COMP1730/COMP6730
Programming for Scientists

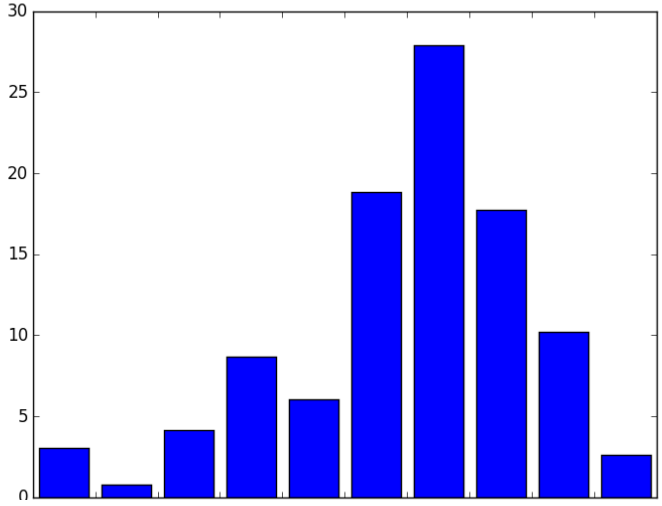
Data science

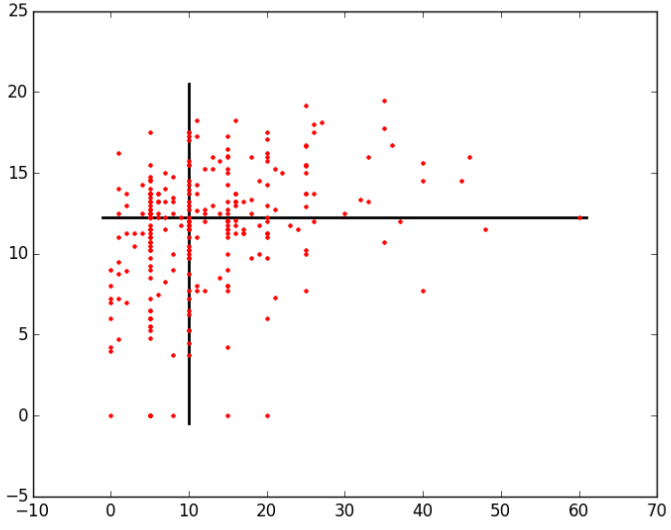
Lecture outline

* 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.

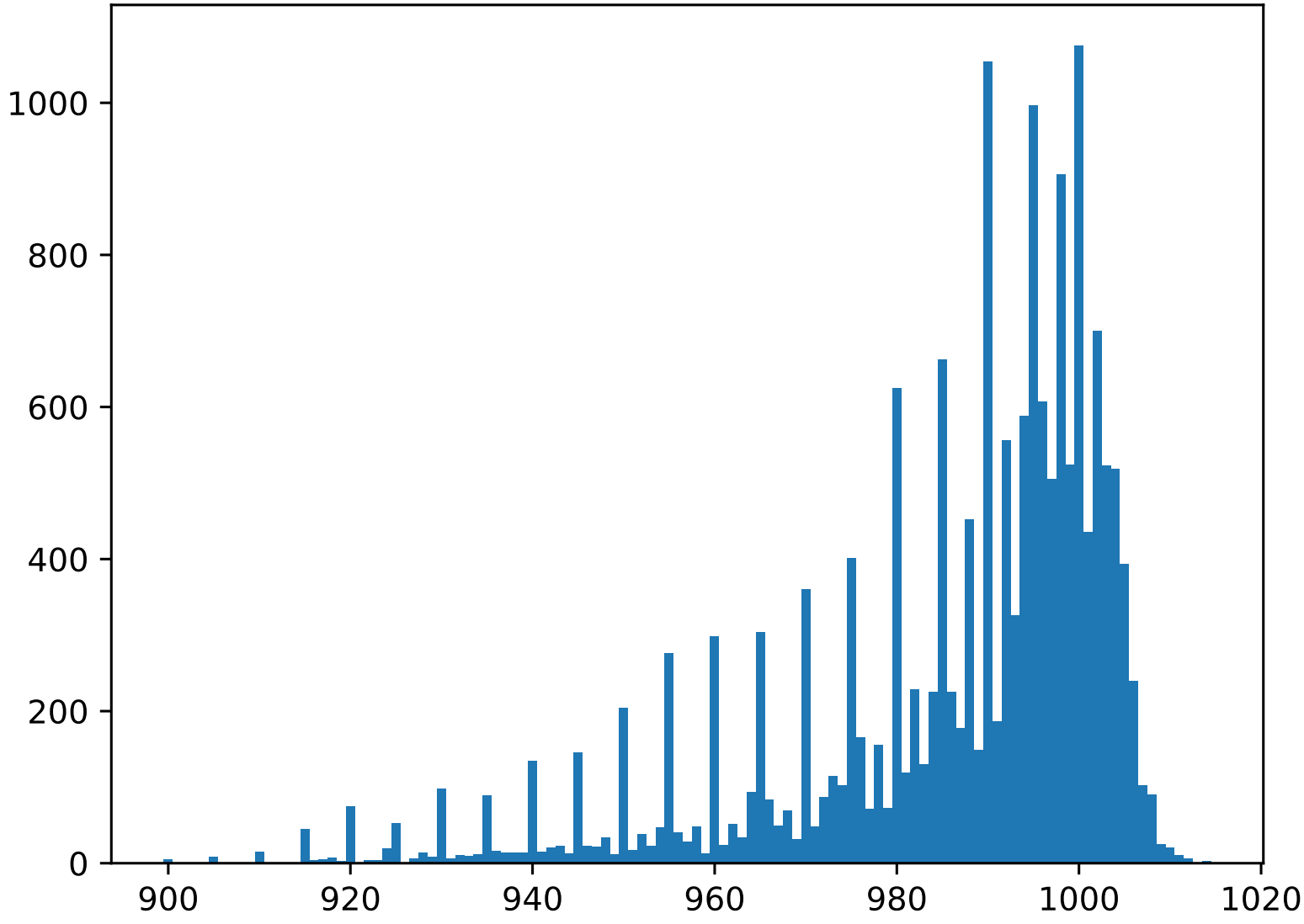
Using `matplotlib`

```
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.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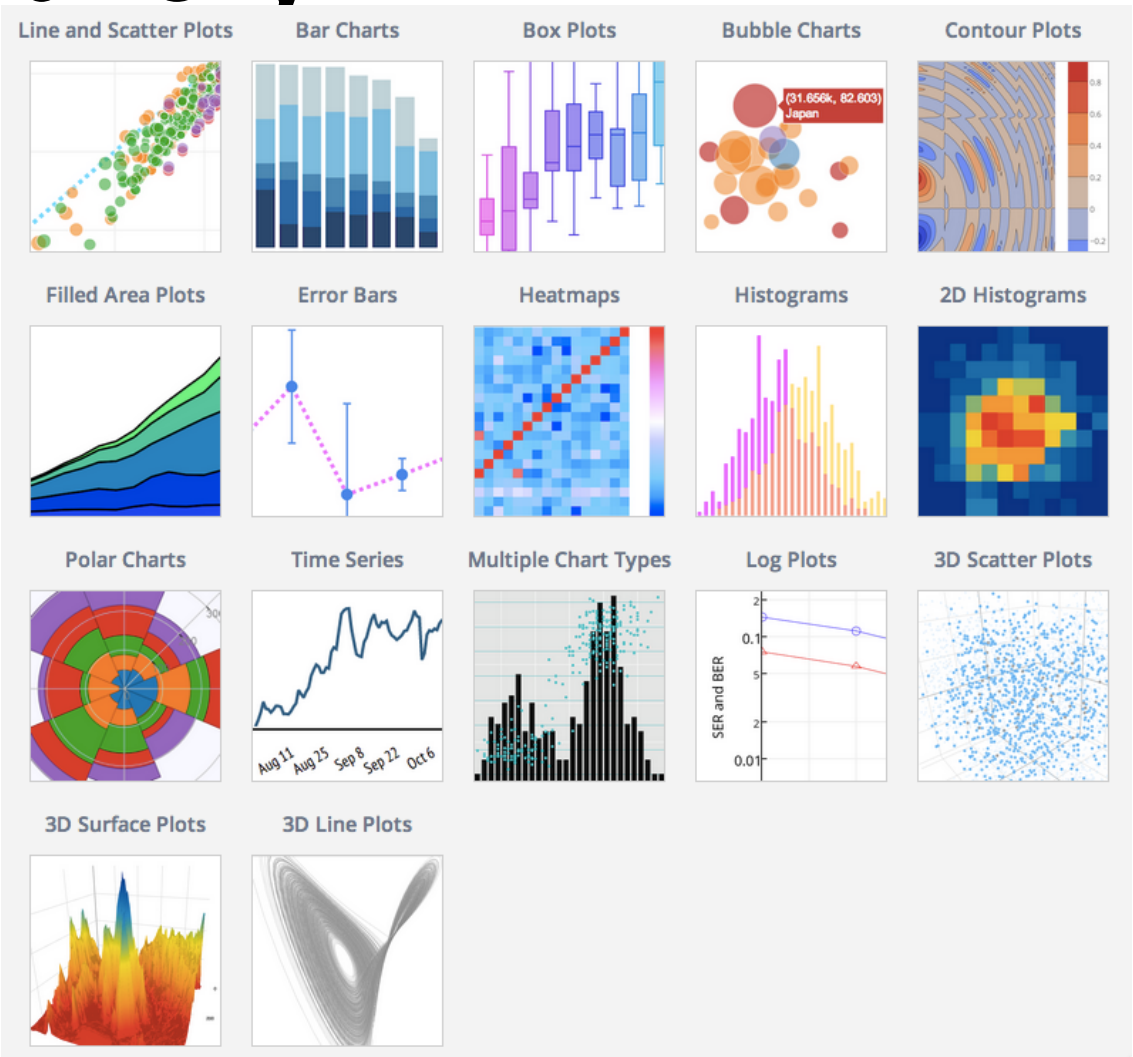
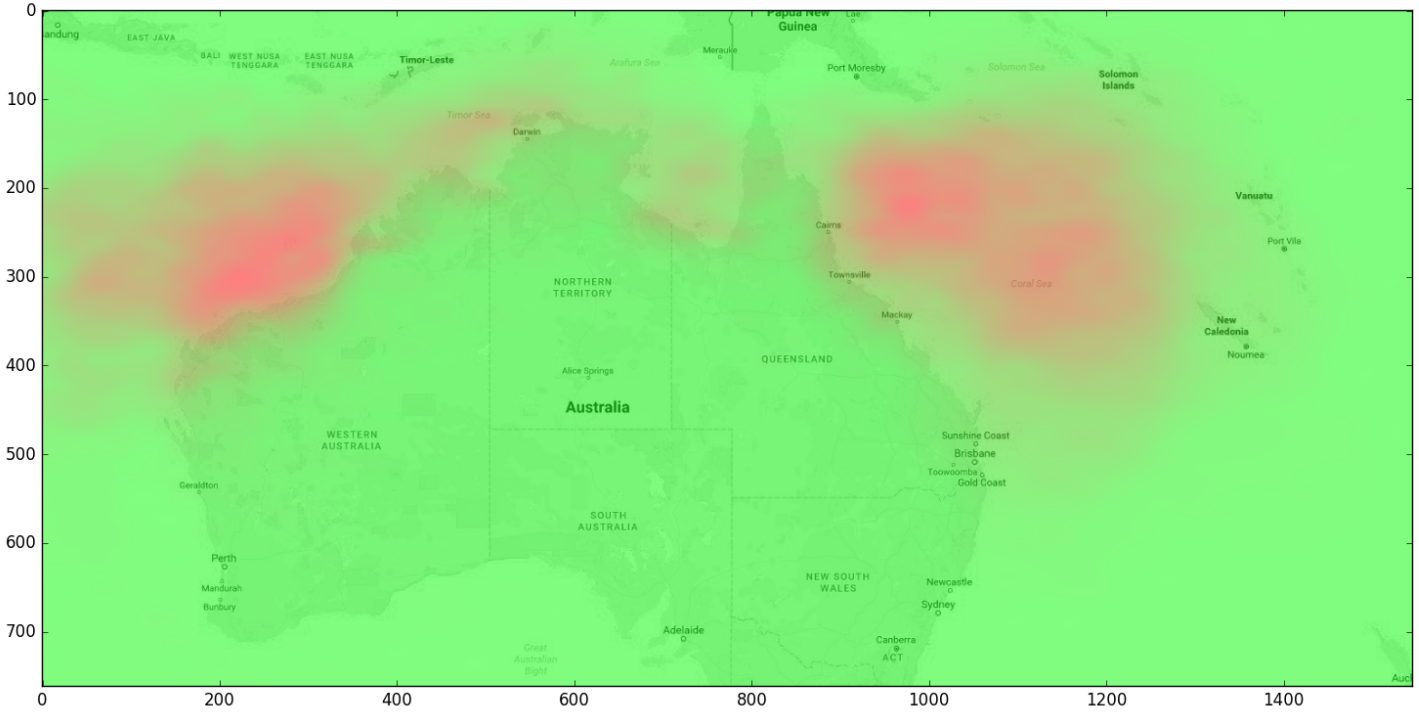
Gallery



Source: https://plot.ly/javascript/basic-charts/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Timor-Leste
Port Moresby
Solomon Islands
Vanuatu
Port Vila
Darwin
Cairns
Townsville
Mackay
New Caledonia
Noumea
NORTHERN TERRITORY
QUEENSLAND
Alice Springs
Australia
WESTERN AUSTRALIA
SOUTH AUSTRALIA
NEW SOUTH WALES
Sunshine Coast
Brisbane
Toowoomba
Gold Coast
Geraldton
Perth
Mandurah
Bunbury
Adelaide
Newcastle
Sydney
Canberra
ACT
Timor Sea
Arafura Sea
Coral Sea
Great Australian Bight

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 you 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 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.