# COMP1730/COMP6730

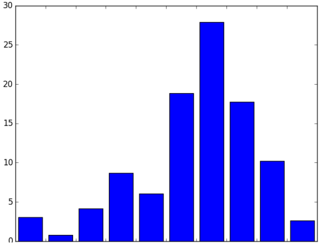
## Programming for Scientists

# Data science

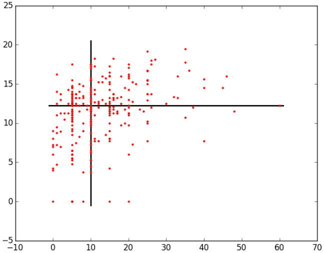
# Lecture outline

- 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`

# Interpretation

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

# 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 elemnts of *A* where *L* is `True` (does not preserve shape).
- If *I* is an array of integers, `A[I]` returns an array with the elemnts 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.