
                    # on last col  
  
sd = sorted(data, key=new_order)
```



# Descriptive statistics

- \* `min(seq)`;
- \* `max(seq)`;
- \* `mean(sum(seq) / len(seq))`;
- \* variance.
- \* No built-in function for median.

```
def median(seq):  
    return sorted(seq)[len(seq) // 2]
```



# Visualisation

- \* The purpose of visualisation is to see or show information – not drawing pretty pictures!
- \* Different kinds of plots show different things:
  - histogram, pie-chart or cumulative distribution
  - scatterplot
  - line and area plot
- \* Use one that best makes the point!
- \* Choose your dimensions carefully.
- \* Label axes, lines, etc.

# Using matplotlib

```
import matplotlib.pyplot as plot

plot.hist([first_col, last_col])
plot.legend(["column A", "column D"])
plot.show()
```

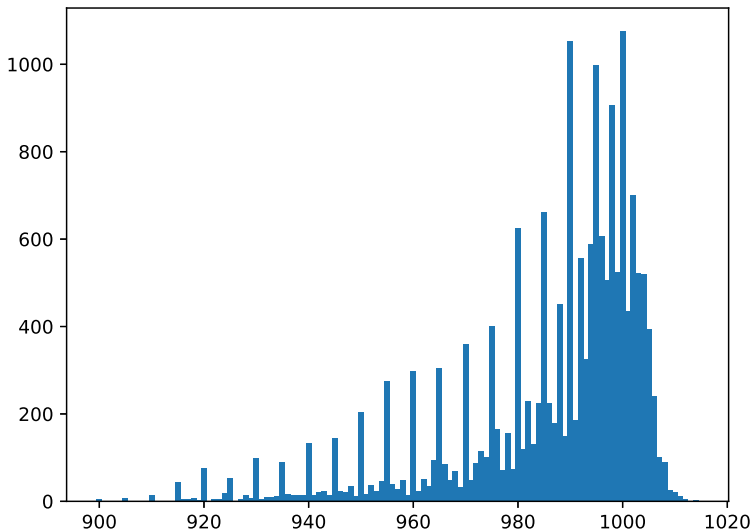
```
plot.plot(first_col, last_col)
plot.xlabel("column A")
plot.ylabel("column D")
plot.show()
```

\* Documentation: [matplotlib.org](http://matplotlib.org)

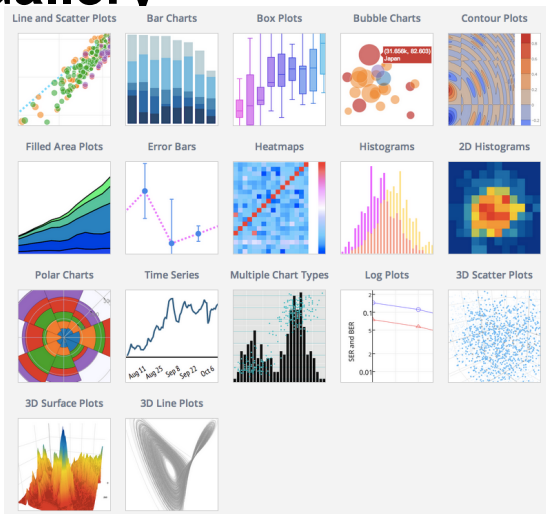


# Interpretation

- \* Understand what the data represents.
- \* Statistical significance.
- \* Over-fitting.
- \* Correlation is not causation.



# Gallery



Source: <https://plot.ly/javascript/basic-charts/>



# Visualisation Tips

- \* Use a chart that is appropriate for your data.
- \* Format your chart appropriately, labels, title, axis, scale, etc., from within the code.
- \* Make sure your colour scheme works well for printed reports (including black and white).
- \* Be consistent with your colours and styles across figures in the same report.

# Animation, Interfaces and Videos

- \* You can produce animations in `matplotlib`.
- \* Think of animation as drawing several individual graphics, one after another.
- \* You can also use `matplotlib` to create interactible graphical user interfaces, with buttons and other controls.
- \* If you have proper codecs installed, you can turn your animation into videos.
- \* There are good tutorials available if you are interested in exploring these topics further (we don't go over them in this course).



# Advanced modules

# NumPy and SciPy

- \* The NumPy and SciPy libraries are not part of the python standard library, but often considered essential for scientific / engineering applications.
- \* The NumPy and SciPy libraries provide
  - an  $n$ -dimensional array data type (`ndarray`);
  - fast math operations on arrays/matrices;
  - linear algebra, Fourier transform, random number generation, signal processing, optimisation, and statistics functions;
  - plotting (via `matplotlib`).
- \* Documentation: `numpy.org` and `scipy.org`.

# NumPy Arrays

- \* `numpy.ndarray` is sequence type, and can also represent  $n$ -dimensional arrays.
  - `len(A)` is the size of the first dimension.
  - Indexing an  $n$ -d array returns an  $(n - 1)$ -d array.
  - `A.shape` is a sequence of the size in each dimension.
- \* All values in an array must be of the same type.
- \* Element-wise operators, functions on arrays.
- \* Read/write functions for some file formats.

# Generalised indexing

- ★ If  $A$  is a 2-d array,
  - $A[i, j]$  is element at  $i, j$  (like  $A[i][j]$ ).
  - $A[i, :]$  is row  $i$  (same as  $A[i]$ ).
  - $A[:, j]$  is column  $j$ .
  - $:$  can be *start:end*.
- ★ If  $L$  is an array of `bool` of the same size as  $A$ ,  $A[L]$  returns an array with the elements of  $A$  where  $L$  is `True` (does not preserve shape).
- ★ If  $I$  is an array of integers,  $A[I]$  returns an array with the elements of  $A$  at indices  $I$  (does not preserve shape).

# Pandas

- \* Library for (tabular) data analysis.
  - Special types for 1-d (`Series`) and 2-d (`DataFrame`) data.
  - General indexing, selection, alignment, grouping, aggregation.
- \* Documentation: `pandas.pydata.org`
- \* *Beware*: Pandas data types do not behave as you expect.