

Python for Healthcare Modelling

Michael Allen: pythonhealthcare.org

April 17, 2018

Contents

1	Python basics	1
1.1	Introduction	2
1.2	Lists	3
1.2.1	Creating a list	3
1.2.2	Deleting a list	3
1.2.3	Returning and printing an element from a list	3
1.2.4	Taking slices of a list	3
1.2.5	Deleting or changing an item in a list	4
1.2.6	Appending an item to a list, and joining two lists	4
1.2.7	Copying a list	5
1.2.8	Inserting an element into a given position in a list	5
1.2.9	Sorting a list	5
1.2.10	Checking whether the list contains a given element	6
1.2.11	Reversing a list	6
1.2.12	Counting the number of elements in a list	6
1.2.13	Returning the index position of an element of a list	6
1.2.14	Removing an element of a list by its value	7
1.2.15	'Popping' an element from a list'	7
1.2.16	Iterating (stepping) through a list	7
1.2.17	Iterating through a list and changing element values	8
1.2.18	Counting the number of times an element exists in a list	8
1.2.19	Turning a sentence into a list of words	8
1.3	Nested lists	9
1.4	Tuples	10
1.4.1	Creating and adding to tuples	10
1.4.2	Converting between tuples and lists, and sorting tuples	10
1.5	Sets	12
1.5.1	Creating sets	12
1.5.2	Adding to a set and removing duplicates	12
1.5.3	Analysing the intersection between sets	12
1.6	Dictionaries	14
1.6.1	Creating and adding to dictionaries	14
1.6.2	Changing a dictionary entry	14
1.6.3	Deleting a dictionary entry	15
1.6.4	Iterating through a dictionary	15
1.6.5	Converting dictionaries to lists of keys and values	15
1.6.6	Using the get method to return a null value if a key does not exist	16
1.6.7	Intersection between dictionaries	16
1.6.8	Other dictionary methods	17
1.6.9	Ordered dictionaries	17
1.7	Accessing math functions through the math module	18
1.8	Variable types	24
1.9	Random numbers and integers	26
1.9.1	Importing the random module and setting a random seed	26
1.9.2	Random numbers	26
1.9.3	Generating random sequences	26

1.10	if, elif, else, while, and logical operators	28
1.10.1	if, else, elif	28
1.10.2	while statements	28
1.10.3	Logical operators	28
1.11	Loops and iterating	30
1.11.1	Breaking out of loops or continuing the loop without action	30
1.11.2	Using pass to replace active code in a loop	31
1.12	List comprehensions: one line loops	32
1.13	Else after while	33
1.14	try ... except (where code might fail)	34
1.15	Decimal places in output	35
1.16	Writing to and reading from files	36
1.16.1	File access modes	36
1.16.2	Creating a file with write	36
1.16.3	Adding to a file	36
1.16.4	Writing multiple lines	37
1.16.5	Reading a file	37
1.17	Functions	38
1.17.1	Defining a function	38
1.17.2	Adding help to a function with a docstring	39
1.17.3	Returning two or more results	39
1.18	Lambda functions (one line functions), and map/filter/reduce	41
1.18.1	Defining one-line lambda functions	41
1.18.2	Applying a lambda function to a list with map	41
1.18.3	Filtering a list with a lambda function	42
1.18.4	Reducing a list with a repeated lambda function call	42
1.18.5	Alternatives to map, filter and reduce	42
1.19	Accessing date and time, and timing code	43
1.19.1	Accessing date and time	43
1.19.2	Timing code	44
2	NumPy and Pandas	45
2.1	Numpy and Pandas	46
2.1.1	NumPy	46
2.1.2	Pandas	46
2.2	Numpy basics: building an array from lists, basic statistics, converting to booleans, refer- encing the array, and taking slices	47
2.2.1	Building an array from lists	47
2.2.2	Performing basic statistics on the array	47
2.2.3	Converting values to a boolean True/False	49
2.2.4	Referencing arrays and taking slices	49
2.3	Pandas basics: building a dataframe from lists, and retrieving data from the dataframe using row and column index references	51
2.3.1	Creating an empty data frame and building it up from lists	51
2.3.2	Setting an index column	51
2.3.3	Accessing data with <i>loc</i> and <i>iloc</i>	52
2.3.4	Selecting rows by index	52
2.3.5	Selecting records by row number	53
2.3.6	Selecting columns by name	53
2.3.7	Selecting columns by number	54
2.3.8	Selecting rows and columns simultaneously	54
2.4	Basic statistics in Pandas	56
2.4.1	Overview statistics	56
2.4.2	List of key statistical methods	57
2.4.3	Returning the index of minimum and maximum	57
2.4.4	Removing rows with incomplete data	58
2.5	Converting between NumPy and Pandas	59
2.5.1	Converting from Pandas to NumPy	59

2.5.2	Converting from NumPy to Pandas	59
2.6	Array maths in NumPy	61
2.6.1	Maths on a single array	61
2.6.2	Maths on two (or more) arrays	62
2.6.3	Matrix multiplication ('dot product')	62
2.7	Reading and writing CSV files using NumPy and Pandas	64
2.7.1	Reading a csv file into a NumPy array	64
2.7.2	Saving a NumPy array as a csv file	64
2.7.3	Reading a csv file into a Pandas dataframe	64
2.7.4	Saving a Pandas dataframe to a CSV file	65
2.8	Applying user-defined functions to NumPy and Pandas	66
2.8.1	Numpy	66
2.8.2	Pandas	66
2.9	Adding data to NumPy arrays and Pandas dataframes	68
2.9.1	Numpy	68
2.10	Using Pandas to merge or lookup data	70
2.11	Sorting and ranking with Pandas	72
2.11.1	Sorting	72
2.11.2	Ranking	72
2.12	Using masks to filter data, and perform search and replace, in NumPy and Pandas	74
2.12.1	NumPy	74
2.12.2	Pandas	79
2.13	Summarising data by groups in Pandas using pivot tables and groupby	82
2.13.1	Pivot tables	82
2.13.2	Groupby	83
2.14	Reshaping Pandas data with stack, unstack, pivot and melt	86
2.14.1	Stack and unstack	87
2.14.2	Melt and pivot	89
2.15	Subgrouping data in Pandas with groupby	91
2.16	Iterating through columns and rows in NumPy and Pandas	93
2.16.1	NumPy	93
2.16.2	Pandas	94
2.17	Removing duplicate data in NumPy and Pandas	96
2.17.1	NumPy	96
2.17.2	Pandas	97
2.18	Setting width and number of decimal places in NumPy print output	99
3	Matplotlib for charting	101
3.1	Simple xy line charts, and simple save to file	102
3.1.1	Plotting a single line	102
3.1.2	Plotting two lines	102
3.1.3	Saving figures	103
3.2	Scatter plot, and labelling axes	104
3.3	Bar charts	105
3.3.1	A simple bar chart	105
3.3.2	Multiple series	105
3.3.3	Stacked bar chart	106
3.3.4	Back to back bar chart	106
3.4	Pie charts, and adding a title	108
3.4.1	A simple bar chart	108
3.5	Plotting histograms with matplotlib and NumPy	109
3.5.1	Plotting histograms with Matplotlib	109
3.5.2	Obtaining histogram data with NumPy	109
3.6	Boxplots	111
3.6.1	Plotting groups	111
3.7	Violin plots	113
3.8	3D wireframe and surface plots	114
3.8.1	Wireframe	114

3.8.2	Surface	114
3.9	Common modifications to charts	116
3.10	A simple heatmap	118
3.11	Adding contour lines to a heat map	119
3.12	Creating a grid of subplots	121
3.13	Adding error bars to charts	123
3.13.1	Adding error bars to line plots	123
3.13.2	Adding error bars to bar charts	123
4	Statistics	125
4.1	Linear regression with <code>scipy.stats</code>	126
4.2	One sample t-test and Wilcoxon signed rank test	127
4.2.1	One sample t-test	127
4.2.2	Wilcoxon signed rank test	127
4.3	t-tests for testing the difference between two groups of data	128
4.3.1	Unpaired t-test	128
4.3.2	Paired t-test	128
4.4	Mann-Whitney U test	130
4.5	Analysis of variance (ANOVA)	131
4.6	Multiple comparisons between groups	132
4.6.1	Setting up the data, and running an ANOVA	132
4.6.2	Tukey's multi-comparison method	133
4.6.3	Holm-Bonferroni Method	133
4.7	Multiple comparison of non-normally distributed data with the Kruskal-Wallis test	135
4.8	Confidence Interval for a single proportion	136
4.9	Chi-squared test	137
4.10	Fisher's exact test	138
5	Clinical pathway simulation with SimPy	139
5.1	A bed occupancy model with SimPy	140
5.1.1	Import the packages	140
5.1.2	Storing variables	140
5.1.3	Generating new arrivals	140
5.1.4	Patient pathway	141
5.1.5	Audit of beds	141
5.1.6	Generate audit report	141
5.1.7	Charting occupancy	141
5.1.8	Main code	142
5.2	An emergency department model in SimPy, with patient prioritisation and capacity limited by doctor availability	144
6	Machine learning with <code>scikit learn</code>	151
6.1	The iris data set	152
6.1.1	Loading the iris data set	152
6.1.2	Data sets in <code>scikit learn</code>	154
6.1.3	Other sources of test data sets	154
6.2	Splitting data into training and test sets	155
6.3	Feature scaling	156
6.4	Using logistic regression to diagnose breast cancer	158
6.5	Adding standard diagnostic performance metrics to a ml diagnosis model	161
6.6	Regularisation	165
6.7	Learning rates: How much data do you need?	170
6.8	Working with ordinal and categorical data	174
6.8.1	Working with ordinal data	174
6.8.2	Working with categorical data	175
6.8.3	Selecting just our new columns	175
6.9	Support Vector Machines (SVMs)	177

Chapter 1

Python basics

1.1 Introduction

Hello

This book is a collection of code snippets that help me use Python for health services research, modelling and analysis. When learning something new I always work on a small code example to understand how something works, and to keep as a handy reference.

I will be looking at data handling, some statistics, data plotting, discrete event simulation, and machine learning.

I will be including use of pure Python as well as commonly used libraries such as NumPy, Pandas, Matplotlib, SciPy, SciKitLearn, TensorFlow and Simpy.

Everything described here is performed in Python 3, based on the Anaconda Scientific Python environment, available for free (for Windows, Mac or Linux). Follow installation instructions from the site <https://www.anaconda.com/download/>

Anaconda comes with its own environments for writing the code: Spyder or Jupyter Notebooks. Both are nice. Other Free and Open Source options are PyCharm for more functionality, Atom, or Visual Studio Code for a modern code text editor, or Vim for a more old-fashioned but very fast and lightweight code text editor.

Occasionally other free libraries may be installed. If so they will be described where appropriate.

I choose to do all my work in GNU/Linux, but everything should also work in Microsoft Windows or Mac OS.

If you are new to this I would recommend installing the Anaconda Scientific Python environment, and then look for 'Spyder' in your computer's application listing. That will open up an 'Integrated Development Environment' (IDE): a posh phrase that means a place where you can both write and run code.

Happy coding!

Michael

1.2 Lists

Lists, tuples, sets and dictionaries are four basic objects for storing data in Python. Later we'll look at libraries that allow for specialised handling and analysis of large or complex data sets.

Lists are a group of text or numbers (or more complex objects) held together in a given order. Lists are recognised by using square brackets, with members of the list separated by commas. Lists are mutable, that is their contents may be changed. Note that when Python numbers a list the first element is referenced by the index zero. Python is a 'zero-indexed' language.

Below is code demonstrating some common handling of lists.

1.2.1 Creating a list

Lists may mix text, numbers, or other Python objects. Here is code to generate and print a list of mixed text and numbers. Note that the text is in speech marks (single or double; both will work). If the speech marks were missing then Python would think the text represented a variable name (such as the name of another list).

```
my_list = ['Gandalf', 'Bilbo', 'Gimli', 10, 30, 40]
print (my_list)
```

OUT:

```
['Gandalf', 'Bilbo', 'Gimli', 10, 30, 40]
```

1.2.2 Deleting a list

The *del* command will delete a list (or any other variable).

```
my_list = ['Gandalf', 'Bilbo', 'Gimli']
del my_list
```

1.2.3 Returning and printing an element from a list

Python lists store their contents in sequence. A particular element may be referenced by its index number. Python indexes start at zero. Watch out for this this will almost certainly trip you up at some point.

The example below prints the second item in the list. The first item would be referenced with 0 (zero).

```
my_list = ['Gandalf', 'Bilbo', 'Gimli', 10, 30, 40]
print (my_list[1])
```

OUT:

```
Bilbo
```

Negative references may be used to refer to position from the end of the list. An index of -1 would be the last item (because -0 is the same as 0 and would be the first item!)

1.2.4 Taking slices of a list

Taking more than one element from a list is called a slice. The slice defines the starting point, and the point just after the end of the slice. The example below takes elements indexed 2 to 4 (but not 5)

```
my_list = [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
slice = my_list[2:5]
print(slice)
```

OUT:

```
[2, 3, 4]
```

Slices can take every *n* elements, the example below takes every second element from index 1 up to, but not including, index 9 (remembering that the first element is index 0):

```
y_list = [0,1,2,3,4,5,6,7,8,9,10]
slice = my_list[2:9:2]
print(slice)
```

OUT:

```
[2, 4, 6, 8]
```

Reverse slices may also be taken by defining the end point before the beginning point and using a negative step:

```
my_list = [0,1,2,3,4,5,6,7,8,9,10]
slice = my_list[9:2:-2]
print(slice)
```

OUT:

```
[9, 7, 5, 3]
```

1.2.5 Deleting or changing an item in a list

Unlike tuples (which are very similar to lists), elements in a list may be deleted or changed.

Here the first element in the list is deleted:

```
my_list = ['Gandalf','Bilbo','Gimli',10,30,40]
del my_list[0]
print (my_list)
```

OUT:

```
['Bilbo', 'Gimli', 10, 30, 40]
```

Here the second element of the list is replaced:

```
my_list = ['Gandalf','Bilbo','Gimli',10,30,40]
my_list[0] = 'Boromir'
print (my_list)
```

OUT:

```
['Boromir', 'Bilbo', 'Gimli', 10, 30, 40]
```

1.2.6 Appending an item to a list, and joining two lists

Individual elements may be added to a list with *append*.

```
my_list = ['Gandalf','Bilbo','Gimli',10,30,40]
my_list.append('Elrond')
print (my_list)
```

OUT:

```
['Gandalf', 'Bilbo', 'Gimli', 10, 30, 40, 'Elrond']
```

Two lists may be joined with a simple +

```
my_list = ['Gandalf','Bilbo','Gimli']
my_second_list = ['Elrond','Boromir']
my_combined_list = my_list + my_second_list
print (my_combined_list)
```

```
OUT:
['Gandalf', 'Bilbo', 'Gimli', 'Elrond', 'Boromir']
```

Or the *extend* method may be used to add a list to an existing list.

```
my_list = ['Gandalf', 'Bilbo', 'Gimli']
my_second_list = ['Elrond', 'Boromir']
my_list.extend(my_second_list)
print (my_list)
```

```
OUT:
['Gandalf', 'Bilbo', 'Gimli', 'Elrond', 'Boromir']
```

1.2.7 Copying a list

If we try to copy a list by saying `mycopy mylist` we do not generate a new copy. Instead we generate an alias, another name that refers to the original list. Any changes to `mycopy` will change `mylist`.

There are two ways we can make a separate copy of a list, where changes to the new copy will not change the original list:

```
my_list = ['Gandalf', 'Bilbo', 'Gimli']
my_copy = my_list.copy()
# Or
my_copy = my_list[:]
```

1.2.8 Inserting an element into a given position in a list

Inserting an element into a given position in a list

An element may be inserted into a list with the *insert* method. Here we specify that the new element will be inserted at index 2 (the third element in the list, remembering that the first element is index 0). In a later post we will look at methods specifically for maintaining a sorted list, but for now let us simply inset an element at a given position in the list.

```
my_list = ['Gandalf', 'Bilbo', 'Gimli']
my_list.insert(2, 'Boromir')
print (my_list)
```

```
OUT:
['Gandalf', 'Bilbo', 'Boromir', 'Gimli']
```

1.2.9 Sorting a list

The *sort* method can work on a list of text or a list of numbers (but not a mixed list text and numbers). Sort order may be reversed if wanted.

A normal sort:

```
x = [10, 5, 24, 5, 8]
x.sort()
print (x)
```

```
OUT:
[5, 5, 8, 10, 24]
```

A reverse sort:

```
x = [10, 5, 24, 5, 8]
x.sort(reverse=True)
print (x)
```

```
OUT:
[24, 10, 8, 5, 5]
```

1.2.10 Checking whether the list contains a given element

The *in* command checks whether a particular element exist in a list. It returns a 'Boolean' True or False.

```
my_list = ['Gandalf','Bilbo','Gimli','Elrond','Boromir']
is_in_list = 'Elrond' in my_list
print (is_in_list)
is_in_list = 'Bob' in my_list
print (is_in_list)
```

```
OUT:
True
False
```

1.2.11 Reversing a list

The method to reverse a list looks a little odd. It is actually creating a 'slice' of a list that steps back from the end of list.

```
my_list = ['Gandalf','Bilbo','Gimli','Elrond','Boromir']
my_list = my_list[::-1]
print (my_list)
```

```
OUT:
['Boromir', 'Elrond', 'Gimli', 'Bilbo', 'Gandalf']
```

1.2.12 Counting the number of elements in a list

Use the len function to return the number of elements in a list.

```
my_list = ['Gandalf','Bilbo','Gimli','Elrond','Boromir']
print (len(my_list))
```

```
OUT:
5
```

1.2.13 Returning the index position of an element of a list

The list *index* will return the position of the first element of the list matching the argument given.

```
my_list = ['Gandalf','Bilbo','Gimli','Elrond','Boromir']
index_pos = my_list.index('Elrond')
print (index_pos)
```

```
OUT:
3
```

If the element is not in the list then the code will error. Later we will look at some different ways of coping with this type of error. For now let us introduce an if/then/else statement (and we'll cover those in more detail later as well).

```
my_list = ['Gandalf','Bilbo','Gimli','Elrond','Boromir']
test_element = 'Elrond'
is_in_list = test_element in my_list
if is_in_list: # this is the same as saying if is_in_list == True
    print (test_element,'is in list at position', my_list.index(test_element))
else:
    print (test_element, 'is not in list')
```

OUT:

Elrond is in list at position 3

1.2.14 Removing an element of a list by its value

An element may be removed from a list by using its value rather than index. Be aware that you might want to put in a method (like the if statement above) to check the value is present before removing it. But here is a simple remove (this will remove the first instance of that particular value:

```
my_list = ['Gandalf','Bilbo','Gimli','Elrond','Boromir']
my_list.remove('Bilbo')
print (my_list)
```

OUT:

['Gandalf', 'Gimli', 'Elrond', 'Boromir']

1.2.15 'Popping' an element from a list

Popping an element from a list means to retrieve an element from a list, removing it from the list at the same time. If no element number is given then the last element of the list will be popped.

```
my_list = ['Gandalf','Bilbo','Gimli','Elrond','Boromir']
print ('Original list:', my_list)
x = my_list.pop()
print (x, 'was popped')
print ('Remaining list:',my_list)
x = my_list.pop(1)
print (x, 'was popped')
print ('Remaining list:', my_list)
```

OUT:

Original list: ['Gandalf', 'Bilbo', 'Gimli', 'Elrond', 'Boromir']
Boromir was popped
Remaining list: ['Gandalf', 'Bilbo', 'Gimli', 'Elrond']
Bilbo was popped
Remaining list: ['Gandalf', 'Gimli', 'Elrond']

1.2.16 Iterating (stepping) through a list

Lists are 'iterable', that is they can be stepped through. The example below prints one element at a time. We use the variable name 'x' here, but any name may be used.

```
my_list = [1,2,3,4,5,6,7,8,9]
for x in my_list:
    print(x, end=' ') # end command replaces a newline with a space
```

OUT:

1 2 3 4 5 6 7 8 9

1.2.17 Iterating through a list and changing element values

Iterating through a list and changing the value in the original list is a little more complicated. Below the range command creates a range of numbers from zero up to the index of the last element of the list. If there were 4 elements, for example, then the range function would produce '0, 1, 2, 3'. This allows us to iterate through the index numbers for the list (the position of each element). Using the index number we can change the value of the element in that position of the list.

```
my_list = [1,2,3,4,5,6,7,8,9]
for index in range(len(my_list)):
    my_list[index] = my_list[index]**2
print ('\nMy list after iterating and mutating:')
print (my_list)
```

OUT:

My list after iterating and mutating:
[1, 4, 9, 16, 25, 36, 49, 64, 81]

1.2.18 Counting the number of times an element exists in a list

The *count* method counts the number of times a value occurs in a list. If the value does not exist a zero is returned.

```
x=[1, 2, 3, 4, 1, 4, 1]
test_value = 1
print ('Count the number of times 1 occurs in',x)
print (x.count(test_value),'\n')
```

OUT:

Count the number of times 1 occurs in [1, 2, 3, 4, 1, 4, 1]
3

1.2.19 Turning a sentence into a list of words

The *split* method allows a long string, such as a sentence, to be separated into individual words. If no separator is defined any white space (such as a space or comma) will be used to divide words.

```
my_sentence="Turn this sentence into a list"
words = my_sentence.split()
print (words)
```

OUT:

['Turn', 'this', 'sentence', 'into', 'a', 'list']

A separator may be specified, such as dividing sentences at commas:

```
my_sentence = 'Hello there, my name is Bilbo'
divided_sentence = my_sentence.split(sep=',')
print(divided_sentence)
```

OUT:

['Hello there', ' my name is Bilbo']

1.3 Nested lists

So far we have looked at lists which contain a simple series of numbers, text, or a mixture of numbers and texts (Python lists can also hold any Python object, but in Healthcare modelling we are usually dealing with numbers or text in a list).

It is possible though to build nested lists. In the example below we generate a list manually, with each nested list on a separate line. This separation by line is just to make it easier to see; it is not needed in Python, but thought to layout of code is important if other people will be looking at your code.

```
my_list = [[1,2,3],
           [4,5,6],
           [7,8,9]]
print (my_list)
```

OUT:

```
[[1, 2, 3], [4, 5, 6], [7, 8, 9]]
```

We can then refer to items by using two reference indices. The first refers to the nested list block (so the first id [1, 2, 3] and the second refers to the position within that block. Remember that Python is zero indexed so the first element of the first list is 0[0].

```
print (my_list[1][1])
```

OUT:

```
5
```

Or we can use other variables to refer to the position:

```
x = 2
y = 0
print (my_list[x][y])
```

OUT:

```
7
```

More complex structures can be built up with further nesting of lists to give multi-dimensional lists.

WARNING: Handling large arrays of data this way is possible but slow. For modelling we are much better off using two libraries dedicated to fast handling of large data sets: NumPy and Pandas. We will be covering those libraries soon.

1.4 Tuples

1.4.1 Creating and adding to tuples

Tuples are like lists in many ways, apart from they cannot be changed - they are immutable. Tuples are defined using curved brackets (unlike square brackets for lists). Tuples may be returned, or be required, by various functions in Python, and tuples may be chosen where immutability would be an advantage (for example, to help prevent accidental changes).

```
my_tuple = ('Hobbit', 'Elf', 'Ork', 'Dwarf')
print (my_tuple[1])
```

```
OUT:
Elf
```

It is possible to add to a tuple. Note that if adding a single item an additional comma is used to indicate to Python that the variable being added is a tuple.

```
my_tuple = my_tuple + ('Man',)
my_tuple += ('Wizard', 'Balrog') # Note that the += is short hand to add something to itself
print (my_tuple)
```

```
OUT:
('Hobbit', 'Elf', 'Ork', 'Dwarf', 'Man', 'Wizard', 'Balrog')
```

It is not possible to change or delete an item in a tuple. To change or delete a tuple a new tuple must be built (but if this is going to happen then a list would be a better choice).

```
my_new_tuple = my_tuple[0:2] + ('Goblin',) + my_tuple[4:]
print (my_new_tuple)
```

```
OUT:
('Hobbit', 'Elf', 'Goblin', 'Man', 'Wizard', 'Balrog')
```

1.4.2 Converting between tuples and lists, and sorting tuples

A tuple may be turned into a list. We can recognise that it is a list by the square brackets.

```
my_list = list(my_tuple)
print (my_list)
```

```
OUT:
['Hobbit', 'Elf', 'Ork', 'Dwarf', 'Man', 'Wizard', 'Balrog']
```

A list may also be converted into a tuple.

```
my_list.sort()
my_new_tuple = tuple(my_list)
print (my_new_tuple)
```

```
OUT:
my_list.sort()
```

```
my_new_tuple = tuple(my_list)
```

```
print (my_new_tuple)
```

```
('Balrog', 'Dwarf', 'Elf', 'Hobbit', 'Man', 'Ork', 'Wizard')
```

In the above example we sorted a list and converted it to a tuple. Tuples cannot be changed (apart from being added to), so it is not possible to directly sort a tuple. The sorted command will act on a tuple to

sort it, but returns a list.

```
print (sorted(my_tuple))
```

OUT:

```
['Balrog', 'Dwarf', 'Elf', 'Hobbit', 'Man', 'Ork', 'Wizard']
```

The tuple may be sorted by converting back to a list in a single step (but think of using lists, rather than tuples, is sorting will be common.

```
my_tuple = tuple(sorted(my_tuple))  
print (my_tuple)
```

OUT:

```
('Balrog', 'Dwarf', 'Elf', 'Hobbit', 'Man', 'Ork', 'Wizard')
```

1.5 Sets

Sets are unordered collections of unique values. Common uses include membership testing, finding overlaps and differences between sets, and removing duplicates from a sequence.

Sets, like dictionaries, are defined using curly brackets.

1.5.1 Creating sets

Creating a set directly:

```
my_set = {'a','e','i','o','u'}
print (my_set)
```

OUT:

```
{'a', 'i', 'u', 'o', 'e'}
```

Creating a set from a list:

```
my_list = ['a','e','i','o','u']
my_set = set(my_list)
print (my_set)
```

OUT:

```
{'a', 'i', 'u', 'o', 'e'}
```

Creating an empty set. This cannot be done simply with

```
my_set = set()
print (my_set)
```

1.5.2 Adding to a set and removing duplicates

Adding one element to a set:

```
my_set.add('y')
print (my_set)
```

OUT:

```
{'a', 'y', 'i', 'u', 'o', 'e'}
```

Adding multiple elements to a set (note that the set has no duplication of entries already present; sets automatically remove duplicate items):

```
my_set.add('y')
print (my_set)
```

OUT:

```
{'a', 'y', 'i', 'u', 'o', 'e'}
```

1.5.3 Analysing the intersection between sets

Sets may be used to explore the intersection between sets. There are usually two forms of syntax which may be used, both of which are given in the examples below.

```
set1 = {'a','b','c','d','e','f'}
set2 = {'a','e','i','o','u'}
```

The difference between two sets:

```
print ('difference')
print (set1.difference(set2))
print (set1 - set2)
```

```
OUT:
difference
{'c', 'f', 'b', 'd'}
{'c', 'f', 'b', 'd'}
```

The intersection between two sets:

```
print ('Intersection')
print (set1.intersection(set2))
print (set1 & set2)
```

```
OUT:
Intersection
{'a', 'e'}
{'a', 'e'}
```

Is a subset? Is set 2 wholly included in set 1?

```
print ('Is subset?')
print (set1.issubset(set2))
print (set1 <= set2)
```

```
OUT:
Is subset?
False
False
```

Is a superset? Does set 1 wholly include set 2?

```
print ('Is superset?')
print (set1.issuperset(set2))
print (set1 >= set2)
```

```
OUT:
Is superset?
False
False
```

The union between two sets:

```
print ('Union')
print (set1.union(set2))
print (set1 | set2)
```

```
OUT:
Union
{'b', 'o', 'a', 'f', 'c', 'i', 'u', 'd', 'e'}
{'b', 'o', 'a', 'f', 'c', 'i', 'u', 'd', 'e'}
```

Symmetric difference: in either but not both (equivalent to xor)

```
print ('Symmetric difference')
print (set1.symmetric_difference(set2))
print (set1 ^ set2)
```

```
OUT:
Symmetric difference
{'c', 'i', 'b', 'u', 'f', 'o', 'd'}
{'c', 'i', 'b', 'u', 'f', 'o', 'd'}
```

1.6 Dictionaries

Dictionaries store objects such as text or numbers (or other Python objects). We saw that lists stored elements in sequence, and that each element can be referred to by an index number, which is the position of that element in a list. The contents of dictionaries are accessed by a unique *key* which may be a number or may be text.

Dictionaries take the form of `key1:value1, key2:value2`

The *value* may be a single number or word, or may be another Python object such as a list or a tuple.

Dictionaries allow fast random-access to data.

1.6.1 Creating and adding to dictionaries

Dictionaries may be created with content, and are referred to by their *key*:

```
fellowship = {'Man': 2, 'Hobbit':4, 'Wizard':1, 'Elf':1, 'Dwarf':1}
print (fellowship['Man'])
```

```
OUT:
2
```

Dictionaries may also be created empty. New content may be added to an empty or an existing dictionary.

```
trilogy = {}
trilogy['Part 1'] = 'The fellowship of the ring'
trilogy['Part 2'] = 'The Two Towers'
trilogy['Part 3'] = 'The return of the king'
print (trilogy['Part 2'])
```

```
OUT:
The Two Towers
```

Dictionaries may contain a mixture of data types.

```
lord_of_the_rings = {'books':3,
                    'author':'JRR Tolkien',
                    'main_characters':['Frodo', 'Sam', 'Gandalf']}
print (lord_of_the_rings['main_characters'])
```

```
OUT:
['Frodo', 'Sam', 'Gandalf']
```

1.6.2 Changing a dictionary entry

Dictionary elements are over-written if a key already exists.

```
trilogy['Part 2'] = 'The Two Towers'
print (trilogy['Part 2'])
```

```
OUT:
The Two Towers
```

Dictionary items may also be updated using another dictionary:

```
entry_update = {'Part 1':'The Fellowship of the Ring',
                'Part 3':'The Return of the King'}
trilogy.update(entry_update)
print (trilogy)
```

OUT:

```
{'Part 1': 'The Fellowship of the Ring', 'Part 2': 'The Two Towers',  
'Part 3': 'The Return of the King'}
```

1.6.3 Deleting a dictionary entry

Dictionary entries may be deleted, by reference to their key, with the *del* command. If the key does not exist an error will be caused, so in the example below we check that the entry exists before trying to delete it.

```
entry_to_delete = 'Part 2'  
if entry_to_delete in trilogy:  
    del trilogy[entry_to_delete]  
    print (trilogy)  
else:  
    print('That key does not exist')
```

OUT:

```
{'Part 1': 'The Fellowship of the Ring', 'Part 3': 'The Return of the King'}
```

1.6.4 Iterating through a dictionary

There are two main methods to iterate through a dictionary. The first retrieves just the key, and the value may then be retrieved from that key. The second method retrieves the key and value together.

```
lord_of_the_rings = {'books':3,  
                    'author':'JRR Tolkien',  
                    'main_characters':['Frodo','Sam','Gandalf']}  
  
# Iterating method 1  
for key in lord_of_the_rings:  
    print (key, '-', lord_of_the_rings[key])  
  
# Iterating method 2  
print()  
for key, value in lord_of_the_rings.items():  
    print (key,'-', value)
```

OUT:

```
books - 3  
author - JRR Tolkien  
main_characters - ['Frodo', 'Sam', 'Gandalf']
```

```
books - 3  
author - JRR Tolkien  
main_characters - ['Frodo', 'Sam', 'Gandalf']
```

1.6.5 Converting dictionaries to lists of keys and values

Dictionary keys and values may be accessed separately. We can also return a list of tuples of keys and values with the *items* method.

```
lord_of_the_rings = {'books':3,  
                    'author':'JRR Tolkien',  
                    'main_characters':['Frodo','Sam','Gandalf']}  
  
# print the keys:
```

```
print ('\nKeys:') # \n creates empty line before text
print (list(lord_of_the_rings.keys()))
```

```
# print the values
print ('\nValues:')
print (list(lord_of_the_rings.values()))
```

```
# print keys and values
print ('\nKeys and Values:')
print (list(lord_of_the_rings.items()))
```

```
OUT:
Keys:
['books', 'author', 'main_characters']
```

```
Values:
[3, 'JRR Tolkien', ['Frodo', 'Sam', 'Gandalf']]
```

```
Keys and Values:
[('books', 3), ('author', 'JRR Tolkien'), ('main_characters', ['Frodo', 'Sam',
'Gandalf'])]
```

1.6.6 Using the get method to return a null value if a key does not exist

Using the usual method of referring to a dictionary element, an error will be returned if the key used does not exist. An 'if key in dictionary' statement could be used to check the key exists. Or the get method will return a null value if the key does not exist. The get method allows for a default value to be returned if a key is not found.

```
print (lord_of_the_rings.get('author'))
print (lord_of_the_rings.get('elves'))
print (lord_of_the_rings.get('books','Key not found - sorry'))
print (lord_of_the_rings.get('dwarfs','Key not found - sorry'))
```

```
JRR Tolkien
None
3
Key not found - sorry
```

1.6.7 Intersection between dictionaries

Like sets the intersection between dictionaries may be evaluated. See the entry on sets for more intersection methods.

```
a = {'x':1,'y':2,'z':3,'zz':2}
b = {'x':10,'w':11,'y':2,'yy':2}
# Show keys in common
print('Keys in common: ',a.keys() & b.keys())
# Show keys in a not in b
print('Keys in a but not b:',a.keys()-b.keys())
# Show keys+values in common (items() return key+value, so both need to be the same)
print('Keys and values in common:',a.items() & b.items())
```

```
OUT:
Keys in common:  {'x', 'y'}
Keys in a but not b: {'z', 'zz'}
Keys and values in common: {('y', 2)}
```

1.6.8 Other dictionary methods

`dictionary.clear()` empties a dictionary

`dictionary.pop(key)` will return an item and remove it from the dictionary

1.6.9 Ordered dictionaries

Like sets, dictionaries do not usually keep the order of entries. If it is useful to keep the order of entry in a dictionary then the `OrderedDict` object is useful. This needs an import statement before it is used (all import statements are usually kept together at the start of code).

```
from collections import OrderedDict
d=OrderedDict()
```

```
d['Gandalf']=1
d['Bilbo']=2
d['Frodo']=3
d['Sam']=4
```

```
for key in d:
    print(key,d[key])
```

OUT:

```
Gandalf 1
Bilbo 2
Frodo 3
Sam 4
```

1.7 Accessing math functions through the math module

Here we are going to use the math module as an introduction to using modules. The math module contains a range of useful mathematical functions that are not built into Python directly. So let's go ahead and start by importing the module. Module imports are usually performed at the start of a programme.

```
import math
```

When this type of import is used Python loads up a link to the module so that module functions and variables may be used. Here for example we access the value of pi through the module.

```
print (math.pi)
```

OUT:

```
3.141592653589793
```

Another way of accessing module contents is to directly load up a function or a variable into Python. When we do this we no longer need to use the module name after the import. This method is not generally recommended as it can lead to conflicts of names, and is not so clear where that function or variable comes from. But here is how it is done.

```
from math import pi
print (pi)
```

OUT:

```
3.141592653589793
```

Multiple methods and variables may be loaded at the same time in this way.

```
from math import pi, tau, log10
print (tau)
print (log10(100))
```

OUT:

```
6.283185307179586
```

```
2.0
```

But usually it is better practice to keep using the library name in the code.

```
print (math.log10(100))
```

OUT:

```
2.0
```

To access help on any Python function use the help command in a Python interpreter.

```
help (math.log10)
```

Help on built-in function log10 in module math:

```
log10(...)
    log10(x)
```

Return the base 10 logarithm of x.

To find out all the methods in a module, and how to use those methods we can simply type help (module.name) into the Python interpreter. The module must first have been imported, as we did for math above.

```
help (math)
```

OUT:

```
Help on module math:
```

NAME

math

MODULE REFERENCE

<https://docs.python.org/3.6/library/math>

The following documentation is automatically generated from the Python source files. It may be incomplete, incorrect or include features that are considered implementation detail and may vary between Python implementations. When in doubt, consult the module reference at the location listed above.

DESCRIPTION

This module is always available. It provides access to the mathematical functions defined by the C standard.

FUNCTIONS

`acos(...)`
`acos(x)`

Return the arc cosine (measured in radians) of x.

`acosh(...)`
`acosh(x)`

Return the inverse hyperbolic cosine of x.

`asin(...)`
`asin(x)`

Return the arc sine (measured in radians) of x.

`asinh(...)`
`asinh(x)`

Return the inverse hyperbolic sine of x.

`atan(...)`
`atan(x)`

Return the arc tangent (measured in radians) of x.

`atan2(...)`
`atan2(y, x)`

Return the arc tangent (measured in radians) of y/x.
Unlike `atan(y/x)`, the signs of both x and y are considered.

`atanh(...)`
`atanh(x)`

Return the inverse hyperbolic tangent of x.

`ceil(...)`
`ceil(x)`

Return the ceiling of x as an Integral.
This is the smallest integer $\geq x$.

`copysign(...)`
`copysign(x, y)`

Return a float with the magnitude (absolute value) of `x` but the sign of `y`. On platforms that support signed zeros, `copysign(1.0, -0.0)` returns `-1.0`.

`cos(...)`
`cos(x)`

Return the cosine of `x` (measured in radians).

`cosh(...)`
`cosh(x)`

Return the hyperbolic cosine of `x`.

`degrees(...)`
`degrees(x)`

Convert angle `x` from radians to degrees.

`erf(...)`
`erf(x)`

Error function at `x`.

`erfc(...)`
`erfc(x)`

Complementary error function at `x`.

`exp(...)`
`exp(x)`

Return `e` raised to the power of `x`.

`expm1(...)`
`expm1(x)`

Return `exp(x)-1`.
This function avoids the loss of precision involved in the direct evaluation of `exp(x)-1` for small `x`.

`fabs(...)`
`fabs(x)`

Return the absolute value of the float `x`.

`factorial(...)`
`factorial(x) -> Integral`

Find `x!`. Raise a `ValueError` if `x` is negative or non-integral.

`floor(...)`
`floor(x)`

Return the floor of x as an Integral.
This is the largest integer $\leq x$.

`fmod(...)`
`fmod(x, y)`

Return `fmod(x, y)`, according to platform C. $x \% y$ may differ.

`frexp(...)`
`frexp(x)`

Return the mantissa and exponent of x , as pair (m, e) .
 m is a float and e is an int, such that $x = m * 2.**e$.
If x is 0, m and e are both 0. Else $0.5 \leq \text{abs}(m) < 1.0$.

`fsum(...)`
`fsum(iterable)`

Return an accurate floating point sum of values in the iterable.
Assumes IEEE-754 floating point arithmetic.

`gamma(...)`
`gamma(x)`

Gamma function at x .

`gcd(...)`
`gcd(x, y) -> int`
greatest common divisor of x and y

`hypot(...)`
`hypot(x, y)`

Return the Euclidean distance, $\text{sqrt}(x*x + y*y)$.

`isclose(...)`
`isclose(a, b, *, rel_tol=1e-09, abs_tol=0.0) -> bool`

Determine whether two floating point numbers are close in value.

`rel_tol`
maximum difference for being considered "close", relative to the magnitude of the input values

`abs_tol`
maximum difference for being considered "close", regardless of the magnitude of the input values

Return True if a is close in value to b , and False otherwise.

For the values to be considered close, the difference between them must be smaller than at least one of the tolerances.

$-\text{inf}$, inf and NaN behave similarly to the IEEE 754 Standard. That is, NaN is not close to anything, even itself. inf and $-\text{inf}$ are only close to themselves.

`isfinite(...)`
`isfinite(x) -> bool`

Return True if x is neither an infinity nor a NaN, and False otherwise.

```
isinf(...)  
    isinf(x) -> bool
```

Return True if x is a positive or negative infinity, and False otherwise.

```
isnan(...)  
    isnan(x) -> bool
```

Return True if x is a NaN (not a number), and False otherwise.

```
ldexp(...)  
    ldexp(x, i)
```

Return $x * (2^{**i})$.

```
lgamma(...)  
    lgamma(x)
```

Natural logarithm of absolute value of Gamma function at x.

```
log(...)  
    log(x[, base])
```

Return the logarithm of x to the given base.
If the base not specified, returns the natural logarithm (base e) of x.

```
log10(...)  
    log10(x)
```

Return the base 10 logarithm of x.

```
log1p(...)  
    log1p(x)
```

Return the natural logarithm of 1+x (base e).
The result is computed in a way which is accurate for x near zero.

```
log2(...)  
    log2(x)
```

Return the base 2 logarithm of x.

```
modf(...)  
    modf(x)
```

Return the fractional and integer parts of x. Both results carry the sign of x and are floats.

```
pow(...)  
    pow(x, y)
```

Return x^{**y} (x to the power of y).

```
radians(...)  
    radians(x)
```

Convert angle x from degrees to radians.

```
sin(...)
sin(x)
```

Return the sine of x (measured in radians).

```
sinh(...)
sinh(x)
```

Return the hyperbolic sine of x .

```
sqrt(...)
sqrt(x)
```

Return the square root of x .

```
tan(...)
tan(x)
```

Return the tangent of x (measured in radians).

```
tanh(...)
tanh(x)
```

Return the hyperbolic tangent of x .

```
trunc(...)
trunc(x:Real) -> Integral
```

Truncates x to the nearest Integral toward 0. Uses the `__trunc__` magic method.

DATA

```
e = 2.718281828459045
inf = inf
nan = nan
pi = 3.141592653589793
tau = 6.283185307179586
```

FILE

```
/home/michael/anaconda3/lib/python3.6/lib-dynload/math.cpython-36m-x86_64-linux-gnu.so
```

So now, for example, we know that to take a square root of a number we can use the `math` module, and use the `sqrt()` function, or use the `pow()` function which can do any power or root.

```
print (math.sqrt(4))
print (math.pow(4,0.5))
```

OUT:

```
2.0
2.0
```

In Python you might read about packages as well as modules. The two names are sometimes used interchangeably, but strictly a package is a collection of modules.

1.8 Variable types

Python is a dynamic language where variable type (e.g. whether a variable is a string or an integer) is not fixed. Sometime though you might like to force a particular type, or convert between types (most common where numbers may be contained within a string).

The most common types of variables in python are integers, float (nearly all types of numbers that are not integers) and strings.

Within python code the function *type* will show what variable type a string is.

```
x = 11 # This is an integer
print (type(x))
```

```
OUT:
<class 'int'>
```

Outside of the code, within the interpreter requesting help on a variable name will give the help for its variable type.

```
help (x)
```

```
OUT:
Help on int object:
```

```
class int(object)
|  int(x=0) -> integer
|  int(x, base=10) -> integer
|
|  Convert a number or string to an integer, or return 0 if no arguments
|  are given.  If x is a number, return x.__int__().  For floating point
|  numbers, this truncates towards zero.
|
|  If x is not a number or if base is given, then x must be a string,
|  bytes, or bytearray instance representing an integer literal in the
|  given base.  The literal can be preceded by '+' or '-' and be surrounded
|  by whitespace.  The base defaults to 10.  Valid bases are 0 and 2-36.
|  Base 0 means to interpret the base from the string as an integer literal.
|  >>> int('0b100', base=0)
|  4
|
|  Methods defined here:
```

```
...
```

Though x is an integer, if we divide it by 2, Python will dynamically change its type to float. This may be common sense to some, but may be irritating to people who are used to coding languages where variables have 'static' types (this particular behaviour is also different to Python2 where the normal behaviours is for integers to remain as integers).

```
x = x/2
print (x)
print (type(x))
```

```
OUT:
5.5
<class 'float'>
```

Python is trying to be helpful, but this dynamic behaviour of variables can sometimes need a little debugging. In our example here, to keep our answer as an integer (if that is what we needed to do) we need to specify that:

```
x = 11
x = int(x/2)
print (x)
print (type(x))
```

```
OUT:
5
<class 'int'>
```

We can convert between types, such as in the follow examples. Numbers may exist as text, particularly in some file imports.

```
x = '10'
print ('Look what happens when we try to multiply a string')
print (x *3)
x = float (x)
print ('Now let us multiply the converted variable')
print (x*3)
```

```
OUT:
Look what happens when we try to multiply a string
101010
Now let us multiply the converted variable
30.0
```

1.9 Random numbers and integers

Here we look at the standard Python random number generator. It uses a *Mersenne Twister*, one of the mostly commonly-used random number generators. The generator can generate random integers, random sequences, and random numbers according to a number of different distributions.

1.9.1 Importing the random module and setting a random seed

```
import random
```

Random numbers can be repeatable in the sequence they are generated if a 'seed' is given. If no seed is given the random number sequence generated each time will be different.

```
random.seed() # This will reset the random seed so that the random number sequence will be different
random.seed(10) # giving a number will lead to a repeatable random number sequence each time
```

1.9.2 Random numbers

Random integers between (and including) a minimum and maximum:

```
i
print (random.randint(0,5))
```

```
OUT:
4
```

Return a random number between 0 and 1:

```
print (random.random())
```

```
OUT:
0.032585065282054626
```

Return a number (floating, not integer) between a & b:

```
print (random.uniform(0,5))
```

```
OUT:
2.412808372754279
```

Select from normal distribution (with mu, sigma):

```
print (random.normalvariate(10,3))
```

```
OUT:
5.3538059684648855
```

Other distributions (see `help(random)` for more info after importing random module):

Lognormal, Exponential, Beta, Gaussian, Gamma, Weibul

1.9.3 Generating random sequences

The random library may also be used to shuffle a list:

```
deck = ['ace', 'two', 'three', 'four']
random.shuffle(deck)
print (deck)
```

```
OUT:
['three', 'ace', 'two', 'four']
```

Sampling without replacement:

```
sample = random.sample([10, 20, 30, 40, 50], k=4) # k is the number of samples to select
print (sample)
```

OUT:

```
[20, 30, 10, 50]
```

Sampling with replacement:

```
pick_from = ['red', 'black', 'green']
sample = random.choices(pick_from, k=10)
print(sample)
```

OUT:

```
['black', 'red', 'black', 'green', 'red', 'red', 'black', 'red', 'black', 'green']
```

Sampling with replacement and weighted sampling:

```
pick_from = ['red', 'black', 'green']
pick_weights = [18, 18, 2]
sample = random.choices(pick_from, pick_weights, k=10)
print(sample)
```

OUT:

```
['black', 'red', 'red', 'red', 'black', 'red', 'red', 'black', 'red', 'black']
```

1.10 if, elif, else, while, and logical operators

Like many programming languages, Python enables code to be run based on testing whether a condition is true. Python uses indented blocks to run code according to these tests.

1.10.1 if, else, elif

emphif statements run a block of code if a particular condition is true. emphelif or 'else if' statements can subsequently run to test more conditions, but these run only if none of the previous emphif or emphelif statements were true. emphelse statements may be used to run code if none of the previous emphif or emphelif were true.

emphif statements may be run alone, with emphelse statements or with emphelif statements. emphelse and emphelif statements require a previous emphif statement.

In the following example we use the input command to ask a user for a password and test against known value.

Here we use just one elif statement, but multiple statements could be used.

Note that the tests of equality uses double = signs

```
password = input ("Password? ") # get user to enter password
if password == "secret":
    print ("Well done")
    print ("You")
elif password=="Secret":
    print ("Close!")
else:
    print("Noodle brain")
```

OUT:

```
Password? Secret
Close!
```

1.10.2 while statements

emphwhile statements may be used to repeat some actions until a condition is no longer true. For example:

```
x = 0
while x <5:
    x +=1 # This is shorthand for x = x + 1
    print (x)
```

OUT:

```
1
2
3
4
5
```

1.10.3 Logical operators

Logical operators

The following are commonly used logical operators:

== Test of identity

`!=` Not equal to

`>` greater than

`<` less than

`>=` equal to or greater than

`<=` less than or equal to

`in` test whether element is in list/tuple/dictionary

`not in` test whether element is not in list/tuple/dictionary

`and` test multiple conditions are true

`or` test one of alternative conditions are true

`any` test whether all elements are true

`all` test whether all elements are true

When Python test conditions they are evaluated as either True or False. These values may also be used directly in tests:

```
x = 10
```

```
y = 20
```

```
z = 30
```

```
# using and/or
```

```
print (x>15)
```

```
print (x>15 and y>15 and z>15)
```

```
print (x>15 or y>15 or z>15)
```

```
print ()
```

```
# Using any and all
```

```
print (any([x>20, y>20, z>20]))
```

```
test_array = [x>20, y>20, z>20]
```

```
print (test_array)
```

```
print (any(test_array))
```

```
print (all(test_array))
```

```
OUT:
```

```
False
```

```
False
```

```
True
```

```
True
```

```
[False, False, True]
```

```
True
```

```
False
```

1.11 Loops and iterating

for loops can be used to step through lists, tuples, and other 'iterable' objects.

Iterating through a list:

```
for item in [10,25,50,75,100]:
    print (item, item**2)
```

OUT:

```
10 100
25 625
50 2500
75 5625
100 10000
```

A *for* loop may be used to generate and loop through a sequence of numbers (note that a 'range' does not include the maximum value specified):

```
for i in range(100,150,10):
    print(i)
```

OUT:

```
100
110
120
130
140
```

A *for* loop may be used to loop through an index of positions in a list:

```
my_list = ['Frodo','Bilbo','Gandalf','Gimli','Sauron']

for i in range(len(my_list)):
    print ('Index:',i,' Value',my_list[i])
```

OUT:

```
Index: 0 , Value Frodo
Index: 1 , Value Bilbo
Index: 2 , Value Gandalf
Index: 3 , Value Gimli
Index: 4 , Value Sauron
```

1.11.1 Breaking out of loops or continuing the loop without action

Though it may not be considered best coding practice, it is possible to prematurely escape a loop with the *break* command:

```
for i in range(10): # This loop would normally go from 0 to 9
    if i == 5:
        break
    else:
        print(i)

print ('Loop complete')
```

OUT:

```
0
1
2
3
4
Loop complete
```

Or, rather than breaking out of a loop, it is possible to effectively skip an iteration of a loop with the *continue* command. This may be places anywhere in the loop and returns the focus to the start of the loop.

```
for i in range (10):
    if i%2 == 0: # This is the integer remainder after dividing i by 2
        continue
    else:
        print (i)

print ('Loop complete')
```

OUT:

```
1
3
5
7
9
Loop complete
```

1.11.2 Using pass to replace active code in a loop

The *pass* command is most useful as a place holder to allow a loop to be built and have contents added later.

```
for i in range (10):
    # Some code will be added here later
    pass

print ('Loop complete')
```

OUT:

```
Loop complete
```

1.12 List comprehensions: one line loops

List comprehensions are a very Pythonic way of condensing loops and action into a single line.

Here is the long form of a loop:

```
my_list=[1,4,5,7,9,10,3,2,16]
my_new_list=[]

for x in my_list:
    if x>5:
        my_new_list.append(x**2)

print (my_new_list)
```

OUT:

```
[49, 81, 100, 256]
```

This may be done by a single line list comprehension:

```
y = [x**2 for x in my_list if x>5]

print (y)
```

OUT:

```
[49, 81, 100, 256]
```

1.13 Else after while

The *else* clause is only executed when your while condition becomes false. If you *break* out of the loop it won't be executed.

The following loop will run the else code:

```
x = 0
while x < 5:
    x += 1
    print (x)
else:
    print ('Else statement has run')
print ('End')
```

OUT:

```
x = 0

while x < 5:

    x += 1

    print (x)

else:

    print ('Else statement has run')

print ('End')
```

OUT:

```
1
2
3
4
5
Else statement has run
End
```

The following loop with a *break* will not run the *else* code:

```
x = 0
while x < 5:
    x += 1
    print (x)
    if x > 3:
        break
else:
    print ('Else statement has run')
print ('End')
```

OUT:

```
1
2
3
4
End
```

1.14 try ... except (where code might fail)

In perfect code all eventualities will be anticipated and code written for all eventualities. Sometimes though we might want to allow for more general failure of code and provide an alternative route.

In the following code we try to perform some code on a list. For the code to work the list must be long enough and the number must be positive. We use try except to perform the calculation where possible and return a null value if not.

In Python an error is called an 'exception'.

```
import math

x = [1, 2, -4]

# Try to take the square root of elements of a list.
# As a user try entering a list index too high (3 or higher)
# or try to enter index 2 (which has a negative value, -4)

test = int(input('Index position?: '))
try:
    print (math.sqrt(x[test]))
except:
    print ('Sorry, no can do')
```

OUT:

```
Index position?: 2
Sorry, no can do
```

Try except may be used in final code (but it is better to allow for all specific circumstances) or may be used during debugging to evaluate variables at the time of code failure

1.15 Decimal places in output

Python allows a lot of control over formatting of output. But here we will just look at controlling decimal places of output.

There are some different ways. Here is perhaps the most common (because it is most similar to other languages).

The number use is represented in the print function as `%x.yf` where `x` is the total number of spaces to use (if defined this will add padding to short numbers to align numbers on different lines, for example), and `y` is the number of decimal places. `f` informs python that we are formatting a float (a decimal number). The `%x.yf` is used as a placeholder in the output (multiple placeholders are possible) and the values are given at the end of the print statement as below:

```
import math
pi = math.pi
pi_square = pi**2

print('Pi is %.3f, and Pi squared is %.3f' %(pi,pi_square))
```

OUT:

```
Pi is 3.142, and Pi squared is 9.870
```

It is also possible to round numbers before printing (or sending to a file). If taking this approach be aware that this may limit the precision of further work using these numbers:

```
import math
pi = math.pi
pi = round(pi,3)
print (pi)
```

OUT:

```
3.142
```

1.16 Writing to and reading from files

For data analytics we will usually be using two libraries called NumPy and Pandas which have their own simple methods for importing data, but here is the standard Python method. This standard method may sometimes have an advantage that data may be written and read one line at a time without having all data held in memory. This may be useful for very large data files.

1.16.1 File access modes

Files may be opened with different access control models

Text file access modes:

"r" Read (if file does not exist there will be an error)

"w" Write If the file exists contents are overwritten. If the file does not exist, it is created.

"a" Append - will add to file, or will create a file if no file exists

"r+" Read from and write to a file

"w+" Write to and read from a text file. If the file exists contents are overwritten. If the file does not exist, it is created.

"a+" Append and read from a text file. If the file exists, new data is appended to it. If the file doesn't exist, it's created.

1.16.2 Creating a file with write

This method where we open a file to save to with the 'w' argument will create a new file or overwrite an old one.

In this standard way of using a file we begin by opening a file and end by closing the file:

```
text_file = open('write_it.txt', 'w')
text_file.write('Line 1\n')
text_file.write('This is line 2\n')
text_file.write('That makes this line 3\n')
text_file.close()
\begin{verbatim}
```

An alternative to open and closing the file is using the with statement:

```
\begin{verbatim}
with open('write_it.txt', 'w') as text_file:
    text_file.write('Line 1\n')
    text_file.write('This is line 2\n')
    text_file.write('That makes this line 3\n')
```

1.16.3 Adding to a file

Using the 'a' mode we will add to an existing file. We will use the with statement below, but the open/close method will work as well.

```
with open('write_it.txt', 'a') as text_file:
    text_file.write('This is a fourth line\n')
```

1.16.4 Writing multiple lines

Multiple lines may be written using a loop with the *write* method, or may we can use *writelines*:

```
'write_it.txt'
text_file = open('write_it.txt', 'w')
lines = ['Line 1\n',
        'This is line 2\n',
        'That makes this line 3\n']
text_file.writelines(lines)
text_file.close()
```

1.16.5 Reading a file

We can read a file in one line at a time (useful for processing very large files which cannot be held in memory), or we can read in all lines.

Here we read one line at a time:

```
text_file = open('write_it.txt', 'r')
text_file = open('write_it.txt', 'r')
print(text_file.readline())
print(text_file.readline())
print(text_file.readline())
text_file.close()
```

OUT:

Line 1

This is line 2

That makes this line 3

Or we can read the entire file in as a list:

```
text_file = open('write_it.txt', 'r')
lines = text_file.readlines()
text_file.close()
print (lines)
```

OUT:

```
['Line 1\n', 'This is line 2\n', 'That makes this line 3\n']
\end{verbatim}
```

A text file may be stepped through as part of a loop:

```
\begin{verbatim}
text_file = open('write_it.txt', 'r')
for line in text_file:
    print(line)
text_file.close()
OUT:
```

Line 1

This is line 2

That makes this line 3

1.17 Functions

Functions are (or should be) short sections of code that may be called from within the main programme, or from another function. They usually take some inputs (arguments) and return one or more results.

Functions may be used for two purposes:

- 1) To avoid repeating code when the same code needs to be run in two or more locations in the main programme.
- 2) To structure the code, breaking the code down into smaller pieces. In functional programming the whole programme would be broken down into functions

If a function is more than 10 lines long you may want to think whether it could be broken down further, with some of the code pulled out as a separate function.

Ideally a function should do just one thing; it should be as simple as possible, and easy for another person to follow.

A docstring may be used at the start of a function to provide help to the user - in this case if the user types `help(function_name)` the docstring will be returned. These docstrings may also give examples of the function.

Any variables defined within functions are destroyed when the function closes. Functions are not usually used to change global variables (those variables defined in the main programme code). If a global variable is passed to a function any changes to that variable made by the function are lost when the function ends (and so global variables are protected from being changed by functions). There is a way to force the function to change the global variable, which we will cover in a later lesson, but this should usually be avoided if possible.

1.17.1 Defining a function

A function is defined with the `def` statement. It is followed by the function's inputs (arguments or 'args') which may also be given a default value. The user may enter the inputs either by name, or in the order in which the function expects them.

It is good practice to use verbs to define functions, to describe what they do.

Let's do a very simple example, raising a number to the power of another number, and we will set a default where, if no other number is given, we will raise to the power of zero (which always returns a value of 1). Note that we define a default value with the `=` sign.

```
def raise_to_power (number, power = 0):  
    result = number ** power  
    return result
```

Once the function has been defined we can call it:

```
print (raise_to_power(2,6))
```

OUT:

64

We could describe the inputs by their names if we wanted to:

```
print (raise_to_power(number = 2, power = 6))
```

OUT:

64

If we define the inputs by name, the order becomes unimportant (without the names the function expects inputs in the order defined in the function):

```
print (raise_to_power(power = 6, number = 2))
```

OUT:

64

And remember that we set a default of power to zero, so if we only pass the first argument ('number'), the power defaults to zero:

```
print (raise_to_power(2))
```

OUT:

1

1.17.2 Adding help to a function with a docstring

A help docstring may be added to a function using triple quotes (' or ") after the function has been defined. This may be called later by the user using help.

```
def raise_to_power (number, power = 0):  
    """  
        This functions takes two numbers, and raises the first number to the power of the second.  
        If no second number, or power, is given then power defaults to zero  
    """  
  
    result = number ** power  
    return result
```

Calling help:

```
help (raise_to_power)
```

OUT:

Help on function raise_to_power in module __main__:

```
raise_to_power(number, power=0)  
    This functions takes two numbers, and raises the first number to the power of the second.  
    If no second number, or power, is given then power defaults to zero
```

1.17.3 Returning two or more results

Sometimes we may wish to return more than one value. There are two ways of doing this:

1) Return the values separately (the code that calls the argument must also refer to both results:

```
def calculate_sum_and_product(a, b):  
    """Return sum and product of two numbers"""  
  
    my_sum = a + b  
    my_product = a * b  
    return my_sum, my_product  
  
# When calling the function we need to put both results generated by the function  
  
calculated_sum, calculated_product = calculate_sum_and_product(5,6)  
print (calculated_sum)  
print (calculated_product)
```

OUT:

11
30

2) A more common way would be to return a single result that is a container (commonly a list or a tuple) of the two results. Here we return a tuple of the two results (remember that tuples are like lists, but they cannot be changed). We can tell that the returned value is a tuple by the use of curved brackets (a list could also be used, which we would spot by square brackets).

```
def calculate_sum_and_product(a, b):  
    """Return sum and product of two numbers"""  
    my_sum = a + b  
    my_product = a * b  
    result = (my_sum, my_product) # this is a tuple  
    return result  
  
results = calculate_sum_and_product(5,6)  
  
# Individual results are obtained by their index:  
  
print (results[0])  
print (results[1])
```

OUT:

11
30

1.18 Lambda functions (one line functions), and map/filter/reduce

Lambda functions are a Pythonic way of writing simple functions in a single line.

They may be applied to a list using the *map* statement.

The function *filter* offers a concise way to filter out all the elements of a list based on the results of a function.

The function *reduce* continually applies a function to a sequence until a single value is returned.

1.18.1 Defining one-line lambda functions

Instead of defining the function with `def`, we define the function with *lambda*.

Here is a 'normal' function:

```
# A named function that returns the power of a number:
```

```
def f(x, y):  
    result = x ** y  
    return result
```

```
print (f(4,3))
```

OUT:

64

Re-writing as a lambda function:

```
g = lambda x,y: x**y
```

```
print (g(4,3))
```

OUT:

64

1.18.2 Applying a lambda function to a list with map

In the example below we define a lambda function to convert Celsius to Fahrenheit, and then apply it to a list.

We will first define lambda separately, and then map, before looking at how they can be combined a single line.

The *map* command generates a 'map object'. To return a list we need to convert that to a list as below

```
celsius = [0, 10, 20, 30]  
g = lambda x: (9/5)*x + 32  
fahrenheit = list(map(g, celsius))
```

```
print (fahrenheit)
```

OUT:

[32.0, 50.0, 68.0, 86.0]

This may be compressed further into one line. But there is always a balance to be had between being as concise as possible, and being as clear for others as possible. It may, however, generally be assumed that other experienced Python coders will be familiar with a combined one-line lambda/map function.

```
celsius = [0, 10, 20, 30]
fahrenheit = list(map(lambda x: (9/5)*x + 32, celsius))

print (fahrenheit)

[32.0, 50.0, 68.0, 86.0]
```

1.18.3 Filtering a list with a lambda function

The function *filter* offers a concise way to filter out all the elements of a list, for which the function returns True. The function `filter(f,l)` needs a function `f` as its first argument. `f` returns a Boolean value, i.e. either True or False.

This function will be applied to every element of the list `l`. Only if `f` returns True will the element of the list be included in the result list.

Here is an example where `filter` is used to return even numbers from a list. As with the `map` example above we will combine the `filter` and `lambda` function in a single line.

```
my_list = [0,1,2,3,4,5,6,7,8,9,10]
result = list(filter(lambda x: x % 2 == 0, my_list))

print (result)
```

OUT:

```
[0, 2, 4, 6, 8, 10]
```

1.18.4 Reducing a list with a repeated lambda function call

The `reduce` function will continually apply a `lambda` function until only a single value is returned. Though it used to be in core python, it is now found in the `functools` module.

A simple example is to use `reduce` to multiply all values in a list. The `reduce` function replaces the first two elements of a list with the product of those two elements. It will continue until one value is left.

```
import functools
my_list = [10,30,34,56,89]
result = functools.reduce(lambda x,y: x*y, my_list)

print (result)
```

OUT:

```
50836800
```

1.18.5 Alternatives to map, filter and reduce

Most results from `map/filter` and `reduce` may also be obtained from using list comprehensions, as previously outlined. Some see list comprehensions as more Pythonic than `map`, `filter` and `reduce`.

1.19 Accessing date and time, and timing code

1.19.1 Accessing date and time

It may sometimes be useful to access the current date and/or time. As an example, when writing code it may be useful to access the time at particular stages to monitor how long different parts of code are taking.

To access date and time we will use the *datetime* module (which is held in a package that is also, a little confusingly called *datetime*!):

```
from datetime import datetime
```

To access the current date and time we can use the `now` method:

```
print (datetime.now())
```

OUT:

```
2018-03-28 08:54:13.623198
```

You might not have expected to get the time to the nearest microsecond! But that may be useful at times when timing short bits of code (which may have to run many times).

But we can access the date and time in different ways:

```
current_datetime = datetime.now()
```

```
print ('Date:', current_datetime.date()) # note the () after date
print ('Year:', current_datetime.year)
print ('Month:', current_datetime.month)
print ('Day:', current_datetime.day)
print ('Time:', current_datetime.time()) # note the () after time
print ('Hour:', current_datetime.hour)
print ('Minute:', current_datetime.minute)
print ('Second:', current_datetime.second)
```

OUT:

```
Date: 2018-03-28
Year: 2018
Month: 3
Day: 28
Time: 08:54:13.636654
Hour: 8
Minute: 54
Second: 13
```

Having microseconds in the time may look a little clumsy. So let's format the date and using the *strftime* method.

```
now = datetime.now()
print (now.strftime('%Y-%m-%d'))
print (now.strftime('%H:%M:%S'))
```

OUT:

```
2018-03-28
08:54:13
```

1.19.2 Timing code

We can use `datetime` to record the time before and after some code to calculate the time taken, but it is a little simpler to use the `time` module which keeps all time in seconds (from January 1st 1970) and gives even more accuracy to the time:

```
import time

time_start = time.time()

for i in range(100000):
    x = i ** 2

time_end = time.time()
time_taken = time_end - time_start

print ('Time taken:', time_taken)
```

OUT:

Time taken: 0.03149104118347168

Chapter 2

NumPy and Pandas

2.1 Numpy and Pandas

For much of healthcare data analytics and modelling we will use NumPy and Pandas as the key containers of our data. These libraries allow efficient manipulation and analysis of very large data sets. They are very considerably faster than using a 'pure Python' approach.

NumPy and Pandas are distributed with all main scientific Python distributions.

2.1.1 NumPy

NumPy is a library for supporting work with large multi-dimensional arrays, with many mathematical functions. NumPy is compatible with many other libraries such as Pandas (see below), Matplotlib (for plotting), and many Python maths, stats and optimisation libraries.

When we import NumPy as a library it is standard practice to use the *as* statement which allows it to be referenced with a shorter name. We will import as *np*:

```
import numpy as np
```

2.1.2 Pandas

Pandas is a library that allows manipulation of large arrays of data. Data may be indexed and manipulated based on index. Data is readily pivoted, reshaped, grouped, merged.

We will use pandas alongside numpy. Generally, NumPy is faster for mathematical functions, but Pandas is more powerful for data manipulation.

As with numpy, we import with a shortened name:

```
import pandas as pd
```

2.2 Numpy basics: building an array from lists, basic statistics, converting to booleans, referencing the array, and taking slices

Most commonly we will be loading files into NumPy arrays, but here we build an array from lists and perform some basic stats on the array.

The examples below construct and use a 2 dimensional array (which may be thought of as 'rows and columns'). Later we will look at higher dimensional arrays.

2.2.1 Building an array from lists

We use the `np.array` function to build an array from existing lists. Here each list represents a row of a data table.

```
import numpy as np

row0 = [23, 89, 100]
row1 = [10, 51, 99]
row2 = [40, 78, 102]
row3 = [35, 81, 110]
row4 = [50, 75, 95]
row5 = [65, 51, 101]

data = np.array([row0, row1, row2, row3, row4, row5])
```

We now have a data array:

```
print (data)
```

OUT:

```
[[ 23  89 100]
 [ 10  51  99]
 [ 40  78 102]
 [ 35  81 110]
 [ 50  75  95]
 [ 65  51 101]]
```

2.2.2 Performing basic statistics on the array

We can see, for example, the mean of all the data

```
print (data.mean())
```

OUT:

```
69.72222222222223
```

Or we can use the *axis* argument to show the mean by column or mean by row:

```
print (np.mean(data,axis=0)) # average all rows in each column
print (np.mean(data,axis=1)) # average all columns in each row
```

OUT:

```
[ 37.16666667  70.83333333 101.16666667]
[70.66666667  53.33333333 73.33333333 75.33333333 73.33333333 72.33333333]
```

Some other commonly used statistics (all of which are by column, or dimension 0, below):

```
print ('Mean:\n', np.mean(data, axis=0))
print ('Median:\n', np.median(data, axis=0))
print ('Sum:\n', np.sum(data, axis=0))
print ('Maximum:\n', np.max(data,axis=0))
print ('Minimum\n:', np.min(data,axis= 0))
print ('Range:\n', np.ptp(data, axis=0))
print ('10th percentile:\n', np.percentile(data, 10, axis=0))
print ('90th percentile:\n', np.percentile(data, 90, axis=0))
print ('Population standard deviation\n', np.std(data, axis=0))
print ('Sample standard deviation:\n', np.std(data, axis=0, ddof=1))
print ('Population variance:\n', np.var(data, axis=0))
print ('Sample variance:\n', np.var(data, axis=0, ddof=1))
```

OUT:

```
Mean:
 [ 37.16666667  70.83333333 101.16666667]
Median:
 [ 37.5  76.5 100.5]
Sum:
 [223 425 607]
Maximum:
 [ 65  89 110]
Minimum
: [10 51 95]
Range:
 [55 38 15]
10th percentile:
 [16.5 51.  97. ]
90th percentile:
 [ 57.5  85. 106. ]
Population standard deviation
 [17.75215167 14.6562463  4.52462399]
Sample standard deviation:
 [19.44650783 16.05511341  4.95647724]
Population variance:
 [315.13888889 214.80555556  20.47222222]
Sample variance:
 [378.16666667 257.76666667  24.56666667]
```

The returned array may be referenced by index number (beginning at zero):

```
results = np.mean(data, axis=0)
```

```
print (results[0])
```

OUT:

```
37.166666666666664
```

Basic python may also be incorporated into the statistics. For example the 10th percentiles, from 0 to 100 may be calculated in a loop (remember that the standard Python range function goes up to, but does not include, the maximum value given, so we need to put a higher maximum than 100 in order to include the 100th percentile in the loop):

```
for percent in range(0,101,10):
    print(percent,'percentile:',np.percentile(data, percent, axis=0))
```

OUT:

```
0 percentile: [10. 51. 95.]
10 percentile: [16.5 51. 97. ]
20 percentile: [23. 51. 99.]
30 percentile: [29. 63. 99.5]
40 percentile: [ 35. 75. 100.]
50 percentile: [ 37.5 76.5 100.5]
60 percentile: [ 40. 78. 101.]
70 percentile: [ 45. 79.5 101.5]
80 percentile: [ 50. 81. 102.]
90 percentile: [ 57.5 85. 106. ]
100 percentile: [ 65. 89. 110.]
```

2.2.3 Converting values to a boolean True/False

We can use test values against some standard. For example, here we test whether a value is equal to, or greater than, the mean of the column.

```
column_mean = np.mean(data, axis=0)
greater_than_mean = data >= column_mean
```

```
print (greater_than_mean)
```

OUT:

```
[[False  True False]
 [False False False]
 [ True  True  True]
 [False  True  True]
 [ True  True False]
 [ True False False]]
```

True/False values in Python may also be used in calculations where False has an equivalent value to zero, and True has an equivalent value to 1.

```
print (np.mean(greater_than_mean, axis=0))
```

OUT:

```
[0.5          0.66666667 0.33333333]
```

2.2.4 Referencing arrays and taking slices

NumPy arrays are referenced similar to lists, except we have two (or more dimensions). For a two dimensional array the reference is [dimension_0, dimension_1], which is equivalent to [row, column].

REMEMBER: Like lists, indices start at index zero, and when taking a slice the slice goes up to, but does not include, the maximum value given.

```
print ('Row zero:\n', data[0,:])
print ('Column one:\n', data[:,1])
# Note in the example below a slice goes up to ,but dot include, the maximum index
print ('Rows 0-3, Column zero:\n', data[0:4,0])
print ('Row 1, Column 2\n', data[1,2])
```

OUT:

```
Row zero:
[ 23  89 100]
Column one:
```

```
[89 51 78 81 75 51]
Rows 0-3, Column zero:
[23 10 40 35]
Row 1, Column 2
99
```

2.3 Pandas basics: building a dataframe from lists, and retrieving data from the dataframe using row and column index references

Here we will repeat basic actions previously described for NumPy. There is significant overlap between NumPy and Pandas (not least because Pandas is built on top of NumPy). Generally speaking Pandas will be used more for data manipulation, and NumPy will be used more for raw calculations (but that is probably somewhat of an over-simplification!).

Pandas allows us to access data using index names or by row/column number. Using index names is perhaps more common in Pandas. You may find having the two different methods available a little confusing at first, but these dual methods are one thing that help make Pandas powerful for data manipulation.

As with NumPy, we will often be importing data from files, but here we will create a dataframe from existing lists.

2.3.1 Creating an empty data frame and building it up from lists

We start with importing pandas (using `pd` as the short name we will use) and then create a dataframe.

```
import pandas as pd
df = pd.DataFrame()
```

Let's create some data in lists and add them to the dataframe:

```
names = ['Gandolf', 'Gimli', 'Frodo', 'Legolas', 'Bilbo']
types = ['Wizard', 'Dwarf', 'Hobbit', 'Elf', 'Hobbit']
magic = [10, 1, 4, 6, 4]
aggression = [7, 10, 2, 5, 1]
stealth = [8, 2, 5, 10, 5]
```

```
df['names'] = names
df['type'] = types
df['magic_power'] = magic
df['aggression'] = aggression
df['stealth'] = stealth
```

We can print the dataframe. Notice that a column to the left has appeared with numbers. This is the index, which has been added automatically.

```
print(df)
```

OUT:

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8
1	Gimli	Dwarf	1	10	2
2	Frodo	Hobbit	4	2	5
3	Legolas	Elf	6	5	10
4	Bilbo	Hobbit	4	1	5

2.3.2 Setting an index column

We can leave the index as it is, or we can make one of the columns the index. Note that to change something in an existing dataframe we use `'inplace=True'`

```
df.set_index('names', inplace=True)
print (df)
```

OUT:

	type	magic_power	aggression	stealth
names				
Gandolf	Wizard	10	7	8
Gimli	Dwarf	1	10	2
Frodo	Hobbit	4	2	5
Legolas	Elf	6	5	10
Bilbo	Hobbit	4	1	5

2.3.3 Accessing data with *loc* and *iloc*

Dataframes have two basic methods of accessing data by row (or index) and by column (or header):

loc selects data by index name and column (header) name.

iloc selects data by row or column number

2.3.4 Selecting rows by index

The *loc* method selects rows by index name, like in Python dictionaries:

```
{print (df.loc['Gandolf']}
```

OUT:

```
print (df.loc['Gandolf'])
```

type	Wizard
magic_power	10
aggression	7
stealth	8

Name: Gandolf, dtype: object

We can pass multiple index references to the *loc* method using a list:

```
to_find = ['Bilbo','Gimli','Frodo']  
print (df.loc[to_find])
```

OUT:

	type	magic_power	aggression	stealth
names				
Bilbo	Hobbit	4	1	5
Gimli	Dwarf	1	10	2
Frodo	Hobbit	4	2	5

Row slices may also be taken. For example let us take a row slice from Gimli to Legolas. Unusually for Python this slice includes both the lower and upper index references.

```
print (df.loc['Gimli':'Legolas'])
```

OUT:

	type	magic_power	aggression	stealth
names				
Gimli	Dwarf	1	10	2
Frodo	Hobbit	4	2	5
Legolas	Elf	6	5	10

As with other Python slices a colon may be used to represent the start or end. :Gimli would take a slice from the beginning to Gimli. Bilbo: would take a row slice from Bilbo to the end.

2.3.5 Selecting records by row number

Rather than using an index, we can use row numbers, using the *iloc* method. As with most references in Python the range given starts from the lower index number and goes up to, but does not include, the upper index number.

	type	magic_power	aggression	stealth
names				
Gandolf	Wizard	10	7	8
Gimli	Dwarf	1	10	2

Discontinuous rows may be accessed with *iloc* by building a list:

```
print (df.iloc[[0,1,4]])
```

OUT:

	type	magic_power	aggression	stealth
names				
Gandolf	Wizard	10	7	8
Gimli	Dwarf	1	10	2
Bilbo	Hobbit	4	1	5

Or, building up a more complex list of row numbers:

```
rows_to_find = list(range(0,2))
rows_to_find += (list(range(3,5)))
```

```
print ('List of rows to find:',rows_to_find)
print()
print (df.iloc[rows_to_find])
```

OUT:

```
List of rows to find: [0, 1, 3, 4]
```

	type	magic_power	aggression	stealth
names				
Gandolf	Wizard	10	7	8
Gimli	Dwarf	1	10	2
Legolas	Elf	6	5	10
Bilbo	Hobbit	4	1	5

2.3.6 Selecting columns by name

Columns are selected using square brackets after the dataframe:

```
print (df['type'])
```

OUT:

```
names
Gandolf    Wizard
Gimli      Dwarf
Frodo      Hobbit
Legolas     Elf
Bilbo      Hobbit
Name: type, dtype: object
```

```
print (df[['type','stealth']])
```

OUT:

	type	stealth
names		
Gandolf	Wizard	8
Gimli	Dwarf	2
Frodo	Hobbit	5
Legolas	Elf	10
Bilbo	Hobbit	5

To take a slice of columns we need to use the *loc* method, using `:` to select all rows.

```
print (df.loc[:, 'magic_power': 'stealth'])
```

	magic_power	aggression	stealth
names			
Gandolf	10	7	8
Gimli	1	10	2
Frodo	4	2	5
Legolas	6	5	10
Bilbo	4	1	5

2.3.7 Selecting columns by number

Columns may also be referenced by number using the *column* method (which allows slicing):

```
print (df[df.columns[1:4]])
```

	magic_power	aggression	stealth
names			
Gandolf	10	7	8
Gimli	1	10	2
Frodo	4	2	5
Legolas	6	5	10
Bilbo	4	1	5

Or *iloc* may be used to select columns by number (the colon shows that we are selecting all rows):

```
print (df.iloc[:, 1:3])
```

OUT:

	magic_power	aggression
names		
Gandolf	10	7
Gimli	1	10
Frodo	4	2
Legolas	6	5
Bilbo	4	1

2.3.8 Selecting rows and columns simultaneously

We can combine row and column references with the *loc* method:

```
rows_to_find = ['Bilbo', 'Gimli', 'Frodo']  
print (df.loc[rows_to_find, 'magic_power': 'stealth'])
```

OUT:

```
rows_to_find = ['Bilbo', 'Gimli', 'Frodo']  
  
print (df.loc[rows_to_find, 'magic_power': 'stealth'])
```

```
      magic_power  aggression  stealth
names
Bilbo           4           1       5
Gimli           1          10       2
Frodo           4           2       5
```

Or with *iloc* (referencing row numbers):

```
print (df.iloc[0:2,2:4])
```

OUT:

```
print (df.iloc[0:2,2:4])
```

```
      aggression  stealth
names
Gandolf         7        8
Gimli          10        2
```

2.4 Basic statistics in Pandas

Like NumPy, Pandas may be used to give us some basic statistics on data.

Let's start by building a very sample dataframe.

```
import pandas as pd
df = pd.DataFrame()

names = ['Gandolf','Gimli','Frodo','Legolas','Bilbo']
types = ['Wizard','Dwarf','Hobbit','Elf','Hobbit']
magic = [10, 1, 4, 6, 4]
aggression = [7, 10, 2, 5, 1]
stealth = [8, 2, 5, 10, None]

df['names'] = names
df['type'] = types
df['magic_power'] = magic
df['aggression'] = aggression
df['stealth'] = stealth
```

2.4.1 Overview statistics

We can get an overview with the `describe()` method.

```
print (df.describe())
```

OUT:

	magic_power	aggression	stealth
count	5.000000	5.000000	4.00
mean	5.000000	5.200000	6.25
std	3.316625	3.420526	3.50
min	1.000000	2.000000	2.00
25%	4.000000	2.000000	4.25
50%	4.000000	5.000000	6.50
75%	6.000000	7.000000	8.50
max	10.000000	10.000000	10.00

We can modify the percentiles reported:

```
print (df.describe(percentiles=[0.05,0.1,0.9,0.95]))
```

OUT:

	magic_power	aggression	stealth
count	5.000000	5.000000	4.00
mean	5.000000	5.200000	6.25
std	3.316625	3.420526	3.50
min	1.000000	2.000000	2.00
5%	1.600000	2.000000	2.45
10%	2.200000	2.000000	2.90
50%	4.000000	5.000000	6.50
90%	8.400000	8.800000	9.40
95%	9.200000	9.400000	9.70
max	10.000000	10.000000	10.00

Specific statistics may be returned:

```
print (df.mean())
```

```
OUT:
magic_power    5.00
aggression     5.20
stealth        6.25
dtype: float64
```

2.4.2 List of key statistical methods

```
mean() = mean
median() = median
min() = minimum
max() = maximum
quantile(x)
var() = variance
std() = standard deviation
mad() = mean absolute variation
skew() = skewness of distribution
kurt() = kurtosis
cov() = covariance
corr() = Pearson Correlation coefficient
autocorr() = autocorelation
diff() = first discrete difference
cumsum() = cummulative sum
comprod() = cumulative product
cummin() = cumulative minimum
```

2.4.3 Returning the index of minimum and maximum

idxmin and *idxmax* will return the index row of the min/max. If two values are equal the first will be returned.

```
print ('Minimum:', df['aggression'].min())
print ('Index row:', df['aggression'].idxmin())
print ('\nFull row:\n', df.iloc[df['aggression'].idxmin()])
```

```
OUT:
Minimum: 2
Index row: 2
```

```
Full row:
names      Frodo
type       Hobbit
magic_power    4
aggression     2
stealth        5
Name: 2, dtype: object
```

2.4.4 Removing rows with incomplete data

We can extract only those rows with a complete data set using the *dropna()* method.

```
print (df.dropna())
```

OUT:

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8.0
1	Gimli	Dwarf	1	10	2.0
2	Frodo	Hobbit	4	2	5.0
3	Legolas	Elf	6	5	10.0

We can use this directly in the describe method.

```
print (df.dropna().describe())
```

OUT:

	magic_power	aggression	stealth
count	4.000000	4.000000	4.00
mean	5.250000	6.000000	6.25
std	3.774917	3.366502	3.50
min	1.000000	2.000000	2.00
25%	3.250000	4.250000	4.25
50%	5.000000	6.000000	6.50
75%	7.000000	7.750000	8.50
max	10.000000	10.000000	10.00

To create a new dataframe with complete rows only, we would simply assign to a new variable name:

```
df_na_dropped = df.dropna()
```

2.5 Converting between NumPy and Pandas

Conversion between NumPy and Pandas is simple.

Let's start with importing NumPy and Pandas, and then make a Pandas dataframe.

```
import numpy as np
import pandas as pd

df = pd.DataFrame()

names = ['Gandolf', 'Gimli', 'Frodo', 'Legolas', 'Bilbo']
types = ['Wizard', 'Dwarf', 'Hobbit', 'Elf', 'Hobbit']
magic = [10, 1, 4, 6, 4]
aggression = [7, 10, 2, 5, 1]
stealth = [8, 2, 5, 10, 5]

df['names'] = names
df['type'] = types
df['magic_power'] = magic
df['aggression'] = aggression
df['stealth'] = stealth

print (df)
```

OUT:

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8
1	Gimli	Dwarf	1	10	2
2	Frodo	Hobbit	4	2	5
3	Legolas	Elf	6	5	10
4	Bilbo	Hobbit	4	1	5

2.5.1 Converting from Pandas to NumPy

We will use the values method to convert from Pandas to NumPy. Notice that we lose our column headers when converting to a NumPy array, and the index field (name) simply becomes the first column.

```
my_array = df.values
```

```
print (my_array)
```

OUT:

```
[['Gandolf' 'Wizard' 10 7 8]
 ['Gimli' 'Dwarf' 1 10 2]
 ['Frodo' 'Hobbit' 4 2 5]
 ['Legolas' 'Elf' 6 5 10]
 ['Bilbo' 'Hobbit' 4 1 5]]
```

2.5.2 Converting from NumPy to Pandas

We will use the dataframe method to convert from a NumPy array to a Pandas dataframe. A new index has been created, and columns have been given numerical headers.

```
my_new_df = pd.DataFrame(my_array)
```

```
print (my_new_df)
```

OUT:

	0	1	2	3	4
0	Gandolf	Wizard	10	7	8
1	Gimli	Dwarf	1	10	2
2	Frodo	Hobbit	4	2	5
3	Legolas	Elf	6	5	10
4	Bilbo	Hobbit	4	1	5

If we have column names, we can supply those to the dataframe during the conversion process. We pass a list to the dataframe method:

```
names = ['name', 'type', 'magic_power', 'aggression', 'strength']
```

```
my_new_df = pd.DataFrame(my_array, columns=names)
```

```
print(my_new_df)
```

OUT:

	name	type	magic_power	aggression	strength
0	Gandolf	Wizard	10	7	8
1	Gimli	Dwarf	1	10	2
2	Frodo	Hobbit	4	2	5
3	Legolas	Elf	6	5	10
4	Bilbo	Hobbit	4	1	5

And, as we have seen previously, we can set the index to a particular column:

```
my_new_df.set_index('name', inplace=True)
```

```
print (my_new_df)
```

OUT:

	type	magic_power	aggression	strength
name				
Gandolf	Wizard	10	7	8
Gimli	Dwarf	1	10	2
Frodo	Hobbit	4	2	5
Legolas	Elf	6	5	10
Bilbo	Hobbit	4	1	5

2.6 Array maths in NumPy

NumPy allows easy standard mathematics to be performed on arrays, as well as more complex linear algebra such as array multiplication.

Let's begin by building a couple of arrays. We'll use the `np.arange` method to create an array of numbers in range 1 to 12, and then reshape the array into a 3 x 4 array.

```
import numpy as np

# note that the arange method is 'half open'
# that is it includes the lower number, and goes up to, but not including,
# the higher number

array_1 = np.arange(1,13)
array_1 = array_1.reshape (3,4)

print (array_1)

OUT:

[[ 1  2  3  4]
 [ 5  6  7  8]
 [ 9 10 11 12]]
```

2.6.1 Maths on a single array

We can multiply an array by a fixed number (or we can add, subtract, divide, raise to power, etc):

```
print (array_1 *4)

OUT:

[[ 4  8 12 16]
 [20 24 28 32]
 [36 40 44 48]]

print (array_1 ** 0.5) # square root of array
```

```
OUT:

[[1.         1.41421356 1.73205081 2.         ]
 [2.23606798 2.44948974 2.64575131 2.82842712]
 [3.         3.16227766 3.31662479 3.46410162]]
```

We can define a vector and multiply all rows by that vector:

```
vector_1 = [1, 10, 100, 1000]

print (array_1 * vector_1)

OUT:

[[ 1  20  300 4000]
 [ 5  60  700 8000]
 [ 9 100 1100 12000]]
```

To multiply by a column vector we will transpose the original array, multiply by our column vector, and transpose back:

```
vector_2 = [1, 10, 100]

result = (array_1.T * vector_2).T

print (result)
```

OUT:

```
[[ 1  2  3  4]
 [ 50 60 70 80]
 [ 900 1000 1100 1200]]
```

2.6.2 Maths on two (or more) arrays

Arrays of the same shape may be multiplied, divided, added, or subtracted.

Let's create a copy of the first array:

```
array_2 = array_1.copy()
```

```
# If we said array_2 = array_1 then array_2 would refer to array_1.
# Any changes to array_1 would also apply to array_2
```

Multiplying two arrays:

```
print (array_1 * array_2)
```

OUT:

```
[[ 1  4  9 16]
 [ 25 36 49 64]
 [ 81 100 121 144]]
```

2.6.3 Matrix multiplication ('dot product')

See <https://www.mathsisfun.com/algebra/matrix-multiplying.html> for an explanation of matrix multiplication, if you are not familiar with it.

We can perform matrix multiplication in numpy with the `np.dot` method.

```
array_2 = np.arange(1,13)
array_2 = array_1.reshape (4,3)

print ('Array 1:')
print (array_1)
print ('\nArray 2:')
print (array_2)
print ('\nDot product of two arrays:')
print (np.dot(array_1, array_2))
```

OUT:

```
Array 1:
[[ 1  2  3  4]
 [ 5  6  7  8]
 [ 9 10 11 12]]
```

```
Array 2:
[[ 1  2  3]
 [ 4  5  6]]
```

```
[ 7  8  9]
[10 11 12]]
```

Dot product of two arrays:

```
[[ 70  80  90]
 [158 184 210]
 [246 288 330]]
```

2.7 Reading and writing CSV files using NumPy and Pandas

Here we will load a CSV called `iris.csv`. This is stored in the same directory as the Python code.

As a general rule, using the Pandas import method is a little more 'forgiving', so if you have trouble reading directly into a NumPy array, try loading in a Pandas dataframe and then converting to a NumPy array.

2.7.1 Reading a csv file into a NumPy array

NumPy's `loadtxt` method reads delimited text. We specify the separator as a comma. The data we are loading also has a text header, so we use `skiprows=1` to skip the header row, which would cause problems for NumPy.

```
import numpy as np

my_array = np.loadtxt('iris_numbers.csv', delimiter=",", skiprows=1)

print (my_array[0:5,:]) # first 5 rows

OUT:

[[5.1 3.5 1.4 0.2 1. ]
 [4.9 3.  1.4 0.2 1. ]
 [4.7 3.2 1.3 0.2 1. ]
 [4.6 3.1 1.5 0.2 1. ]
 [5.  3.6 1.4 0.2 1. ]]
```

2.7.2 Saving a NumPy array as a csv file

We use the `savetxt` method to save to a csv.

```
np.savetxt("saved_numpy_data.csv", my_array, delimiter=",")
```

2.7.3 Reading a csv file into a Pandas dataframe

The `read_csv` will read a CSV into Pandas. This import assumes that there is a header row. If there is no header row, then the argument `header = None` should be used as part of the command. Notice that a new index column is created.

```
import pandas as pd

df = pd.read_csv('iris.csv')

print (df.head(5)) # First 5 rows

OUT:

   sepal.length  sepal.width  petal.length  petal.width  variety
0           5.1           3.5           1.4           0.2   Setosa
1           4.9           3.0           1.4           0.2   Setosa
2           4.7           3.2           1.3           0.2   Setosa
3           4.6           3.1           1.5           0.2   Setosa
4           5.0           3.6           1.4           0.2   Setosa
```

2.7.4 Saving a Pandas dataframe to a CSV file

The *to_csv* will save a dataframe to a CSV. By default column names are saved as a header, and the index column is saved. If you wish not to save either of those use *header=True* and/or *index=True* in the command. For example, in the command below we save the dataframe with headers, but not with the index column.

```
df.to_csv('my_pandas_dataframe.csv', index=False)
```

2.8 Applying user-defined functions to NumPy and Pandas

Both NumPy and Pandas allow user to functions to applied to all rows and columns (and other axes in NumPy, if multidimensional arrays are used)

2.8.1 Numpy

In NumPy we will use the *apply_along_axis* method to apply a user-defined function to each row and column.

Let's first set up a array and define a function. We will use a simple user-defined function for illustrative purposes - one that returns the position of the highest value in the slice passed to the function. In NumPy we use *argmax* for finding the position of the highest value.

```
import numpy as np
import pandas as pd

my_array = np.array([[10,2,13],
                     [21,22,23],
                     [31,32,33],
                     [10,57,20],
                     [20,20,20],
                     [101,91,10]])
```

```
def my_function(x):
    position = np.argmax(x)
    return position
```

Using *axis=0* we can apply that function to all columns:

```
print (np.apply_along_axis(my_function, axis=0, arr=my_array))
```

```
OUT:
[5 5 2]
```

Using *axis=1* we can apply that function to all rows:

```
print (np.apply_along_axis(my_function, axis=1, arr=my_array))
```

```
OUT:
[2 2 2 1 0 0]
```

2.8.2 Pandas

Pandas has a similar method, the *apply* method for applying a user function by either row or column. The Pandas method for determining the position of the highest value is *idxmax*.

We will convert our NumPy array to a Pandas dataframe, define our function, and then apply it to all columns. Notice that because we are working in Pandas the returned value is a Pandas series (equivalent to a DataFrame, but with one one axis) with an index value.

```
import pandas as pd

df = pd.DataFrame(my_array)

def my_function(x):
    z= x.idxmax()
    return z
```

```
print(df.apply(my_function, axis=0))
```

OUT:

```
0    5
1    5
2    2
dtype: int64
```

And applying it to all rows:

```
print(df.apply(my_function, axis=1))
```

OUT:

```
0    2
1    2
2    2
3    1
4    0
5    0
dtype: int64
```

2.9 Adding data to NumPy arrays and Pandas dataframes

2.9.1 Numpy

Adding more rows of data

To add more rows to an existing numpy array use the *vstack* method which can add multiple or single rows. New data may be in the form of a numpy array or a list. All combined data must have the same number of columns.

```
import numpy as np

# Starting with a NumPy array
array1 = np.array([[1,2,3,4,5],
                  [6,7,8,9,10],
                  [11,12,13,14,15]])

# An additional 2d list
array2 = [[16,17,18,19,20],
          [21,22,23,24,25]]

# An additional single row Numpy array
array3 = np.array([26,27,28,29,30])

# We will combine all data into existing array, array1
# But a new name could be given
array1 = np.vstack([array1, array2, array3])

print (array1)
```

OUT:

```
[[ 1  2  3  4  5]
 [ 6  7  8  9 10]
 [11 12 13 14 15]
 [16 17 18 19 20]
 [21 22 23 24 25]
 [26 27 28 29 30]]
```

Adding more columns of data

To add more columns to an existing numpy array use the *hstack* method which can add multiple or single rows. All combined data must have the same number of rows.

```
df1 = pd.DataFrame()
names = ['Gandolf','Gimli','Frodo','Legolas','Bilbo']
types = ['Wizard','Dwarf','Hobbit','Elf','Hobbit']

df1['names'] = names
df1['type'] = types

print (df1)

# Add another column
magic = [10, 1, 4, 6, 4]
df1['magic'] = magic
```

```
print ('\n Added column:\n',df1)
```

OUT:

	names	type
0	Gandolf	Wizard
1	Gimli	Dwarf
2	Frodo	Hobbit
3	Legolas	Elf
4	Bilbo	Hobbit

Added column:

	names	type	magic
0	Gandolf	Wizard	10
1	Gimli	Dwarf	1
2	Frodo	Hobbit	4
3	Legolas	Elf	6
4	Bilbo	Hobbit	4

We can use *concat* also to add multiple columns (in the form of another dataframe), in which case the data will be combined based on the index column. We pass the argument *axis=1* to the *concat* statement to instruct the method to combine by column (it defaults to *axis=0*, or row concatenation).

```
df1 = pd.DataFrame()
names = ['Gandolf','Gimli','Frodo','Legolas','Bilbo']
types = ['Wizard','Dwarf','Hobbit','Elf','Hobbit']
```

```
df1['names'] = names
df1['type'] = types
```

```
print (df1)
```

```
df2 = pd.DataFrame()
```

```
magic = [10, 1, 4, 6, 4]
aggression = [7, 10, 2, 5, 1]
stealth = [8, 2, 5, 10, 5]
```

```
df2['magic_power'] = magic
df2['aggression'] = aggression
df2['stealth'] = stealth
```

```
df1 = pd.concat([df1,df2], axis=1)
print(df1)
```

OUT:

```
df1 = pd.concat([df1,df2], axis=1)
```

```
print(df1)
```

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8
1	Gimli	Dwarf	1	10	2
2	Frodo	Hobbit	4	2	5
3	Legolas	Elf	6	5	10
4	Bilbo	Hobbit	4	1	5

There is more information here: <https://pandas.pydata.org/pandas-docs/stable/merging.html>

2.10 Using Pandas to merge or lookup data

Sometimes we may want to cross-reference data between different data tables. This may be in order to perform a full merge of data, or just to produce a summary lookup table referencing across different tables.

```
import numpy as np
import pandas as pd

# Set up the first data frame

df1 = pd.DataFrame()

names = ['Gandolf', 'Gimli', 'Frodo', 'Legolas', 'Bilbo']
types = ['Wizard', 'Dwarf', 'Hobbit', 'Elf', 'Hobbit']
magic = [10, 1, 4, 6, 4]
aggression = [7, 10, 2, 5, 1]
stealth = [8, 2, 5, 10, 5]

df1['names'] = names
df1['type'] = types
df1['magic_power'] = magic
df1['aggression'] = aggression
df1['stealth'] = stealth

# Set up the second dataframe

names = ['Gandolf', 'Gimli', 'Frodo', 'Aragorn', 'Sauron']
popularity = ['High', 'Medium', 'High', 'Medium', 'Low']

df2 = pd.DataFrame()

df2['name'] = names
df2['popularity'] = popularity
```

We will look here at where the reference fields are not the index fields. We are going to want to merge using 'names' in df1 and 'name' in df2, and we are going to keep all records from df1, and add data from df2 where it is available.

```
merged_df = pd.merge(df1, df2,
                      left_on = 'names',
                      right_on = 'name',
                      how='left')

print (merged_df)
```

OUT:

	names	type	magic_power	aggression	stealth	name	popularity
0	Gandolf	Wizard	10	7	8	Gandolf	High
1	Gimli	Dwarf	1	10	2	Gimli	Medium
2	Frodo	Hobbit	4	2	5	Frodo	High
3	Legolas	Elf	6	5	10	NaN	NaN
4	Bilbo	Hobbit	4	1	5	NaN	NaN

We can keep all data from both databases by using *how=outer* (an outer database join).

```
merged_df = pd.merge(df1, df2,
                      left_on = 'names',
                      right_on = 'name',
```

```

        how='outer')

print (merged_df)

```

OUT:

	names	type	magic_power	aggression	stealth	name	popularity
0	Gandolf	Wizard	10.0	7.0	8.0	Gandolf	High
1	Gimli	Dwarf	1.0	10.0	2.0	Gimli	Medium
2	Frodo	Hobbit	4.0	2.0	5.0	Frodo	High
3	Legolas	Elf	6.0	5.0	10.0	NaN	NaN
4	Bilbo	Hobbit	4.0	1.0	5.0	NaN	NaN
5	NaN	NaN	NaN	NaN	NaN	Aragorn	Medium
6	NaN	NaN	NaN	NaN	NaN	Sauron	Low

Or we could use *how=inner* to produce a dataframe for only the rows with reference columns in both dataframes, or *how=right* to keep all rows in df2 and add data from df1 where it exists.

In the above examples we have returned all fields both both dataframes. We can choose to select just the fields we wish to return (though we need the reference field from both dataframes):

```

merged_df = pd.merge(df1[['names','type']],
                    df2[['name','popularity']],
                    left_on = 'names',
                    right_on = 'name',
                    how='left')

```

```

print (merged_df)

```

OUT:

	names	type	name	popularity
0	Gandolf	Wizard	Gandolf	High
1	Gimli	Dwarf	Gimli	Medium
2	Frodo	Hobbit	Frodo	High
3	Legolas	Elf	NaN	NaN
4	Bilbo	Hobbit	NaN	NaN

Using this method we need our reference fields, used to join data, as part of the dataframe and not as the index. To use this method where there is an index column that you wish to use as a joining field you will need to reset the index to a new numbered column. That is done by the command *df.reset_index()*. Alternatively you can use a method that joins using the index fields of each dataframe, as described in the link below.

There are many ways of joining and merging Pandas dataframes. I have set out just one method here. See <https://pandas.pydata.org/pandas-docs/stable/merging.html> for all methods.

2.11 Sorting and ranking with Pandas

2.11.1 Sorting

Pandas allows easy and flexible sorting.

As usual, let's first build a dataframe:

```
import pandas as pd
df = pd.DataFrame()

names = ['Gandolf', 'Gimli', 'Frodo', 'Legolas', 'Bilbo']
types = ['Wizard', 'Dwarf', 'Hobbit', 'Elf', 'Hobbit']
magic = [10, 1, 4, 6, 4]
aggression = [7, 10, 2, 5, 1]
stealth = [8, 2, 5, 10, 5]

df['names'] = names
df['type'] = types
df['magic_power'] = magic
df['aggression'] = aggression
df['stealth'] = stealth
```

And now let's sort first by magic power and then (in reverse order aggression.

```
new_df = df.sort_values(['magic_power', 'aggression'], ascending=[False, True])
print (new_df)
```

OUT:

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8
3	Legolas	Elf	6	5	10
4	Bilbo	Hobbit	4	1	5
2	Frodo	Hobbit	4	2	5
1	Gimli	Dwarf	1	10	2

Usually it is fine to use the default sorting method. Sometimes though you may wish to do a series of sequential sorts where you maintain the previous order within the sorted the dataframe. In that case use a mergesort by passing *kind = 'mergesort'* as one of the arguments.

We can use *sort_index* to sort by the index field. Let's sort our new dataframe by reverse index order:

```
print (new_df.sort_index(ascending=False))
i
```

	names	type	magic_power	aggression	stealth
4	Bilbo	Hobbit	4	1	5
3	Legolas	Elf	6	5	10
2	Frodo	Hobbit	4	2	5
1	Gimli	Dwarf	1	10	2
0	Gandolf	Wizard	10	7	8

2.11.2 Ranking

Pandas allows easy ranking of dataframes by a single column. Where two values are identical the result is the average of the number of ranks they would cover. Notice that a higher number is a higher rank.

```
i
print (df['magic_power'].rank())
```

OUT:

```
0    5.0
1    1.0
2    2.5
3    4.0
4    2.5
Name: magic_power, dtype: float64
```

Pandas does not offer a direct method for ranking using multiple columns. One way would be to sort the dataframe, reset the index with *df.reset_index()* and compare the index values to the original table.

2.12 Using masks to filter data, and perform search and replace, in NumPy and Pandas

In both NumPy and Pandas we can create masks to filter data. Masks are 'Boolean' arrays - that is arrays of true and false values and provide a powerful and flexible method to selecting data.

2.12.1 NumPy

creating a mask

Let's begin by creating an array of 4 rows of 10 columns of uniform random number between 0 and 100.

```
import numpy as np

array1 = np.random.randint(0,100,size=(4,10))

print (array1)
```

OUT:

```
[[68 56 72 91 64 98  3 54 49 67]
 [ 1  6 54 65 24 97 68  9 28 47]
 [30 88 52 11 22 12 35 65 66  3]
 [13 83 81 32 87 74 79 34 26  1]]
```

Now we'll create a mask to show those numbers greater than 70.

```
mask = array1 > 70

print(mask)
```

OUT:

```
[[False False  True  True False  True False False False False]
 [False False False False False  True False False False False]
 [False  True False False False False False False False False]
 [False  True  True False  True  True  True False False False]]
```

We can use that mask to extract the numbers:

```
print (array1[mask])
```

OUT:

```
[72 91 98 97 88 83 81 87 74 79]
```

Using *any* and *all*

any and all allow us to check for all true or all false.

We can apply that to the whole array:

```
print (mask.any())
print (mask.all())
```

OUT:

```
True
False
```

Or we can apply it column-wise (by passing *axis=1*) or row-wise (by passing *axis=1*).

```
print ('All tests in a column are true:')
print (mask.all(axis=0))
print ('\nAny test in a row is true:')
print (mask.any(axis=1))
```

OUT:

```
All tests in a column are true:
[False False False False False False False False False]
```

```
Any test in a row is true:
[False  True  True  True]
```

We can use `!=` to invert a mask if needed (all trues become false, and all falses become true). This can be useful, but can also become a little confusing!

```
inverted_mask = mask!=True
print (inverted_mask)
```

OUT:

```
[[ True  True  True  True  True  True  True  True  True  True]
 [ True  True False False  True False  True False False False]
 [False False False  True False  True  True  True False  True]
 [ True False  True  True  True  True  True  True  True  True]]
```

Adding or averaging trues

Boolean values (True/False) in Python also take the values 1 and 0. This can be useful for counting trues/false, for example:

```
print ('Number of trues in array:')
print (mask.sum())
```

OUT:

```
Number of trues in array:
12
```

```
print('Number of trues in array by row:')
print (mask.sum(axis=1))
```

OUT:

```
Number of trues in array by row:
[0 6 5 1]
```

```
print('Average of trues in array by column:')
print (mask.mean(axis=0))
```

OUT:

```
Average of trues in array by column:
[0.25 0.5  0.5  0.25 0.25 0.25 0.  0.25 0.5  0.25]
```

Selecting rows or columns based on one value in that row or column

Let's select all columns where the value of the first element is equal to, or greater than 50:

```
mask = array1[0,:] >= 50 # colon indicates all columns, zero indicates row 0
```

```
print ('\nHere is the mask')
print (mask)
print ('\nAnd here is the mask applied to all columns')
print (array1[:,mask]) # colon represents all rows of chosen columns
```

OUT:

```
Here is the mask
[ True  True False False  True False False False  True]
```

```
And here is the mask applied to all columns
[[60 68 57 57]
 [47 52 64 74]
 [77 78 79 21]
 [11 78  5 14]]
```

Similarly if we wanted to select all rows where the 2nd element was equal to, or greater, than 50

```
mask = array1[:,1] >= 50 # colon indicates all rows, 1 indicates row 1)
print ('\nHere is the mask')
print (mask)
print ('\nAnd here is the mask applied to all rows')
print (array1[mask,:]) # colon represents all rows of chosen columns
```

OUT:

```
Here is the mask
[ True  True  True  True]
```

```
And here is the mask applied to all rows
[[60 68 34 25 57 33 49  5 33 57]
 [47 52 78 89 64 75  8 98 93 74]
 [77 78 74 41 79 50 43 21 81 21]
 [11 78 39 18  5 67 69  1 50 14]]
```

Using *and* and *or*, and combining filters from two arrays

We may create and combine multiple masks. For example we may have two masks that look for values less than 20 or greater than 80, and then combine those masks with or which is represented by `—` (stick).

```
print ('Mask for values <20:')
mask1 = array1 < 20
print (mask1)

print ('\nMask for values >80:')
mask2 = array1 > 80
print (mask2)

print ('\nCombined mask:')
mask = mask1 | mask2 # | (stick) is used for 'or' with two boolean arrays
print (mask)

print ('\nSelected values using combined mask')
print (array1[mask])
```

OUT:

```
Mask for values <20:
```

```
[[False False False False False False False True False False]
 [False False False False False False True False False False]
 [False False False False False False False False False False]
 [ True False False  True  True False False  True False  True]]
```

Mask for values >80:

```
[[False False False False False False False False False False]
 [False False False  True False False False  True  True False]
 [False False False False False False False False  True False]
 [False False False False False False False False False False]]
```

Combined mask:

```
[[False False False False False False False True False False]
 [False False False  True False False  True  True  True False]
 [False False False False False False False False  True False]
 [ True False False  True  True False False  True False  True]]
```

Selected values using combined mask

```
[ 5 89  8 98 93 81 11 18  5  1 14]
```

We can combine these masks in a single line:

```
mask = (array1 < 20) | (array1 > 80)
print (mask)
```

OUT:

```
mask = (array1 < 20) | (array1 > 80)
```

```
print (mask)
```

```
[[False False False False False False False True False False]
 [False False False  True False False  True  True  True False]
 [False False False False False False False False  True False]
 [ True False False  True  True False False  True False  True]]
```

We can combine masks derived from different arrays, so long as they are the same shape. For example let's produce an another array of random numbers and check for those element positions where corresponding positions of both arrays have values of greater than 50. When comparing boolean arrays we represent 'and' with &.

```
array2 = np.random.randint(0,100,size=(4,10))
```

```
print ('Mask for values of array1 > 50:')
mask1 = array1 > 50
print (mask1)
```

```
print ('\nMask for values of array2 > 50:')
mask2 = array2 > 50
print (mask2)
```

```
print ('\nCombined mask:')
mask = mask1 & mask2
print (mask)
```

OUT:

Mask for values of array1 > 50:

```
[[ True  True False False  True False False False False  True]
 [False  True  True  True  True  True False  True  True  True]]
```

```
[ True  True  True False  True False False False  True False]
[False  True False False False  True  True False False False]]
```

Mask for values of array2 > 50:

```
[[ True False  True False False  True  True False False  True]
 [ True False  True  True False  True  True  True False False]
 [False  True  True False  True False  True  True  True False]
 [ True False  True False False  True  True  True  True  True]]
```

Combined mask:

```
[[ True False False False False False False False False  True]
 [False False  True  True False  True False  True False False]
 [False  True  True False  True False False False  True False]
 [False False False False False  True  True False False False]]
```

We could shorten this to:

```
mask = (array1 > 50) & (array2 > 50)
print (mask)
```

OUT:

```
[[ True False False False False False False False False  True]
 [False False  True  True False  True False  True False False]
 [False  True  True False  True False False False  True False]
 [False False False False False  True  True False False False]]
```

Setting values based on mask

We can use masks to reassign values only for elements that meet the given criteria. For example we can set the values of all cells with a value less than 50 to zero, and set all other values to 1.

```
print ('Array at sttart:')
print (array1)
mask = array1 < 50
array1[mask] = 0
mask = mask != True # invert mask
array1[mask] = 1
print('\nNew array')
print (array1)
```

OUT:

```
Array at sttart:
[[60 68 34 25 57 33 49  5 33 57]
 [47 52 78 89 64 75  8 98 93 74]
 [77 78 74 41 79 50 43 21 81 21]
 [11 78 39 18  5 67 69  1 50 14]]
```

```
New array
[[1 1 0 0 1 0 0 0 0 1]
 [0 1 1 1 1 1 0 1 1 1]
 [1 1 1 0 1 1 0 0 1 0]
 [0 1 0 0 0 1 1 0 1 0]]
```

We can shorten this, by making the mask implicit in the assignment command.

```
array2[array2<50] = 0
array2[array2>=50] = 1
```

```
print('New array2:')
print(array2)
```

OUT:

```
New array2:
[[1 0 1 0 0 1 1 0 0 1]
 [1 0 1 1 0 1 1 1 0 0]
 [0 1 1 0 1 0 1 1 1 0]
 [1 0 1 0 0 1 1 1 1 1]]
```

Miscellaneous examples

Select columns where the average value across the column is greater than the average across the whole array, and return both the columns and the column number.

```
array = np.random.randint(0,100,size=(4,10))
number_of_columns = array.shape[1]
column_list = np.arange(0, number_of_columns) # create a list of column ids
array_average = array.mean()
column_average = array.mean(axis=0)
column_average_greater_than_array_average = column_average > array_average
selected_columns = column_list[column_average_greater_than_array_average]
selected_data = array[:,column_average_greater_than_array_average]

print ('Selected columns:')
print (selected_columns)
print ('\nSeelcted data:')
print (selected_data)
```

OUT:

```
Selected columns:
[1 2 4 9]

Seelcted data:
[[56 48 97 78]
 [26 87  6 45]
 [56 65 71 59]
 [41 34 98 70]]
```

2.12.2 Pandas

Filtering with masks in Pandas is very similar to numpy. It is perhaps more usual in Pandas to be creating masks testing specific columns, with resulting selection of rows. For example let's use a mask to select characters meeting conditions on magical power and aggression:

```
i
import pandas as pd

df = pd.DataFrame()

names = ['Gandolf','Gimli','Frodo','Legolas','Bilbo']
types = ['Wizard','Dwarf','Hobbit','Elf','Hobbit']
magic = [10, 1, 4, 6, 4]
aggression = [7, 10, 2, 5, 1]
stealth = [8, 2, 5, 10, 5]
```

```

df['names'] = names
df['type'] = types
df['magic_power'] = magic
df['aggression'] = aggression
df['stealth'] = stealth

mask = (df['magic_power'] > 3) & (df['aggression'] < 5)
print ('Mask:')
print (mask) # notice mask is a 'series'; a one dimensional DataFrame
# when passing a Boolean series to a dataframe we select the appropriate rows
filtered_data = df[mask]
print (filtered_data)

```

OUT:

```

Mask:
0    False
1    False
2     True
3    False
4     True
dtype: bool
   names  type  magic_power  aggression  stealth
2  Frodo  Hobbit           4           2        5
4  Bilbo  Hobbit           4           1        5

```

Though creating masks based on particular columns will be most common in Pandas. We can also filter on the entire dataframe. Look what happens when we filter on values >3:

```

mask = df > 3
print('Mask:')
print (mask)
print ('\nMasked data:')
df2 = df[mask]
print (df2)

```

OUT:

```

Mask:
   names  type  magic_power  aggression  stealth
0   True  True          True          True    True
1   True  True         False          True   False
2   True  True          True         False    True
3   True  True          True          True    True
4   True  True          True         False    True

Masked data:
   names  type  magic_power  aggression  stealth
0  Gandolf  Wizard        10.0          7.0        8.0
1   Gimli  Dwarf         NaN          10.0         NaN
2   Frodo  Hobbit          4.0          NaN        5.0
3  Legolas   Elf          6.0          5.0       10.0
4   Bilbo  Hobbit          4.0          NaN        5.0

```

The structure of the dataframe is maintained, and all text is maintained. Those values not >3 have been removed (NaN represents 'Not a Number').

Conditional replacing of values in Pandas

Replacing values in Pandas, based on the current value, is not as simple as in NumPy. For example, to replace all values in a given column, given a conditional test, we have to (1) take one column at a time, (2) extract the column values into an array, (3) make our replacement, and (4) replace the column values with our adjusted array.

For example to replace all values less than 4 with zero (in our numeric columns):

```
columns = ['magic_power', 'aggression', 'stealth']
# note: to get a list of all columns you can use list(df)

for column in columns: # loop through our column list
    values = df[column].values # extract the column values into an array
    mask = values < 4 # create Boolean mask
    values[mask] = 0 # apply Boolean mask
    df[column] = values # replace the dataframe column with the array

print (df)
```

OUT:

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8
1	Gimli	Dwarf	0	10	0
2	Frodo	Hobbit	4	0	5
3	Legolas	Elf	6	5	10
4	Bilbo	Hobbit	4	0	5

2.13 Summarising data by groups in Pandas using pivot tables and groupby

Pandas offers two methods of summarising data - groupby and pivot_table*. The data produced can be the same but the format of the output may differ.

*pivot_table summarises data. There is a similar command, pivot, which we will use in the next section which is for reshaping data.

As usual let's start by creating a dataframe.

```
import pandas as pd
df = pd.DataFrame()

names = ['Gandolf',
         'Gimli',
         'Frodo',
         'Legolas',
         'Bilbo',
         'Sam',
         'Pippin',
         'Boromir',
         'Aragorn',
         'Galadriel',
         'Meriadoc']
types = ['Wizard',
        'Dwarf',
        'Hobbit',
        'Elf',
        'Hobbit',
        'Hobbit',
        'Hobbit',
        'Hobbit',
        'Man',
        'Man',
        'Elf',
        'Hobbit']
magic = [10, 1, 4, 6, 4, 2, 0, 0, 2, 9, 0]
aggression = [7, 10, 2, 5, 1, 6, 3, 8, 7, 2, 4]
stealth = [8, 2, 5, 10, 5, 4, 5, 3, 9, 10, 6]

df['names'] = names
df['type'] = types
df['magic_power'] = magic
df['aggression'] = aggression
df['stealth'] = stealth
```

2.13.1 Pivot tables

To return the median values by type:

```
import numpy as np # we will use a numpy method to summarise data

pivot = df.pivot_table(index='type',
                        values=['magic_power', 'aggression', 'stealth'],
                        aggfunc=[np.mean],
                        margins=True) # margins summarises all

# note: addgunc can be any valid function that can act on data provided
```

```
print (pivot)
```

OUT:

	mean		
	aggression	magic_power	stealth
type			
Dwarf	10.0	1.000000	2.000000
Elf	3.5	7.500000	10.000000
Hobbit	3.2	2.000000	5.000000
Man	7.5	1.000000	6.000000
Wizard	7.0	10.000000	8.000000
All	5.0	3.454545	6.090909

Or we may group by more than one index. In this case we'll return the average and summed values by type and magical power:

```
pivot = df.pivot_table(index=['type','magic_power'],
                        values=['aggression', 'stealth'],
                        aggfunc=[np.mean,np.sum],
                        margins=True) # margins summarises all
```

```
print (pivot)
```

OUT:

		mean		sum	
		aggression	stealth	aggression	stealth
type	magic_power				
Dwarf	1	10.0	2.000000	10	2
Elf	6	5.0	10.000000	5	10
	9	2.0	10.000000	2	10
Hobbit	0	3.5	5.500000	7	11
	2	6.0	4.000000	6	4
	4	1.5	5.000000	3	10
Man	0	8.0	3.000000	8	3
	2	7.0	9.000000	7	9
Wizard	10	7.0	8.000000	7	8
All		5.0	6.090909	55	67

2.13.2 Groupby

Grouby is a very powerful method in Pandas which we shall return to in the next section. Here we will use groupby simply to summarise data.

```
print(df.groupby('type').median())
```

OUT:

	magic_power	aggression	stealth
type			
Dwarf	1.0	10.0	2.0
Elf	7.5	3.5	10.0
Hobbit	2.0	3.0	5.0
Man	1.0	7.5	6.0
Wizard	10.0	7.0	8.0

Instead of built in methods we can also apply user-defined functions. To illustrate we'll define a simple

function to return the lower quartile.

```
def my_func(x):
    return (x.quantile(0.25))

print(df.groupby('type').apply(my_func))

# Note we need not apply a lambda function
# We may apply any user-defined function
```

OUT:

0.25	magic_power	aggression	stealth
type			
Dwarf	1.00	10.00	2.0
Elf	6.75	2.75	10.0
Hobbit	0.00	2.00	5.0
Man	0.50	7.25	4.5
Wizard	10.00	7.00	8.0

As with pivot-table we can have more than one index column.

```
print(df.groupby(['type', 'magic_power']).median())
```

OUT:

		aggression	stealth
type	magic_power		
Dwarf	1	10.0	2.0
Elf	6	5.0	10.0
	9	2.0	10.0
Hobbit	0	3.5	5.5
	2	6.0	4.0
	4	1.5	5.0
Man	0	8.0	3.0
	2	7.0	9.0
Wizard	10	7.0	8.0

Or we can return just selected data columns.

```
print(df.groupby('type').median()[['magic_power', 'stealth']])
```

OUT:

	magic_power	stealth
type		
Dwarf	1.0	2.0
Elf	7.5	10.0
Hobbit	2.0	5.0
Man	1.0	6.0
Wizard	10.0	8.0

To return multiple types of results we use the *agg* argument.

```
print(df.groupby('type').agg([min, max]))
```

OUT:

	names		magic_power		aggression		stealth	
	min	max	min	max	min	max	min	max
type								
Dwarf	Gimli	Gimli	1	1	10	10	2	2

Elf	Galadriel	Legolas	6	9	2	5	10	10
Hobbit	Bilbo	Sam	0	4	1	6	4	6
Man	Aragorn	Boromir	0	2	7	8	3	9
Wizard	Gandolf	Gandolf	10	10	7	7	8	8

Pandas built-in groupby functions

Remember that apply can be used to apply any user-defined function

```
.all # Boolean True if all true
.any # Boolean True if any true
.count count of non null values
.size size of group including null values
.max
.min
.mean
.median
.sem
.std
.var
.sum
.prod
.quantile
.agg(functions) # for multiple outputs
.apply(func)
.last # last value
.nth # nth row of group
```

2.14 Reshaping Pandas data with stack, unstack, pivot and melt

Sometimes data is best shaped where the data is in the form of a wide table where the description is in a column header, and sometimes it is best shaped as as having the data descriptor as a variable within a tall table.

To begin with you may find it a little confusing what happens to the index field as we switch between different formats. But hang in there and you'll get the hang of it!

Lets look at some examples, beginning as usual with creating a dataframe.

```
import pandas as pd
df = pd.DataFrame()

names = ['Gandolf',
         'Gimli',
         'Frodo',
         'Legolas',
         'Bilbo',
         'Sam',
         'Pippin',
         'Boromir',
         'Aragorn',
         'Galadriel',
         'Meriadoc']
types = ['Wizard',
        'Dwarf',
        'Hobbit',
        'Elf',
        'Hobbit',
        'Hobbit',
        'Hobbit',
        'Hobbit',
        'Man',
        'Man',
        'Elf',
        'Hobbit']
magic = [10, 1, 4, 6, 4, 2, 0, 0, 2, 9, 0]
aggression = [7, 10, 2, 5, 1, 6, 3, 8, 7, 2, 4]
stealth = [8, 2, 5, 10, 5, 4 ,5, 3, 9, 10, 6]
```

```
df['names'] = names
df['type'] = types
df['magic_power'] = magic
df['aggression'] = aggression
df['stealth'] = stealth
```

When we look at this table, the data descriptors are columns, and the data table is 'wide'.

```
print (df)
```

OUT:

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8
1	Gimli	Dwarf	1	10	2
2	Frodo	Hobbit	4	2	5
3	Legolas	Elf	6	5	10
4	Bilbo	Hobbit	4	1	5

5	Sam	Hobbit	2	6	4
6	Pippin	Hobbit	0	3	5
7	Boromir	Man	0	8	3
8	Aragorn	Man	2	7	9
9	Galadriel	Elf	9	2	10
10	Meriadoc	Hobbit	0	4	6

2.14.1 Stack and unstack

We can convert between the two formats of data with *stack* and *unstack*. To convert from a wide table to a tall and skinny, use *stack*. Notice this creates a more complex index which has two levels the first level is person id, and the second level is the data header. This is called a multi-index.

```
df_stacked = df.stack()
print(df_stacked.head(20)) # print first 20 rows
```

OUT:

```
0  names      Gandolf
   type      Wizard
   magic_power      10
   aggression       7
   stealth         8
1  names      Gimli
   type      Dwarf
   magic_power       1
   aggression      10
   stealth         2
2  names      Frodo
   type      Hobbit
   magic_power       4
   aggression       2
   stealth         5
3  names      Legolas
   type      Elf
   magic_power       6
   aggression       5
   stealth        10
```

dtype: object

We can convert back to wide table with *unstack*. This recreates a single index for each line of data.

```
df_unstacked = df_stacked.unstack()
print (df_unstacked)
```

OUT:

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8
1	Gimli	Dwarf	1	10	2
2	Frodo	Hobbit	4	2	5
3	Legolas	Elf	6	5	10
4	Bilbo	Hobbit	4	1	5
5	Sam	Hobbit	2	6	4
6	Pippin	Hobbit	0	3	5
7	Boromir	Man	0	8	3
8	Aragorn	Man	2	7	9
9	Galadriel	Elf	9	2	10
10	Meriadoc	Hobbit	0	4	6

Returning to our stacked data, we can convert our multi-index to two separate fields by resetting the index. By default this method names the separated index field 'level_0' and 'level_1' (multi-level indexes may have further levels as well), and the data field '0'. Let's rename them as well (comment out that row with a # to see what it would look like without renaming them). You can see the effect below:

```
reindexed_stacked_df = df_stacked.reset_index()
reindexed_stacked_df.rename(
    columns={'level_0': 'ID', 'level_1': 'variable', 0:'value'},inplace=True)

print (reindexed_stacked_df.head(20)) # print first 20 rows
```

OUT:

	ID	variable	value
0	0	names	Gandolf
1	0	type	Wizard
2	0	magic_power	10
3	0	aggression	7
4	0	stealth	8
5	1	names	Gimli
6	1	type	Dwarf
7	1	magic_power	1
8	1	aggression	10
9	1	stealth	2
10	2	names	Frodo
11	2	type	Hobbit
12	2	magic_power	4
13	2	aggression	2
14	2	stealth	5
15	3	names	Legolas
16	3	type	Elf
17	3	magic_power	6
18	3	aggression	5
19	3	stealth	10

We can return to a multi-index, if we want to, by setting the index to the two fields to be combined. Whether a multi-index is preferred or not will depend on what you wish to do wit the dataframe, so it useful to know how to convert back and forth between multi-index and single-index.

```
reindexed_stacked_df.set_index(['ID', 'variable'], inplace=True)
print (reindexed_stacked_df.head(20))
```

OUT:

		value
ID	variable	
0	names	Gandolf
	type	Wizard
	magic_power	10
	aggression	7
	stealth	8
1	names	Gimli
	type	Dwarf
	magic_power	1
	aggression	10
	stealth	2
2	names	Frodo
	type	Hobbit
	magic_power	4

```

    aggression      2
    stealth          5
3  names            Legolas
    type             Elf
    magic_power      6
    aggression       5
    stealth           10

```

2.14.2 Melt and pivot

melt and *pivot* are like *stack* and *unstack*, but offer some other options.

melt de-pivots data (into a tall skinny table)

pivot will re-pivot data into a wide table.

Let's return to our original dataframe created (which we called 'df') and create a tall skinny table of selected fields using *melt*. We will separate out one or more of the fields, such as 'names' as an ID field, as below:

```

unpivoted = df.melt(id_vars=['names'], value_vars=['type', 'magic_power'])
print (unpivoted)

```

OUT:

	names	variable	value
0	Gandolf	type	Wizard
1	Gimli	type	Dwarf
2	Frodo	type	Hobbit
3	Legolas	type	Elf
4	Bilbo	type	Hobbit
5	Sam	type	Hobbit
6	Pippin	type	Hobbit
7	Boromir	type	Man
8	Aragorn	type	Man
9	Galadriel	type	Elf
10	Meriadoc	type	Hobbit
11	Gandolf	magic_power	10
12	Gimli	magic_power	1
13	Frodo	magic_power	4
14	Legolas	magic_power	6
15	Bilbo	magic_power	4
16	Sam	magic_power	2
17	Pippin	magic_power	0
18	Boromir	magic_power	0
19	Aragorn	magic_power	2
20	Galadriel	magic_power	9
21	Meriadoc	magic_power	0

And we can use the *pivot* method to re-pivot the data, defining which field identifies the data to be grouped together, which column contains the new column headers, and which field contains the data.

```

pivoted = unpivoted.pivot(index='names', columns='variable', values='value')
print (pivoted_2)

```

OUT:

	variable	magic_power	type
names			
Aragorn		2	Man

Bilbo	4	Hobbit
Boromir	0	Man
Frodo	4	Hobbit
Galadriel	9	Elf
Gandolf	10	Wizard
Gimli	1	Dwarf
Legolas	6	Elf
Meriadoc	0	Hobbit
Pippin	0	Hobbit
Sam	2	Hobbit

2.15 Subgrouping data in Pandas with groupby

A very powerful feature in Pandas is to use groupby to create groups of data. Each group may then be further acted on as if it were an independent dataframe. This allows for very sophisticated operations broken down by group.

Here we will create a very simple example to illustrate this.

Let's create our usual dataframe:

```
import pandas as pd
df = pd.DataFrame()

names = ['Gandolf',
         'Gimli',
         'Frodo',
         'Legolas',
         'Bilbo',
         'Sam',
         'Pippin',
         'Boromir',
         'Aragorn',
         'Galadriel',
         'Meriadoc']
types = ['Wizard',
        'Dwarf',
        'Hobbit',
        'Elf',
        'Hobbit',
        'Hobbit',
        'Hobbit',
        'Hobbit',
        'Man',
        'Man',
        'Elf',
        'Hobbit']
magic = [10, 1, 4, 6, 4, 2, 0, 0, 2, 9, 0]
aggression = [7, 10, 2, 5, 1, 6, 3, 8, 7, 2, 4]
stealth = [8, 2, 5, 10, 5, 4, 5, 3, 9, 10, 6]

df['names'] = names
df['type'] = types
df['magic_power'] = magic
df['aggression'] = aggression
df['stealth'] = stealth
```

And now we will create an object 'groups' that allows us to work on those groups individually. We will group just by one parameter (type), but the groups can combine more parameters (each group produced will have identical values for the parameters used for the grouping).

We create an 'iterable' object (an object that can be stepped through using groupby. We can step through members of that new groupby object. Each member has an index and a dataframe of data.

Lets just print out the index and the data for each group.

```
groups = df.groupby('type') # creates a new object of groups of data
for index, group_df in groups: # each group has an index and a dataframe of data
    print ('group index:', index)
    print ('\nData')
    print (group_df)
```

OUT:

group index: Dwarf

Data

	names	type	magic_power	aggression	stealth
1	Gimli	Dwarf	1	10	2

group index: Elf

Data

	names	type	magic_power	aggression	stealth
3	Legolas	Elf	6	5	10
9	Galadriel	Elf	9	2	10

group index: Hobbit

Data

	names	type	magic_power	aggression	stealth
2	Frodo	Hobbit	4	2	5
4	Bilbo	Hobbit	4	1	5
5	Sam	Hobbit	2	6	4
6	Pippin	Hobbit	0	3	5
10	Meriadoc	Hobbit	0	4	6

group index: Man

Data

	names	type	magic_power	aggression	stealth
7	Boromir	Man	0	8	3
8	Aragorn	Man	2	7	9

group index: Wizard

Data

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8

See what happened? We created six smaller dataframes, each of which was one group of the original data. We can then perform any amount of code in each of those sections. As an example, below is some code for a rather crazy method that extracts the third member of the group, but if there are fewer than three members of the group it will take the highest member that it can (the last).

```
col_names = list(df) # get column names from existing dataframe
groups = df.groupby('type') # creates a new object of groups of data
output_df = pd.DataFrame(columns = col_names) # create empty dataframe to store new data
```

```
for index, group_df in groups: # each group has an index and a dataframe of data
    number_of_members = len(group_df)
    get_index = min (3, number_of_members)
    get_index -= 1 # subtract 1 to correct for zero-indexing
    retrieved_data = group_df.iloc[get_index].values
    output_df.loc[index] = retrieved_data
```

```
print (output_df)
```

OUT:

	names	type	magic_power	aggression	stealth
Dwarf	Gimli	Dwarf	1	10	2
Elf	Galadriel	Elf	9	2	10
Hobbit	Sam	Hobbit	2	6	4
Man	Aragorn	Man	2	7	9
Wizard	Gandolf	Wizard	10	7	8

2.16 Iterating through columns and rows in NumPy and Pandas

Using *apply_along_axis* (NumPy) or *apply* (Pandas) is a more Pythonic way of iterating through data in NumPy and Pandas. But there may be occasions you wish to simply work your way through rows or columns in NumPy and Pandas. Here is how it is done.

2.16.1 NumPy

NumPy is set up to iterate through rows when a loop is declared.

```
import numpy as np

# Create an array of random numbers (3 rows, 5 columns)
array = np.random.randint(0,100,size=(3,5))

print ('Array:')
print (array)
print ('\nAverage of rows:')

# iterate through rows:
for row in array:
    print (row.mean())
```

OUT:

```
Array:
[[12 40 30 93 99]
 [62 85 89 26 17]
 [93 34 67 59 56]]
```

```
Average of rows:
54.8
55.8
61.8
```

To iterate through columns we transpose the array with `.T` so that rows become columns (and vice versa):

```
print('\nTranposed array:')
print (array.T)
print ('\nAverage of original columns:')

for row_t in array.T:
    print (row_t.mean())
```

```
Transposed array:
[[12 62 93]
 [40 85 34]
 [30 89 67]
 [93 26 59]
 [99 17 56]]
```

```
Average of original columns:
55.666666666666664
53.0
62.0
```

```
59.333333333333336
57.333333333333336
```

2.16.2 Pandas

Lets first create our data:

```
import pandas as pd
df = pd.DataFrame()

names = ['Gandolf',
         'Gimli',
         'Frodo',
         'Legolas',
         'Bilbo',
         'Sam',
         'Pippin',
         'Boromir',
         'Aragorn',
         'Galadriel',
         'Meriadoc']
types = ['Wizard',
        'Dwarf',
        'Hobbit',
        'Elf',
        'Hobbit',
        'Hobbit',
        'Hobbit',
        'Hobbit',
        'Man',
        'Man',
        'Elf',
        'Hobbit']
magic = [10, 1, 4, 6, 4, 2, 0, 0, 2, 9, 0]
aggression = [7, 10, 2, 5, 1, 6, 3, 8, 7, 2, 4]
stealth = [8, 2, 5, 10, 5, 4, 5, 3, 9, 10, 6]

df['names'] = names
df['type'] = types
df['magic_power'] = magic
df['aggression'] = aggression
df['stealth'] = stealth
```

To iterate throw rows in a Pandas dataframe we use `.iterrows()`:

```
for index, row in df.iterrows():
    print(row[0], 'is a', row[1])
```

OUT:

```
Gandolf is a Wizard
Gimli is a Dwarf
Frodo is a Hobbit
Legolas is a Elf
Bilbo is a Hobbit
Sam is a Hobbit
Pippin is a Hobbit
Boromir is a Man
Aragorn is a Man
Galadriel is a Elf
```

Meriadoc is a Hobbit

To iterate through columns we need to do just a bit more manual work, creating a list of dataframe columns and then iterating through that list to pull out the dataframe columns:

```
columns = list(df)
for column in columns:
    print (df[column][2]) # print the third element of the column
```

OUT:

```
Frodo
Hobbit
4
2
5
```

2.17 Removing duplicate data in NumPy and Pandas

Both NumPy and Pandas offer easy ways of removing duplicate rows. Pandas offers a more powerful approach if you wish to remove rows that are partly duplicated.

2.17.1 NumPy

With numpy we use *np.unique()* to remove duplicate rows or columns (use the argument *axis=0* for unique rows or *axis=1* for unique columns).

```
import numpy as np

array = np.array([[1,2,3,4],
                  [1,2,3,4],
                  [5,6,7,8],
                  [1,2,3,4],
                  [3,3,3,3],
                  [5,6,7,8]])

unique = np.unique(array, axis=0)
print (unique)
```

OUT:

```
[[1 2 3 4]
 [3 3 3 3]
 [5 6 7 8]]
```

We can return the index values of the kept rows with the argument *return_index=True* (the argument *return_inverse=True* would return the discarded rows):

```
array = np.array([[1,2,3,4],
                  [1,2,3,4],
                  [5,6,7,8],
                  [1,2,3,4],
                  [3,3,3,3],
                  [5,6,7,8]])

unique, index = np.unique(array, axis=0, return_index=True)
print ('Unique rows:')
print (unique)
print ('\nIndex of kept rows:')
print (index)
```

OUT:

```
Unique rows:
[[1 2 3 4]
 [3 3 3 3]
 [5 6 7 8]]
```

```
Index of kept rows:
[0 4 2]
```

We can also count the number of times a row is repeated with the argument *return_counts=True*:

```
array = np.array([[1,2,3,4],
                  [1,2,3,4],
                  [5,6,7,8],
                  [1,2,3,4],
```

```

        [3,3,3,3],
        [5,6,7,8]])

unique, index, count = np.unique(array, axis=0,
                                return_index=True,
                                return_counts=True)

print ('Unique rows:')
print (unique)
print ('\nIndex of kept rows:')
print (index)
print ('\nCount of duplicate rows')
print (count)

```

OUT:

```

Unique rows:
[[1 2 3 4]
 [3 3 3 3]
 [5 6 7 8]]

```

```

Index of kept rows:
[0 4 2]

```

```

Count of duplicate rows
[3 1 2]

```

2.17.2 Pandas

With Pandas we use *drop_duplicates*.

```

import pandas as pd
df = pd.DataFrame()

names = ['Gandolf','Gimli','Frodo', 'Gimli', 'Gimli']
types = ['Wizard','Dwarf','Hobbit', 'Dwarf', 'Dwarf']
magic = [10, 1, 4, 1, 3]
aggression = [7, 10, 2, 10, 2]
stealth = [8, 2, 5, 2, 5]

```

```

df['names'] = names
df['type'] = types
df['magic_power'] = magic
df['aggression'] = aggression
df['stealth'] = stealth

```

Let's remove duplicated rows:

```

df_copy = df.copy() # we'll work on a copy of the dataframe
df_copy.drop_duplicates(inplace=True)
print (df_copy)

```

OUT:

```

df_copy = df.copy() # we'll work on a copy of the dataframe

df_copy.drop_duplicates(subset=['names','type'], inplace=True)

```

```
print (df_copy)
```

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8
1	Gimli	Dwarf	1	10	2
2	Frodo	Hobbit	4	2	5

We can choose to keep the last entered row with the argument *keep='last'*:

```
df_copy = df.copy() # we'll work on a copy of the dataframe
df_copy.drop_duplicates(subset=['names','type'], inplace=True, keep='last')
print (df_copy)
```

OUT:

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8
2	Frodo	Hobbit	4	2	5
4	Gimli	Dwarf	3	2	5

We can also remove all duplicate rows by using the argument *keep=False*:

```
df_copy = df.copy() # we'll work on a copy of the dataframe
df_copy.drop_duplicates(subset=['names','type'], inplace=True, keep=False)
print (df_copy)
```

OUT:

	names	type	magic_power	aggression	stealth
0	Gandolf	Wizard	10	7	8
2	Frodo	Hobbit	4	2	5

More complicated logic for choosing which record to keep would best be performed using a groupby method.

2.18 Setting width and number of decimal places in NumPy print output

The function below may be used to set both the number of decimal places and the fixed width of NumPy print out. If no width is given it defaults to zero (no extra padding added). Setting width will ensure alignment of output.

```
import numpy as np

# We can set NumPy to print to a fixed number of decimal places:
# e.g. the 8 decimal places that are standard, with no set width

np.set_printoptions(formatter={'float': lambda x: "{0:0.8f}".format(x)})

# Or to make things more flexible/clearer in the code we can set up a function.
# This function will define both fixed width and decimal placed/
# If no width is given it will default to zero, with no extra spacing added

def set_numpy_decimal_places(places, width=0):
    set_np = '{0:' + str(width) + '.' + str(places) + 'f}'
    np.set_printoptions(formatter={'float': lambda x: set_np.format(x)})
```

Let's generate some random number data:

```
x = np.random.rand(3,3)
```

The array as originally printed:

```
print (x)
```

OUT:

```
[[0.50873497 0.60515928 0.41612647]
 [0.56755605 0.58378952 0.11467147]
 [0.49378493 0.99466011 0.70781679]]
```

Setting the number of decimal places:

```
set_numpy_decimal_places(3)
print (x)
```

OUT:

```
set_numpy_decimal_places(3)
```

```
print (x)
```

```
[[0.509 0.605 0.416]
 [0.568 0.584 0.115]
 [0.494 0.995 0.708]]
```

Setting the number of decimal places and a fixed width:

```
set_numpy_decimal_places(3, 6)
print (x)
```

OUT:

```
set_numpy_decimal_places(3, 6)
```

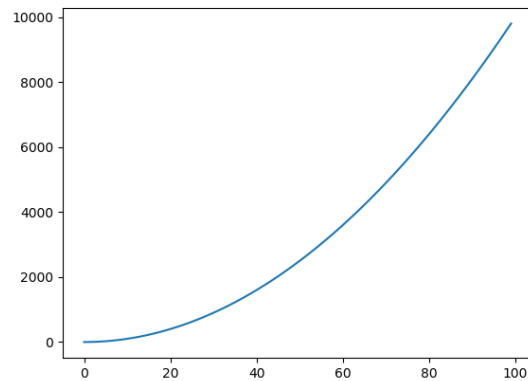
```
print (x)
```

```
[[ 0.509  0.605  0.416]
 [ 0.568  0.584  0.115]
 [ 0.494  0.995  0.708]]
```

Chapter 3

Matplotlib for charting

Figure 3.1: A simple xy line chart



3.1 Simple xy line charts, and simple save to file

Matplotlib is a powerful library for plotting data. Data may be in the form of lists, or data from NumPy and Pandas may be used directly. Charts are very highly configurable, but here we'll focus on the key basics first.

A useful resource for matplotlib is a gallery of charts with associated code: <https://matplotlib.org/gallery.html>

3.1.1 Plotting a single line

The following code plots a simple line plot and saves the file in png format. Other formats may be used (e.g. jpg), but png offers an open source high quality format which is ideal for charts.

```
import matplotlib.pyplot as plt

# The following line is only needed to display chart in Jupyter notebooks
%matplotlib inline

X=range(100)
Y=[value ** 2 for value in X] # (A list comprehension)

plt.plot(X,Y)
plt.show()
plt.savefig('plot_01.png') # optional save as png file
```

3.1.2 Plotting two lines

To plot two lines we simply add another plot before generating the chart with `plt.show()`

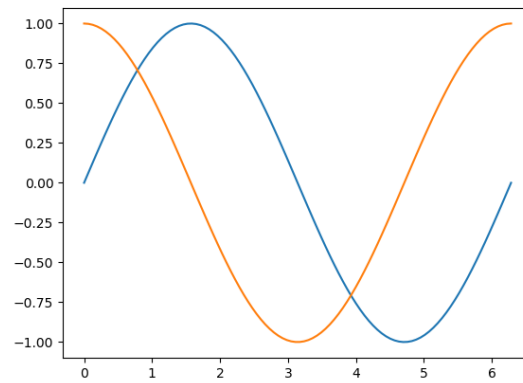
```
import numpy as np

import matplotlib.pyplot as plt

# The following line is only needed to display chart in Jupyter notebooks
%matplotlib inline

# np.linspace creates an array of equally spaced numbers
X=np.linspace(0,2*np.pi,100) # 100 points between 0 and 2*pi
```

Figure 3.2: A simple xy line chart with two lines



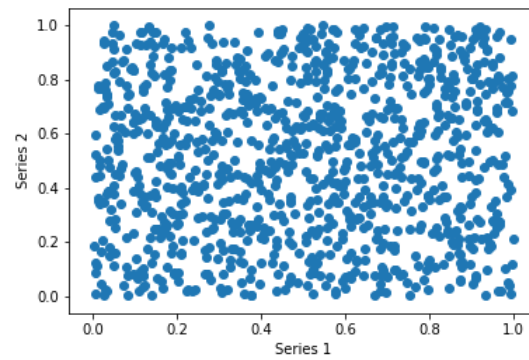
```
Ya=np.sin(X)
Yb=np.cos(X)

plt.plot(X,Ya)
plt.plot(X,Yb)
plt.show()
```

3.1.3 Saving figures

To save a figure use `plt.savefig('my_figname.png')` before `plt.show()` to save as png format (best for figures, but you can also use jpg or tif).

Figure 3.3: A scatter plot



3.2 Scatter plot, and labelling axes

```
import matplotlib.pyplot as plt
import numpy as np

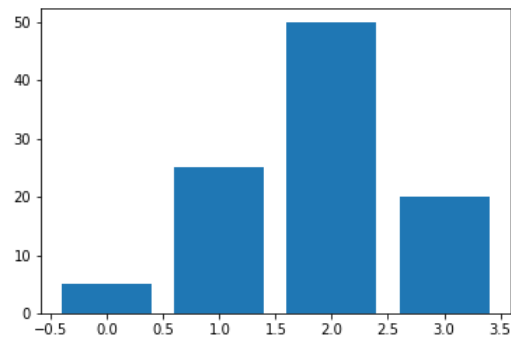
# Create a 1024 by 2 array of random points
data=np.random.rand(1024,2)

x = data[:,0]
y = data[:,1]
plt.scatter(x, y)

plt.xlabel ('Series 1')
plt.ylabel ('Series 2')

plt.show()
```

Figure 3.4: A simple bar chart



3.3 Bar charts

3.3.1 A simple bar chart

```
import matplotlib.pyplot as plt
import numpy as np

import matplotlib.pyplot as plt
import numpy as np

data =[5.,25.,50.,20.]
x = range(len(data)) # creates a range of 0 to 4

plt.bar(x, data)

plt.show()
```

3.3.2 Multiple series

```
import matplotlib.pyplot as plt
import numpy as np

data =[[5.,25.,50.,20],
       [4.,23.,51.,17],
       [6., 22.,52.,19]]

X=np.arange(4)

plt.bar(X+0.00,data[0],color='b',width=0.25) # colour is blue
plt.bar(X+0.25,data[1],color='g',width=0.25) # colour is green
plt.bar(X+0.50,data[2],color='r',width=0.25) # colour is red

plt.show()
```

For larger data sets we could automate the creation of the bars:

```
import matplotlib.pyplot as plt
import numpy as np

data =[[5.,25.,50.,20],
       [4.,23.,51.,17],
       [6., 22.,52.,19]]
```

Figure 3.5: A multiple series bar chart

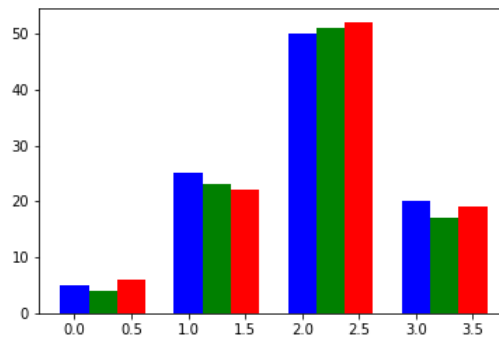
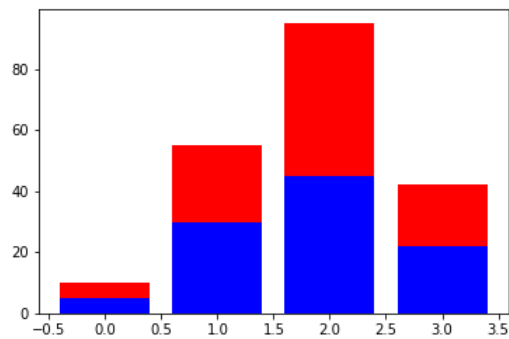


Figure 3.6: A stacked bar chart



```
color_list=['b','g','r']
gap=0.8/len(data)

for i, row in enumerate(data): # creates int i and list row
    X=np.arange(len(row))
    plt.bar(X+i*gap,row,width=gap,color=color_list[i])
plt.show()
```

3.3.3 Stacked bar chart

```
a=[5.,30.,45.,22.]
b=[5.,25.,50.,20.]
x=range(4)

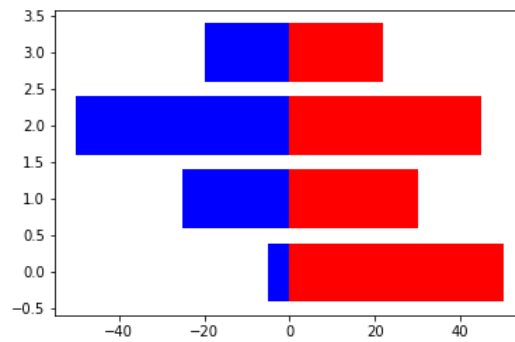
plt.bar(x,a,color='b')
plt.bar(x,b,color='r',bottom=a) # bottom specifies the starting position for a bar

plt.show()
```

3.3.4 Back to back bar chart

```
women_pop=np.array([50,30,45,22])
men_pop=np.array([5,25,50,20])
x=np.arange(4)
```

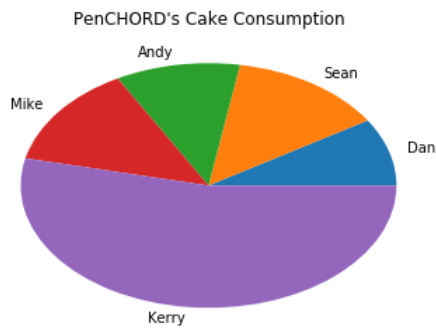
Figure 3.7: A back to back bar chart



```
plt.barh(x,women_pop,color='r')
plt.barh(x,-men_pop,color='b') # the minus sign creates an opposite bar

plt.show()
```

Figure 3.8: A pie chart



3.4 Pie charts, and adding a title

3.4.1 A simple bar chart

As with all matplotlib charts, pie charts are highly configurable. Here we just show the simplest of pie charts.

```
import matplotlib.pyplot as plt

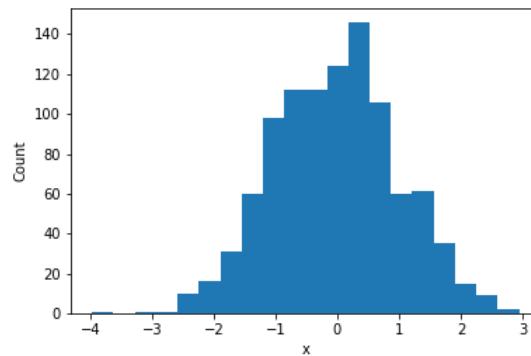
labels = 'Dan','Sean','Andy','Mike','Kerry'

cake_consumption = [10, 15, 12, 30, 100]

plt.pie(cake_consumption, labels=labels)
plt.title ("PenCHORD's Cake Consumption")

plt.show()
```

Figure 3.9: A histogram with defined number of bins



3.5 Plotting histograms with matplotlib and NumPy

Matplotlib has an easy method for plotting data. NumPy has an easy method for obtaining histogram data.

3.5.1 Plotting histograms with Matplotlib

Plotting a histogram with a defined number of bins:

```
import matplotlib.pyplot as plt
import numpy as np

%matplotlib inline

x=np.random.randn(1000) # samples from a normal distribution

plt.hist(x,bins=20)
plt.title ('Defined number of bins')
plt.xlabel ('x')
plt.ylabel ('Count')

plt.show()
```

Plotting a histogram with a defined range of bins:

```
x=np.random.randn(1000) # samples from a normal distribution

# Use np.arange to create bins from -4 to +4 in steps of 0.5
# A custom list could also be used

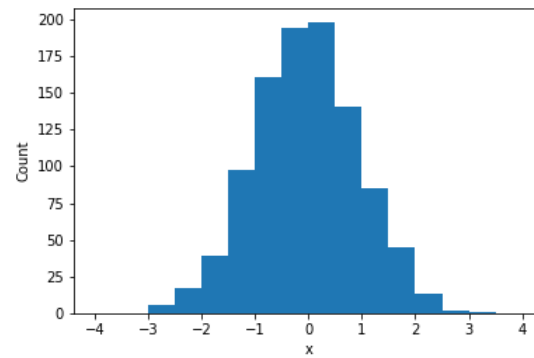
plt.hist(x,bins=np.arange(-4,4.5,0.5))
plt.title ('Defined bin range and width')
plt.xlabel ('x')
plt.ylabel ('Count')

plt.show()
```

3.5.2 Obtaining histogram data with NumPy

If histogram data is needed in addition to, or instead of, a plot, NumPy may be used. Here a defined number of bins is used:

Figure 3.10: A histogram with defined bin range and width



```
import numpy as np
count, bins = np.histogram(x, bins=20)
print ('Bins:')
print (bins)
print ('\nCount:')
print (count)
```

OUT:

```
Bins:
[-2.88652288 -2.57566476 -2.26480664 -1.95394852 -1.6430904  -1.33223228
 -1.02137416 -0.71051604 -0.39965792 -0.0887998   0.22205832  0.53291644
  0.84377456  1.15463268  1.4654908   1.77634892  2.08720704  2.39806516
  2.70892328  3.0197814   3.33063952]
```

```
Count:
[  5   9  12  22  32  69  80 113 125 116 108  94  77  59  40  22  10   4
  1   2]
```

And here a defined bin range is used.

```
import numpy as np
count, bins = np.histogram(x, bins=np.arange(-5,6,1))
print ('Bins:')
print (bins)
print ('\nCount:')
print (count)
```

OUT:

```
Bins:
[-5 -4 -3 -2 -1  0  1  2  3  4  5]
```

```
Count:
[  0  0  20 134 332 340 154  18   2   0]
```

Figure 3.11: A simple boxplot

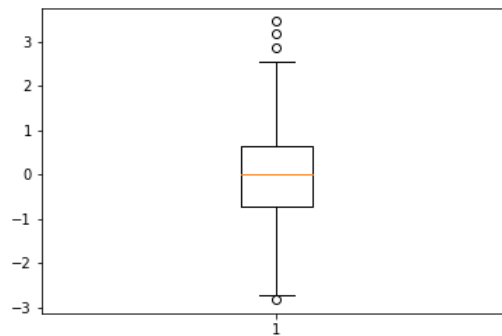
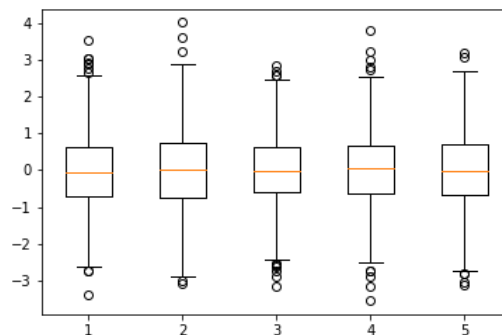


Figure 3.12: A grouped boxplot from a single NumPy array



3.6 Boxplots

Matplotlib allows easy creation of boxplots. These traditionally show median (middle line across box), upper and lower quartiles (box), range excluding outliers (whiskers) and outliers (points). The default setting for outliers is points more than $1.5 \times \text{IQR}$ above or below the quartiles.

*IQR = inter-quartile range.

```
import matplotlib.pyplot as plt
import numpy as np
```

```
x=np.random.randn(500) # samples from a normal distribution
```

```
plt.boxplot(x)
```

```
plt.show()
```

3.6.1 Plotting groups

Boxplot can take data from multiple columns in a NumPy array.

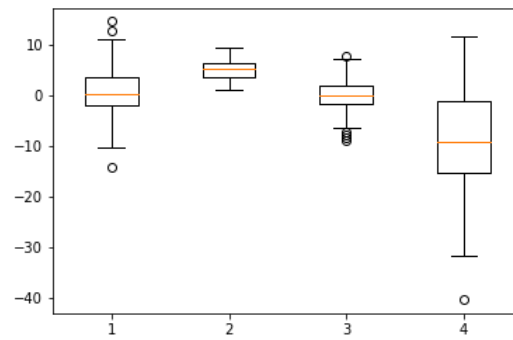
```
x=np.random.randn(1000,5) # samples from a normal distribution
```

```
plt.boxplot(x)
```

```
plt.show()
```

Or data may come from separate sources:

Figure 3.13: A grouped boxplot from multiple sources



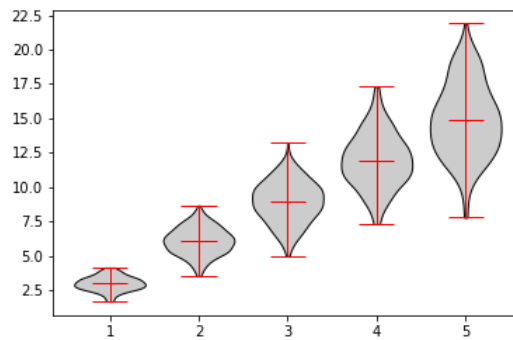
```
x1=list(np.random.randn(100)*5)
x2=list((np.random.randn(50)*2)+5)
x3=list(np.random.randn(250)*3)
x4=list((np.random.randn(70)*10)-10)

x=[x1,x2,x3,x4]

plt.boxplot(x)

plt.show()
```

Figure 3.14: Violin plot



3.7 Violin plots

Violin plots are an alternative to box plots. They show the spread of data in the form of a distribution plot along the y axis. Some people love them. Others don't! See what you think.

```
import numpy as np
import matplotlib.pyplot as plt

%matplotlib inline

n_violins = 5
groups = np.arange(1,n_violins+1)

# Use Python list comprehension to build distributions
# Mean is i (group #), standard deviation is 0.5 * i
samples = [np.random.normal(3*i,0.5*i,250) for i in groups]

violins = plt.violinplot (samples,
                           groups,
                           points=300, # the more the smoother
                           widths=0.8,
                           showmeans=False,
                           showextrema=True,
                           showmedians=True)

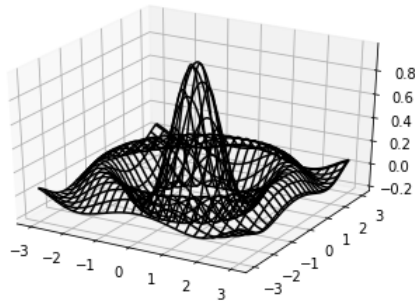
# Change the bodies to grey

for v in violins['bodies']:
    v.set_facecolor('0.8')
    v.set_edgecolor('k')
    v.set_linewidth(1)
    v.set_alpha(1)

# Make all the violin statistics marks red:
for partname in ('cbars','cmins','cmaxes','cmedians'):
    vp = violins[partname]
    vp.set_edgecolor('r')
    vp.set_linewidth(1)

plt.show()
```

Figure 3.15: A 3D wireframe



3.8 3D wireframe and surface plots

We can create 3D wireframe or surface plots easily in Matplotlib

3.8.1 Wireframe

```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm

# Create a 3D array
# meshgrid produces all combinations of given x and y
x=np.linspace(-3,3,256) # x goes from -3 to 3, with 256 steps
y=np.linspace(-3,3,256) # y goes from -3 to 3, with 256 steps
X,Y=np.meshgrid(x,y) # combine all x with all y

# A function of x and y for demo purposes
Z=np.sinc(np.sqrt(X**2 + Y**2))

fig=plt.figure()
ax=fig.gca(projection='3d')

# rstride: Array row stride (step size), defaults to 1
# cstride: Array column stride (step size), defaults to 1
# rcount: Use at most this many rows, defaults to 50
# ccount: Use at most this many columns, defaults to 50

ax.plot_wireframe(X,Y,Z,color='k',rcount=25,ccount=25)

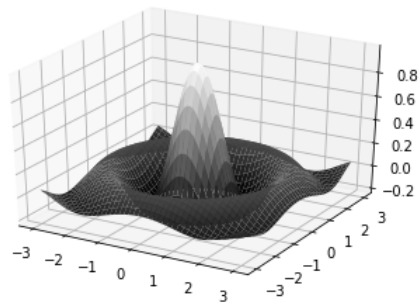
plt.show()
```

3.8.2 Surface

```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib import cm

# Create a 3D array
```

Figure 3.16: A 3D surface plot



```
# meshgrid produces all combinations of given x and y
x=np.linspace(-3,3,256) # x goes from -3 to 3, with 256 steps
y=np.linspace(-3,3,256) # y goes from -3 to 3, with 256 steps
X,Y=np.meshgrid(x,y) # combine all x with all y

# A function of x and y for demo purposes
Z=np.sinc(np.sqrt(X**2 + Y**2))

fig=plt.figure()
ax=fig.gca(projection='3d')
ax.plot_surface(X,Y,Z,cmap=cm.gray)

plt.show()}
```

3.9 Common modifications to charts

Here we show some common modifications to charts. These include:

- Changing scatter plot point style
- Changing line plot line and marker style
- Adding a legend
- Adding some text
- Changing axis scales
- Changing axis ticks
- Adding a grid
- Adding axis tiles
- Adding chart title

```
import matplotlib.pyplot as plt
import numpy as np
import matplotlib.ticker as ticker

data=np.random.rand(100,2)

# To give us maximum control over axes we set up the figure in this way:

ax1 = plt.figure().add_subplot(111)

# Add scatter plot
# Adjust scatter plot points by shape (marker), size (s),
# color, and edgcolour. Add a label for legend.

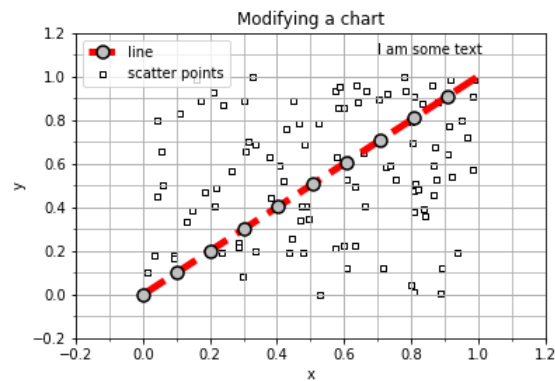
ax1.scatter(data[:,0],data[:,1],
            marker='s',
            s = 20,
            color = 'w',
            edgecolors = 'k',
            label = 'scatter points')

x = np.linspace(0,1,100)
y = np.linspace(0,1,100)

# Add line plot
# Adjust line for colour, style, and width, and marker
# shape, frequency, and coloring. Colours may be given by letter
# or by a number between '0.0' (black) and '1.0' (white)
# Add a label for legend.

ax1.plot(x,y,
        color = 'r',
        linestyle = '--',
        linewidth = 5,
        marker = 'o',
        markevery = 10,
        markersize=9,
        markeredgewidth=1.5,
        markerfacecolor='0.75',
        markeredgewidth='k',
        label = 'line')
```

Figure 3.17: A modified chart



```
# Adjust axes limits

ax1.set_xlim(-0.2,1.2)
ax1.set_ylim(-0.2,1.2)

# Adjust axes tickmarks

ax1.xaxis.set_major_locator(ticker.MultipleLocator(0.2))
ax1.xaxis.set_minor_locator(ticker.MultipleLocator(0.1))
ax1.yaxis.set_major_locator(ticker.MultipleLocator(0.2))
ax1.yaxis.set_minor_locator(ticker.MultipleLocator(0.1))

# Add a grid

ax1.grid(True, which='both') # which may be major, minor or both

# Add axis titles

ax1.set_xlabel('x', size = 15)
ax1.set_ylabel('y', size = 15)
# Add a title

ax1.set_title('Modifying a chart', size = 20)

# Add some text at a given position

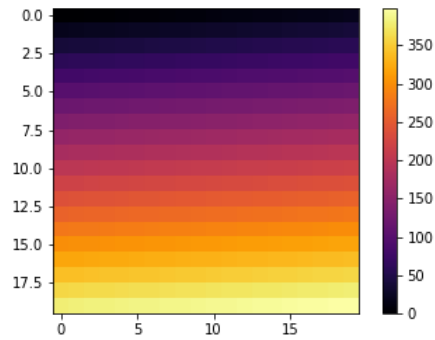
plt.text(0.7,1.1,'I am some text')

# Add the legend

ax1.legend() # see help (plt.legend) for options

plt.show()
```

Figure 3.18: A simple heat map



3.10 A simple heatmap

Heatmaps may be generated with *imshow*.

We import a colour map from the library *cm*.

For a list of colour maps available see: https://matplotlib.org/examples/color/colormaps_reference.html

```
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import cm # This allows different color schemes

# Generate an array of increasing values
a=np.arange(0,400)
a = a.reshape(20,20)

# Plot the heatmap using 'inferno' from the cm colour schemes

plt.imshow(a,interpolation='nearest', cmap=cm.inferno)

# Add a scale bar

plt.colorbar()

plt.show()
```

3.11 Adding contour lines to a heat map

Here we will add contour lines to a heat map.

We'll use something a little more interesting for the array of values, we'll define a Mandelbrot fractal function. We have build a 1,000 and 1,000 array and calculate z as a Mandelbrot function of x and y.

The heatmap is drawn with *plt.imshow*, and then contour lines are added with *plt.contour*.

See if you can follow how the arrays are built up, and the Mandelbrot function used to calculate Z, but the main purpose is to demonstrate adding contour lines to a heat map.

The Mandelbrot function may take up to 30 seconds to calculate (maybe longer on an old computer).

```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.cm as cm

%matplotlib inline

# Mandelbrot function - a fractal

def iter_count(c,max_iter):
    x=c
    for n in range(max_iter):
        if abs(x)>2:
            return (n)
        x=x**2+c
    return (max_iter)

# Build a 512 * 512 array of x, y

n=1000
max_iter=75
# xmin,xmax,ymin,ymax = -0.32,0,0.8,0.1
xmin,xmax,ymin,ymax = -0.32,0.1,0.7,1.1
x_series=np.linspace(xmin,xmax,n)
y_series=np.linspace(ymin,ymax,n)

# Create an empty array for z (which will be calculated from all x and y)

z=np.empty((n,n))

# Calculate z based on the Mandelbrot function

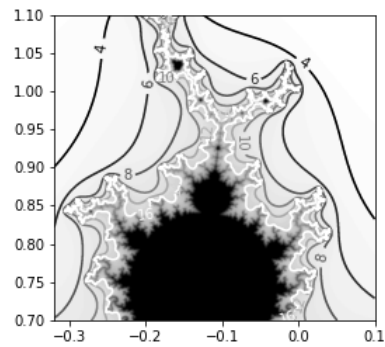
for i,y in enumerate(y_series):
    for j,x in enumerate(x_series):
        z[i,j]=iter_count(complex(x,y),max_iter)

# THE CHART

# Show a grey scale heatmap with imshow

plt.imshow(z,
            cmap=cm.binary,
            interpolation='bicubic',
            origin='lower',
            extent=(xmin,xmax,ymin,ymax))
```

Figure 3.19: Adding contour lines to a heatmap



```
# Extent (above) defines the axes values which are not held in the
# results array (z) itself

# Add contours

levels=[2, 4, 6, 8, 10, 12, 14, 16] # Define levels

ct=plt.contour(x_series,y_series,z,levels,cmap=cm.gray)

# Add contour labels

plt.clabel(ct,fmt='%d')

plt.show()
```

3.12 Creating a grid of subplots

There are various ways of creating subplots in Matplotlib.

Here we will use `add_subplot` to bring four plots together.

It is also worth looking at *subplot2grid* if you want plots of different sizes brought together.

```
import numpy as np
import matplotlib.pyplot as plt

%matplotlib inline

# Define the size of the overall figure
fig = plt.figure(figsize=(8,8)) # 8 inch * 8 inch

# Create subplot 1

ax1 = fig.add_subplot(221) # Grid of 2x2, this is subplot 1

x=range(100)
y=[value ** 2 for value in x]

ax1.plot(x,y)

ax1.set_xlabel('x')
ax1.set_ylabel('x squared')
ax1.set_title('Subplot 1: A line chart')

# Create subplot 2

ax2 = fig.add_subplot(222) # Grid of 2x2, this is subplot 2

data=np.random.rand(1024,2)

ax2.scatter(data[:,0],data[:,1])

ax2.set_xlabel('x')
ax2.set_ylabel('y')
ax2.set_title('Subplot 2: A Scatter plot')

# Create subplot 3

ax3 = fig.add_subplot(223) # Grid of 2x2, this is subplot 3

data=[5.,25.,50.,20.]

ax3.bar(range(len(data)),data)

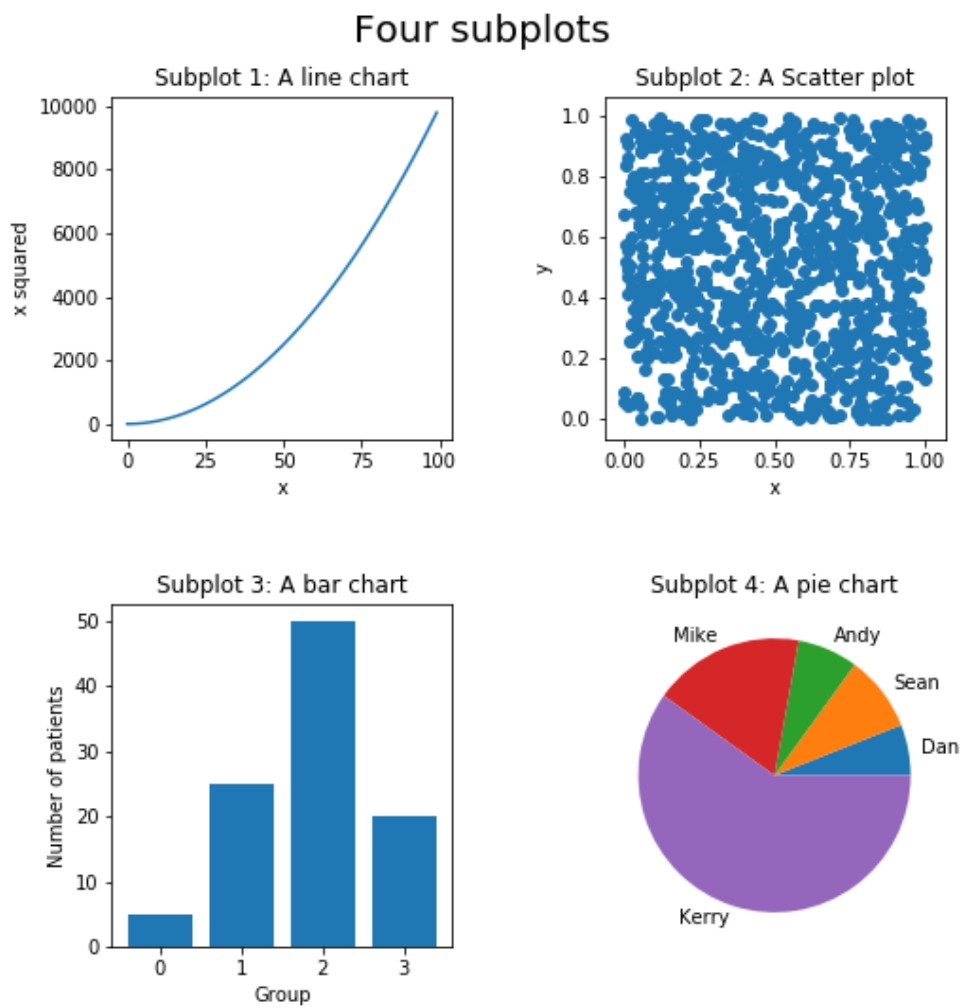
ax3.set_xlabel('Group')
ax3.set_ylabel('Number of patients')
ax3.set_title('Subplot 3: A bar chart')

# Create subplot 4

ax4 = fig.add_subplot(224) # Grid of 2x2, this is subplot 4

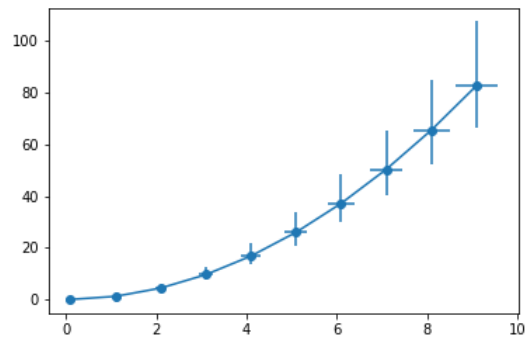
labels = 'Dan','Sean','Andy','Mike','Kerry'
cake_consumption = [10, 15, 12, 30, 100]
```

Figure 3.20: Creating a grid of subplots



```
ax4.pie(cake_consumption, labels=labels)
ax4.set_title("Subplot 4: A pie chart")
# Add an overall title
plt.suptitle('Four subplots', size = 20)
# Adjust the spacing between plots
plt.tight_layout(pad=4)
# Show plot
plt.show()
```


Figure 3.21: Error bars on a line chart



3.13 Adding error bars to charts

3.13.1 Adding error bars to line plots

```
import numpy as np
import matplotlib.pyplot as plt

%matplotlib inline

# example data
x = np.arange(0.1, 10, 1)
y = x ** 2

# calculate example errors (could also be from list or NumPy array)
lower_y_error = y * 0.2
upper_y_error = y * 0.3
y_error = [lower_y_error, upper_y_error]
lower_x_error = x * 0.05
upper_x_error = x * 0.05
x_error = [lower_x_error, upper_x_error]

# To use only x or y errors simple omit the relevant argument

plt.errorbar(x, y, yerr = y_error, xerr = x_error, fmt='-o')

plt.show()
```

3.13.2 Adding error bars to bar charts

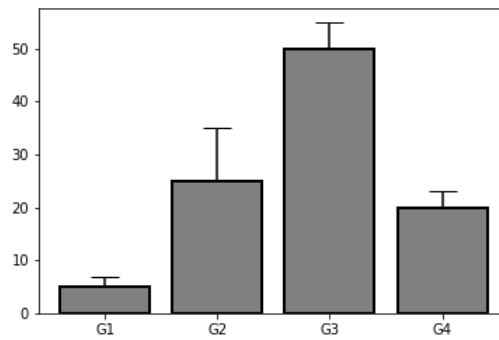
```
import matplotlib.pyplot as plt
import numpy as np

%matplotlib inline

x=[1,2,3,4]
y=[5.,25.,50.,20.]
yerr_upper=[2,10,5,3]
yerr_lower=np.zeros(len(yerr_upper))

fig, ax = plt.subplots()
ax.bar(x,y,
```

Figure 3.22: Error bars on a barchart

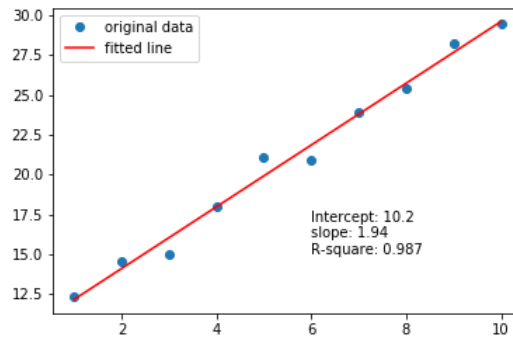


```
width=0.8,  
color='0.5',  
edgecolor='k',  
yerr=[yerr_lower,yerr_upper],  
linewidth = 2,  
capsize=10)  
  
ax.set_xticks(x)  
ax.set_xticklabels(('G1', 'G2', 'G3', 'G4'))  
  
plt.savefig('plot_21.png')  
  
plt.show()
```

Chapter 4

Statistics

Figure 4.1: Linear regression with scipy.stats



4.1 Linear regression with scipy.stats

```
%matplotlib inline

import numpy as np
import matplotlib.pyplot as plt
from scipy import stats

# Set up x any arrays

x=np.array([1,2,3,4,5,6,7,8,9,10])
y=np.array([2.3,4.5,5.0,8,11.1,10.9,13.9,15.4,18.2,19.5])
y=y+10

# scipy linear regression

gradient, intercept, r_value, p_value, std_err = stats.linregress(x,y)

# Calculated fitted y

y_fit=intercept + (x*gradient)

# Plot data

plt.plot(x, y, 'o', label='original data')
plt.plot(x, y_fit, 'r', label='fitted line')

# Add text box and legend

text='Intercept: %.1f\nslope: %.2f\nR-square: %.3f' %(intercept,gradient,r_value**2)
plt.text(6,15,text)
plt.legend()

# Display plot

plt.show()
```

4.2 One sample t-test and Wilcoxon signed rank test

The following test for a difference between the centre of a sample of data and a given reference point. The one sample t-test assumes normally distributed data, whereas the Wilcoxon signed rank test can be used with any data.

4.2.1 One sample t-test

```
import numpy as np
import scipy.stats as stats

# generate the data
normDist = stats.norm(loc=7.5, scale=3)
data = normDist.rvs(100)

# Define a value to check against
checkVal = 6.5

# T-test
# --- >>> START stats <<< ---
t, tProb = stats.ttest_1samp(data, checkVal)
# --- >>> STOP stats <<< ---

print ('P value:')
print (tProb)
```

OUT:

```
P value:
0.007269398564245046
```

4.2.2 Wilcoxon signed rank test

```
# Note the test value is subtracted from all data (test is then effectively against zero)

rank, pVal = stats.wilcoxon(data-checkVal)

print ('P value:')
print (pVal)
```

OUT:

```
P value:
0.006010251964988403
```

4.3 t-tests for testing the difference between two groups of data

t-tests are ideally suited to groups of data that are normally distributed.

4.3.1 Unpaired t-test

Statistical test for testing the difference between independent groups (e.g. measure the weight of men and women).

```
import numpy as np
import scipy.stats as stats

# Create two random groups of data with a mean difference of 1

mu, sigma = 10, 2.5 # mean and standard deviation
group1 = np.random.normal(mu, sigma, 50)

mu, sigma = 11, 2.5 # mean and standard deviation
group2 = np.random.normal(mu, sigma, 50)

# Calculate t and probability of a difference

t_statistic, p_value = stats.ttest_ind(group1, group2)

# Print results

print ('P value:')
print (p_value)

OUT:

P value:
0.030724260024008986
```

4.3.2 Paired t-test

Statistical test for testing the difference between paired samples (e.g. measuring the weight of people at the start and at the end of an experiment).

```
# Create a random group of data
# The add an average difference of 1 (but with variation)

mu, sigma = 10, 2.5 # mean and standard deviation
t_0 = np.random.normal(mu, sigma, 50)

mu, sigma = 1, 2.5 # mean and standard deviation
diff = np.random.normal(mu, sigma, 50)
t_1 = t_0 + diff

# Calculate t and probability of a difference

t_statistic, p_value = stats.ttest_rel(t_0, t_1)

# Print results

print ('P value:')
print (p_value)
```

OUT:

P value:

3.600736720529075e-05

4.4 Mann-Whitney U test

The Mann-Whitney U test allows comparison of two groups of data where the data is not normally distributed.

```
import numpy as np
import scipy.stats as stats

# Create two groups of data

group1 = [1, 5 ,7 ,3 ,5 ,8 ,34 ,1 ,3 ,5 ,200, 3]
group2 = [10, 18, 11, 12, 15, 19, 9, 17, 1, 22, 9, 8]

# Calculate u and probability of a difference

u_statistic, pVal = stats.mannwhitneyu(group1, group2)

# Print results

print ('P value:')
print (pVal)
```

OUT:

```
P value:
0.02081882005772675
```

4.5 Analysis of variance (ANOVA)

One way analysis of variance (ANOVA) tests whether multiple groups all belong to the same population or not.

If a conclusion is reached that the groups do not all belong to the same population, further tests may be utilised to identify the differences.

```
import numpy as np
import scipy.stats as stats

# Create four random groups of data with a mean difference of 1

mu, sigma = 10, 3 # mean and standard deviation
group1 = np.random.normal(mu, sigma, 50)

mu, sigma = 11, 3 # mean and standard deviation
group2 = np.random.normal(mu, sigma, 50)

mu, sigma = 12, 3 # mean and standard deviation
group3 = np.random.normal(mu, sigma, 50)

mu, sigma = 13, 3 # mean and standard deviation
group4 = np.random.normal(mu, sigma, 50)

# Test whether all groups belong to the same population

F_statistic, pVal = stats.f_oneway(group1, group2, group3, group4)

print ('P value:')
print (pVal)

OUT:

P value:
7.905723172217297e-09
```

4.6 Multiple comparisons between groups

If an ANOVA test has identified that not all groups belong to the same population, then methods may be used to identify which groups are significantly different to each other.

Below are two commonly used methods: Tukey's and Holm-Bonferroni.

These two methods assume that data is approximately normally distributed.

4.6.1 Setting up the data, and running an ANOVA

```
import numpy as np
import scipy.stats as stats

# Create four random groups of data with a mean difference of 1

mu, sigma = 10, 3 # mean and standard deviation
group1 = np.random.normal(mu, sigma, 50)

mu, sigma = 11, 3 # mean and standard deviation
group2 = np.random.normal(mu, sigma, 50)

mu, sigma = 12, 3 # mean and standard deviation
group3 = np.random.normal(mu, sigma, 50)

mu, sigma = 13, 3 # mean and standard deviation
group4 = np.random.normal(mu, sigma, 50)

# Show the results for Anova

F_statistic, pVal = stats.f_oneway(group1, group2, group3, group4)

print ('P value:')
print (pVal)
```

OUT:

```
P value:
1.6462001201818463e-08
```

For the multicomparison tests we will put the data into a dataframe. And then reshape it to a stacked dataframe

```
# Put into dataframe

df = pd.DataFrame()
df['treatment1'] = group1
df['treatment2'] = group2
df['treatment3'] = group3
df['treatment4'] = group4

# Stack the data (and rename columns):

stacked_data = df.stack().reset_index()
stacked_data = stacked_data.rename(columns={'level_0': 'id',
                                           'level_1': 'treatment',
                                           0: 'result'})

# Show the first 8 rows:
```

```
print (stacked_data.head(8))
```

OUT:

```
   id  treatment    result
0  0  treatment1  12.980445
1  0  treatment2   8.444603
2  0  treatment3  10.713692
3  0  treatment4  10.777762
4  1  treatment1  14.350560
5  1  treatment2   9.436072
6  1  treatment3  12.715509
7  1  treatment4  15.016419
```

4.6.2 Tukey's multi-comparison method

See https://en.wikipedia.org/wiki/Tukey's_range_test

This method tests at $P \leq 0.05$ (correcting for the fact that multiple comparisons are being made which would normally increase the probability of a significant difference being identified). A results of 'reject = True' means that a significant difference has been observed.

```
from statsmodels.stats.multicomp import (pairwise_tukeyhsd,
                                         MultiComparison)

# Set up the data for comparison (creates a specialised object)
MultiComp = MultiComparison(stacked_data['result'],
                             stacked_data['treatment'])

# Show all pair-wise comparisons:

# Print the comparisons

print(MultiComp.tukeyhsd().summary())
```

OUT:

```
Multiple Comparison of Means - Tukey HSD,FWER=0.05
=====
group1    group2    meandiff  lower  upper  reject
-----
treatment1 treatment2    1.5021  -0.0392  3.0435  False
treatment1 treatment3     1.47   -0.0714  3.0113  False
treatment1 treatment4    3.8572   2.3159  5.3985   True
treatment2 treatment3   -0.0322  -1.5735  1.5091  False
treatment2 treatment4    2.355    0.8137  3.8963   True
treatment3 treatment4    2.3872    0.8459  3.9285   True
```

4.6.3 Holm-Bonferroni Method

See: https://en.wikipedia.org/wiki/Holm%E2%80%93Bonferroni_method

The Holm-Bonferroni method is an alternative method.

```
comp = MultiComp.allpairtest(stats.ttest_rel, method='Holm')
print (comp[0])
```

OUT:

```

Test Multiple Comparison ttest_rel
FWER=0.05 method=Holm
alphacSidak=0.01, alphacBonf=0.008
=====
  group1    group2    stat    pval    pval_corr reject
-----
treatment1 treatment2 -2.1234 0.0388    0.0776  False
treatment1 treatment3 -2.4304 0.0188    0.0564  False
treatment1 treatment4 -6.4443  0.0      0.0      True
treatment2 treatment3  0.0457 0.9637    0.9637  False
treatment2 treatment4 -3.7878 0.0004    0.0017  True
treatment3 treatment4 -5.0246  0.0      0.0      True

```

4.7 Multiple comparison of non-normally distributed data with the Kruskal-Wallace test

For data that is not normally distributed, the equivalent test to the ANOVA test (for normally distributed data) is the Kruskal-Wallace test. This tests whether all groups are likely to be from the same population.

```
import numpy as np
from scipy import stats

grp1 = np.array([69, 93, 123, 83, 108, 300])
grp2 = np.array([119, 120, 101, 103, 113, 80])
grp3 = np.array([70, 68, 54, 73, 81, 68])
grp4 = np.array([61, 54, 59, 4, 59, 703])

h, p = stats.kruskal(grp1, grp2, grp3, grp4)

print ('P value of there being a significant difference:')
print (p)
```

OUT:

```
P value of there being a significant difference:
0.013911742382969793
```

If the groups do not belong to the same population, between group analysis needs to be undertaken. One method would be to use repeated Mann-Whitney U-tests, but with the P value needed to be considered significant modified by the Bonferroni correction (divide the required significant level by the number of comparisons being made). This however may be overcautious.

4.8 Confidence Interval for a single proportion

We can use statsmodels to calculate the confidence interval of the proportion of given 'successes' from a number of trials. This may be the frequency of occurrence of a gene, the intention to vote in a particular way, etc.

```
import statsmodels.stats.proportion as smp

# e.g. 35 out of a sample 120 (29.2%) people have a particular gene type.
# What are the 95% confidence intervals on the proportion?

lower, upper = smp.proportion_confint (35, 120, alpha=0.05, method='normal')

print ('Lower confidence interval:', lower)
print ('Upper confidence interval:', upper)

OUT:

Lower confidence interval: 0.21034248403748906
Upper confidence interval: 0.3729908492958443
```

4.9 Chi-squared test

See https://en.wikipedia.org/wiki/Chi-squared_test

Without other qualification, 'chi-squared test' often is used as short for Pearson's chi-squared test. The chi-squared test is used to determine whether there is a significant difference between the expected frequencies and the observed frequencies in one or more categories.

Example chi-squared test for categorical data:

Suppose there is a city of 1,000,000 residents with four neighborhoods: A, B, C, and D. A random sample of 650 residents of the city is taken and their occupation is recorded as "white collar", "blue collar", or "no collar". The null hypothesis is that each person's neighborhood of residence is independent of the person's occupational classification. The data are tabulated as follows:

```
import numpy as np
import pandas as pd
import scipy.stats as stats

cols = ['A', 'B', 'C', 'D']
data = pd.DataFrame(columns=cols)

data.loc['White Collar'] = [90, 60, 104, 95]
data.loc['Blue Collar'] = [30, 50, 51, 20]
data.loc['No collar'] = [30, 40, 45, 35]

print (data)
```

OUT:

	A	B	C	D
White Collar	90	60	104	95
Blue Collar	30	50	51	20
No collar	30	40	45	35

We can use the chi-squared test whether area effects the numbers of each collar type. That is, are the values in each row affected by the column? We can reported an expected distribution if column does not effect the values in each row (other than each column having a different total).

```
V, p, dof, expected = stats.chi2_contingency(data)
# add correction=False for uncorrected Chi-square

print ('P value for effect of area on proportion of each collar:')
print (p)
print ('\nExpected numbers if area did not effect proportion of each collar:')
print (expected)
```

OUT:

```
P value for effect of area on proportion of each collar:
0.0004098425861096696
```

```
Expected numbers if area did not effect proportion of each collar:
[[ 80.53846154  80.53846154 107.38461538  80.53846154]
 [ 34.84615385  34.84615385  46.46153846  34.84615385]
 [ 34.61538462  34.61538462  46.15384615  34.61538462]]
```

Note. In Chi-square at least 80% of the of the cells should have a value of at least 5, and all cells where values are expected should be at least 1. If this is not the case then use Fisher exact test.

4.10 Fisher's exact test

Fisher's exact test is similar to the Chi-squared test, but is suitable for small sample sizes. As a rule it should be used if at least 20% of values are less than 5 or any value is zero. Although in practice it is employed when sample sizes are small, it is valid for all sample sizes.

For example, let us look at an example where a group of 16 people may choose tennis or football. In the group of 16 there are six boys and ten girls. The tennis group has one boy and eight girls. The football group has five boys and two girls. Does the sport affect the proportion of boys and girls choosing it?

```
import numpy as np
import scipy.stats as stats

obs = np.array([[1,5], [8,2]])
fisher_result = stats.fisher_exact(obs)

p_val = fisher_result[1]

print ('Data:')
print (obs)

print ('\nProbability that column does not effect row values:')
print (p_val)
```

OUT:

```
Data:
[[1 5]
 [8 2]]
```

```
Probability that column does not effect row values:
0.03496503496503495
```


Chapter 5

Clinical pathway simulation with SimPy

5.1 A bed occupancy model with SimPy

SimPy is a process-based discrete-event simulation framework based on standard Python.

The purpose of the examples presented here is not to give basic training in SimPy. For that please go to:

<https://simpy.readthedocs.io/en/latest/contents.html>

The purpose of the examples here are to show how SimPy may be used for healthcare pathway modelling.

We will start with a relatively simple hospital ward bed occupancy model.

Patients arrive at a given average rate, with the time between any two patients sampled from an exponential distribution. Length of stay in the hospital is again sampled from an exponential distribution. We assume here that the hospital ward can expand to cope with peaks in demand, and use the model to look at the expected natural variation in ward bed occupancy.

5.1.1 Import the packages

IMPORTANT: SimPy is not in the Anaconda environment. To download, open a command line environment and type:

```
pip install simpy
```

```
import simpy
import random
import pandas as pd
import matplotlib.pyplot as plt
```

```
# For Jupyter Notebook use only:
% matplotlib inline
```

5.1.2 Storing variables

We'll store global variables in a class, `g`. Variables are then referred to as `g.var_name`. It is not strictly necessary, but is a convenient way of allowing functions to directly change global variables (well, I like doing it this way anyway!).

For those more familiar with object-based programming, you will notice that we just use the class itself, rather than creating an individual instance of the class.

```
class g():
    # Global variables
    bed_count=0
    inter_arrival_time=1
    los=10 # length of stay
    sim_duration=500
    audit_time=[]
    audit_beds=[]
    audit_interval=1 # bed occupancy is measured at this interval
```

5.1.3 Generating new arrivals

The new arrival function continuously generated new arrivals.

```
def new_admission(env, interarrival_time, los):
    i=0
    while True:
```

```

i+=1
p_los=random.expovariate(1/los) # sample length of stay for patient
p=patient(env,i,p_los) # generate a patient
env.process(p) # activate the patient
next_p=random.expovariate(1/interarrival_time) # sample next arrival time
# print('Next patient in %f3.2' %next_p)
yield env.timeout(next_p) # set up next arrival

```

5.1.4 Patient pathway

When a new patient arrives, hospital bed occupancy is increased by one. A delay is then triggered for that patient according to their length of stay. At the end of that time-out the patient leaves and bed occupancy is reduced by one.

```

def patient(env,i,p_los):
    g.bed_count+=1 # adjust global variable for occupied beds
    # print('Patient %d arriving %7.2f, bed count %d' %(i,env.now,g.bed_count))
    yield env.timeout(p_los) # set delay according to length of stay
    g.bed_count-=1
    # print('Patient %d leaving %7.2f, bed count %d' %(i,env.now,g.bed_count))

```

5.1.5 Audit of beds

The audit runs at regular time intervals. Each time it runs, it adds to two global lists - one recording the simulated time, and the other the number of beds currently occupied.

```

def audit_beds(env,delay):
    yield env.timeout(delay)
    while True:
        g.audit_time.append(env.now)
        g.audit_beds.append(g.bed_count)
        yield env.timeout(g.audit_interval)

```

5.1.6 Generate audit report

At the end of the simulation run, an audit report is generated to summarise hospital bed occupancy variation. This may be viewed directly, but is used here in the occupancy chart produced.

```

def build_audit_report():
    audit_report=pd.DataFrame()
    audit_report['Time']=g.audit_time
    audit_report['Occupied_beds']=g.audit_beds
    audit_report['Median_beds']=audit_report['Occupied_beds'].quantile(0.5)
    audit_report['Beds_5_percent']=audit_report['Occupied_beds'].quantile(0.05)
    audit_report['Beds_95_percent']=audit_report['Occupied_beds'].quantile(0.95)
    return audit_report

```

5.1.7 Charting occupancy

At the end of the run a chart of bed occupancy is produced.

```

def chart():
    plt.plot(g.audit_dataframe['Time'],
             g.audit_dataframe['Occupied_beds'],
             color='k',marker='o',linestyle='solid',
             markevery=1,label='Occupied beds')

```

```

plt.plot(g.audit_dataframe['Time'],
         g.audit_dataframe['Beds_5_percent'],
         color='0.5',linestyle='dashdot',
         markevery=1,label='5th percentile')

plt.plot(g.audit_dataframe['Time'],
         g.audit_dataframe['Median_beds'],
         color='0.5',linestyle='dashed',
         label='Median')

plt.plot(g.audit_dataframe['Time'],
         g.audit_dataframe['Beds_95_percent'],
         color='0.5',linestyle='dashdot',
         label='95th percentile')

plt.xlabel('Day')
plt.ylabel('Occupied beds')
plt.title('Occupied beds (individual days with 5th, 50th and 95th percentiles)')
#plt.legend()
plt.show()

```

5.1.8 Main code

The main code sets up the simulation environment, and initialises the first admission and the first audit (these then maintain themselves by triggering the next admission/audit). It then starts the simulation environment and sets the run time. At the end of the run functions to summarise and plot occupancy are called.

```

# Initialise environment
env=simpy.Environment()
# Initialise processes (admissions & bed audit)
env.process(new_admission(env,g.inter_arrival_time,g.los))
env.process(audit_beds(env,delay=20))
# Start simulation run
env.run(until=g.sim_duration)
# Build audit table
g.audit_dataframe=build_audit_report()
chart()

```

Occupied beds (individual days with 5th, 50th and 95th percentiles)

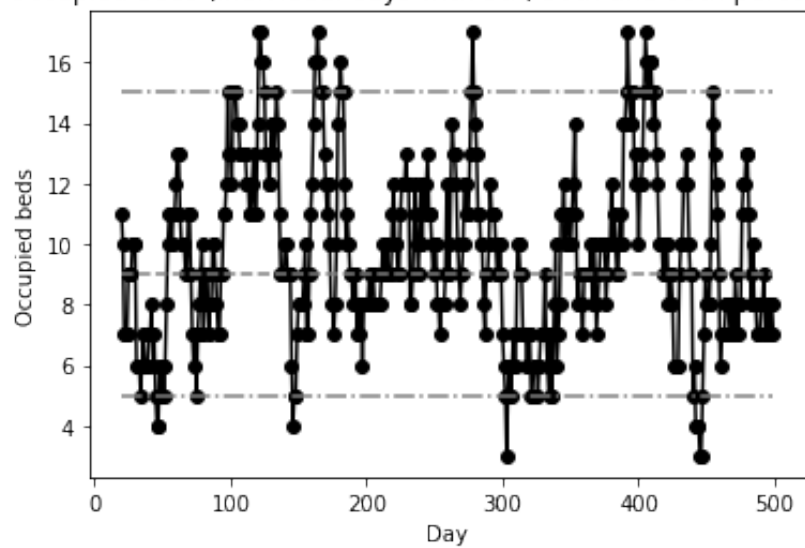
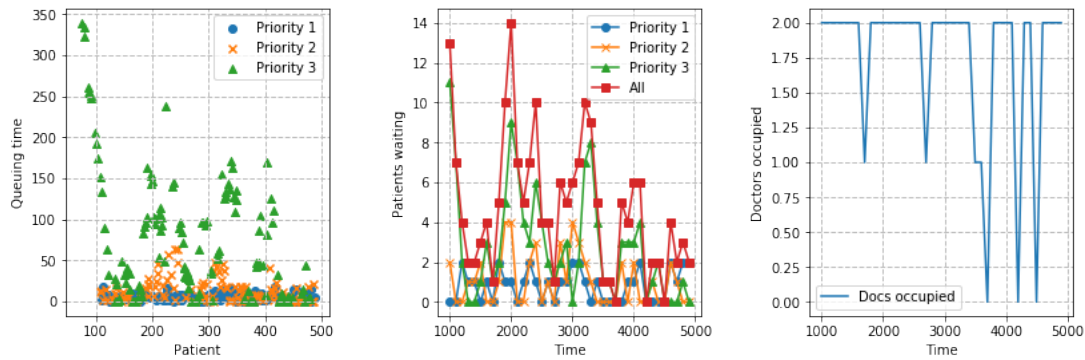


Figure 5.1: ED model summary results



5.2 An emergency department model in SimPy, with patient prioritisation and capacity limited by doctor availability

This model mimics the random arrival of patients at an emergency department (ED). The patients are assessed as being low, medium or high priority. Higher priority patients are always selected next (but do not displace lower priority patients already being seen by a doctor).

This model requires some understanding of object-oriented programming in Python.

There are four classes of object in the model:

- 1) A global variables class. These are stored directly, and may be edited, in the class definition.
- 2) A model class. There is one instance of this class created. This holds the SimPy model.
- 3) A patient class. A new instance of this class is triggered with each patient arrival. The patient object holds all relevant information about individual patients (such as their priority level).
- 4) A resources class. There is one instance of this class created which holds the doctors (if other resources were required they could also be held here).

There is a warm-up period before the auditing of results starts.

```
import simpy
import random
import pandas as pd
import matplotlib.pyplot as plt
import numpy as np

%matplotlib inline

class Global_vars:
    """Storage of global variables. No object instance created"""

    appointment_time_mean = 18
    appointment_time_sd = 7
    audit_time = []
    audit_interval = 100
    audit_patients_in_ED = []
    audit_patients_waiting = []
    audit_patients_waiting_p1 = []
    audit_patients_waiting_p2 = []
    audit_patients_waiting_p3 = []
    audit_reources_used = []
    inter_arrival_time = 10
    number_of_docs = 2
```

```

patient_count = 0
patients_waiting = 0
patients_waiting_by_priority = [0, 0, 0]
patient_queuing_results = pd.DataFrame(columns=['priority', 'q_time', 'consult_time'])
results = pd.DataFrame()
sim_duration = 5000
warm_up = 1000

class Model:
    """ The model object holds the model and the methods directly relevant to the model."""

    def __init__(self):
        """Creates instance of SimPy model environemnt"""

        self.env = simpy.Environment()

    def build_audit_results(self):
        """Compiles audit results into dataframe held in Glov_vars"""

        Global_vars.results['time'] = Global_vars.audit_time

        Global_vars.results['patients in ED'] = (
            Global_vars.audit_patients_in_ED)

        Global_vars.results['all patients waiting'] = (
            Global_vars.audit_patients_waiting)

        Global_vars.results['priority 1 patients waiting'] = (
            Global_vars.audit_patients_waiting_p1)

        Global_vars.results['priority 2 patients waiting'] = (
            Global_vars.audit_patients_waiting_p2)

        Global_vars.results['priority 3 patients waiting'] = (
            Global_vars.audit_patients_waiting_p3)

        Global_vars.results['resources occupied'] = (
            Global_vars.audit_reources_used)

    def chart(self):
        """Plots results at end of run"""

        # Define figure size and defintion
        fig = plt.figure(figsize=(12, 4.5))
        # Create two charts side by side

        # Figure 1: patient level results
        ax1 = fig.add_subplot(131) # 1 row, 3 cols, chart position 1
        x = Global_vars.patient_queuing_results.index
        # Chart loops through 3 priorities
        markers = ['o', 'x', '^']
        for priority in range(1, 4):
            x = (Global_vars.patient_queuing_results[Global_vars.patient_queuing_results
                                                        ['priority'] == priority].index)

            y = (Global_vars.patient_queuing_results
                 [Global_vars.patient_queuing_results['priority'] == priority]['q_time'])

```

```

ax1.scatter(x, y, marker=markers[priority - 1], label='Priority ' + str(priority))
ax1.set_xlabel('Patient')
ax1.set_ylabel('Queuing time')
ax1.legend()
ax1.grid(True, which='both', lw=1, ls='--', c='.75')

# Figure 2: ED level queuing results
ax2 = fig.add_subplot(132) # 1 row, 3 cols, chart position 2
x = Global_vars.results['time']
y1 = Global_vars.results['priority 1 patients waiting']
y2 = Global_vars.results['priority 2 patients waiting']
y3 = Global_vars.results['priority 3 patients waiting']
y4 = Global_vars.results['all patients waiting']
ax2.plot(x, y1, marker='o', label='Priority 1')
ax2.plot(x, y2, marker='x', label='Priority 2')
ax2.plot(x, y3, marker='^', label='Priority 3')
ax2.plot(x, y4, marker='s', label='All')
ax2.set_xlabel('Time')
ax2.set_ylabel('Patients waiting')
ax2.legend()
ax2.grid(True, which='both', lw=1, ls='--', c='.75')

# Figure 3: ED staff usage
ax3 = fig.add_subplot(133) # 1 row, 3 cols, chart position 3
x = Global_vars.results['time']
y = Global_vars.results['resources occupied']
ax3.plot(x, y, label='Docs occupied')
ax3.set_xlabel('Time')
ax3.set_ylabel('Doctors occupied')
ax3.legend()
ax3.grid(True, which='both', lw=1, ls='--', c='.75')

# Create plot
plt.tight_layout(pad=3)
plt.show()

def perform_audit(self):
    """Monitors modelled ED at regular intervals (as defined by audit
    interval in global_vars)"""

    # Delay before first audit if length of warm-up
    yield self.env.timeout(Global_vars.warm_up)
    # The trigger repeated audits
    while True:
        # Record time
        Global_vars.audit_time.append(self.env.now)
        # Record patients waiting by referencing global variables
        Global_vars.audit_patients_waiting.append(Global_vars.patients_waiting)

        (Global_vars.audit_patients_waiting_p1.append
         (Global_vars.patients_waiting_by_priority[0]))

        (Global_vars.audit_patients_waiting_p2.append
         (Global_vars.patients_waiting_by_priority[1]))

        (Global_vars.audit_patients_waiting_p3.append
         (Global_vars.patients_waiting_by_priority[2]))

```

```

        # Record patients waiting by asking length of dictionary of all patients
        # (another way of doing things)
        Global_vars.audit_patients_in_ED.append(len(Patient.all_patients))
        # Record resources occupied
        Global_vars.audit_reources_used.append(self.doc_resources.docs.count)
        # Trigger next audit after interval
        yield self.env.timeout(Global_vars.audit_interval)

def run(self):
    """Runs the model: Sets up resources, initialises model process, and starts
    running the model environment. At the end of the run raw model data is saved
    to file, and summary figure and results are displayed."""

    # Set up resources
    self.doc_resources = Resources(self.env, Global_vars.number_of_docs)
    # Initialise processes that will run on model run
    self.env.process(self.trigger_admissions())
    self.env.process(self.perform_audit())
    # Run
    self.env.run(until=Global_vars.sim_duration)

    # End of simulation run. Build and save results.
    # The saved results are the raw audit data
    Global_vars.patient_queuing_results.to_csv('patient results.csv')
    self.build_audit_results()
    Global_vars.results.to_csv('operational results.csv')
    # Plot a chart of results
    self.chart()
    # Pront text summary of results
    self.summarise()

def see_doc(self, p):
    """Mangages waiting for doctor resorce. Records time waiting to see doc"""

    with self.doc_resources.docs.request(priority=p.priority) as req:
        Global_vars.patients_waiting += 1
        # Wait for resources to become available
        yield req
        # Resources now available
        # Record queuing times in patient object and Global dataframe
        p.time_see_doc = self.env.now
        p.queuing_time = self.env.now - p.time_in
        _results = [p.priority, p.queuing_time]
        yield self.env.timeout(p.consultation_time)
        _results.append(self.env.now - p.time_see_doc)
        # Record results if warm-up complete
        if self.env.now >= Global_vars.warm_up:
            Global_vars.patient_queuing_results.loc[p.id] = _results
        # Reduce patients waiting counts
        Global_vars.patients_waiting_by_priority[p.priority - 1] -= 1
        Global_vars.patients_waiting -= 1
        # Delete patient (removal from patient dictionary removes only
        # reference to patient and Python then automatically cleans up)
        del Patient.all_patients[p.id]

def summarise(self):
    """Produces displayed text summary of model run"""

```

```

# For each patient calculate time in system as time in queue + time with doc
Global_vars.patient_queuing_results['system_time'] = (
    Global_vars.patient_queuing_results['q_time'] +
    Global_vars.patient_queuing_results['consult_time'])

# Display results summaries
print ('Patient-centred metrics:')
print ('-----\n')
print ('Lower quartile time in system by priority:')
print (Global_vars.patient_queuing_results.groupby('priority').quantile(0.25))
print ('\nMedian time in system by priority:')
print (Global_vars.patient_queuing_results.groupby('priority').quantile(0.50))
print ('\nUpper quartile time in system by priority:')
print (Global_vars.patient_queuing_results.groupby('priority').quantile(0.75))
print ('\nMaximum time in system by priority:')
print (Global_vars.patient_queuing_results.groupby('priority').quantile(1))
print ('\nED-centred metrics:')
print ('-----\n')
print (Global_vars.results.describe())

def trigger_admissions(self):
    """Produces patient arrivals. Initialises a patient object (from Patient class),
    passes the patient over to the see_doc method, and sets the next admission
    time/event"""

    # While loop continues generating new patients
    while True:
        # Initialise new patient (pass environment to be used to record
        # current simulation time)
        p = Patient(self.env)
        # Add patient to dictionary of patients
        Patient.all_patients[p.id] = p
        # Pass patient to see_doc method
        self.env.process(self.see_doc(p))
        # Sample time for next admissions
        next_admission = random.expovariate(1 / Global_vars.inter_arrival_time)
        # Schedule next admission
        yield self.env.timeout(next_admission)

class Patient:
    """Class of patient objects. The class also holds a list of all patient objects in
    all_patients dictionary"""

    # The following dictionaries store patients
    all_patients = {}

    # New patient instance
    def __init__(self, env):
        Global_vars.patient_count += 1

        self.consultation_time = (
            random.normalvariate(Global_vars.appointment_time_mean,
                                Global_vars.appointment_time_sd))

        self.consultation_time = 0 if self.consultation_time < 0 else self.consultation_time
        self.id = Global_vars.patient_count
        self.priority = random.randint(1, 3)

```

```

        self.queuing_time = 0
        self.time_in = env.now
        self.time_see_doc = 0
        self.time_out = 0
        # 1 is subtracted from priority to align priority (1-3) with zero indexed list (0-2)
        Global_vars.patients_waiting_by_priority[self.priority - 1] += 1

class Resources:
    """Resources required by processes in the model.
    Just holds doctors as the only limiting resource"""

    def __init__(self, env, number_of_docs):
        self.docs = simpy.PriorityResource(env, capacity=number_of_docs)

if __name__ == '__main__':
    """Start model running"""
    model = Model() # calls method to set up model environment
    model.run() # calls method to run model

```

OUT:

Patient-centred metrics:

Lower quartile time in system by priority:

0.25	consult_time	q_time	system_time
priority			
1.0	12.804572	1.945121	17.481070
2.0	14.027237	2.903354	19.862303
3.0	13.037387	45.798714	65.487228

Median time in system by priority:

0.5	consult_time	q_time	system_time
priority			
1.0	18.258018	6.313626	26.046536
2.0	18.177676	9.276112	28.713375
3.0	17.646766	135.581720	155.499640

Upper quartile time in system by priority:

0.75	consult_time	q_time	system_time
priority			
1.0	23.390835	12.422608	33.696397
2.0	23.683261	21.640748	41.999221
3.0	22.340090	230.462964	248.254876

Maximum time in system by priority:

1	consult_time	q_time	system_time
priority			
1.0	39.415063	29.704864	53.879094
2.0	36.161817	80.892908	109.380811
3.0	33.433588	401.793694	422.526345

ED-centred metrics:

	time	patients in ED	all patients waiting \
count	40.000000	40.000000	40.000000
mean	2950.000000	8.200000	8.200000

std	1169.045194	4.696971	4.696971
min	1000.000000	0.000000	0.000000
25%	1975.000000	4.750000	4.750000
50%	2950.000000	8.500000	8.500000
75%	3925.000000	12.000000	12.000000
max	4900.000000	18.000000	18.000000

	priority 1 patients waiting	priority 2 patients waiting \
count	40.000000	40.000000
mean	0.900000	1.200000
std	0.928191	1.090754
min	0.000000	0.000000
25%	0.000000	0.000000
50%	1.000000	1.000000
75%	1.000000	2.000000
max	3.000000	4.000000

	priority 3 patients waiting	resources occupied
count	40.000000	40.000000
mean	6.100000	1.875000
std	4.19279	0.404304
min	0.000000	0.000000
25%	1.750000	2.000000
50%	6.000000	2.000000
75%	9.000000	2.000000
max	14.000000	2.000000

Chapter 6

Machine learning with scikit learn

6.1 The iris data set

This is a classic 'toy' data set used for machine learning testing is the iris data set.

The data set consists of 50 samples from each of three species of Iris (Iris setosa, Iris virginica and Iris versicolor). Four features were measured from each sample: the length and the width of the sepals and petals, in centimetres.

6.1.1 Loading the iris data set

The iris data set comes preloaded in scikit learn. Let's load it and have a look at it.

```
import numpy as np
from sklearn import datasets

iris=datasets.load_iris()

# The iris dataset is an object that contains a number of elements:

print (list(iris))

OUT:

['data', 'target', 'target_names', 'DESCR', 'feature_names']

# feature_names shows data field titles:

print (iris.feature_names)

OUT:

['sepal length (cm)', 'sepal width (cm)', 'petal length (cm)', 'petal width (cm)']

# data is the data for each sample; columns described by feature_names:
# lets' print just the first 10 roes
print (iris.data[0:10])

OUT:

# data is the data for each sample; columns described by feature_names:

# lets' print just the first 10 roes

print (iris.data[0:10])

[[5.1 3.5 1.4 0.2]
 [4.9 3.  1.4 0.2]
 [4.7 3.2 1.3 0.2]
 [4.6 3.1 1.5 0.2]
 [5.  3.6 1.4 0.2]
 [5.4 3.9 1.7 0.4]
 [4.6 3.4 1.4 0.3]
 [5.  3.4 1.5 0.2]
 [4.4 2.9 1.4 0.2]
 [4.9 3.1 1.5 0.1]]
```

```

# target_names lists types of iris identified:

print (iris.target_names)

OUT:

['setosa' 'versicolor' 'virginica']

# target lists the type of iris in each row of data:
# this maps to the target_names

print (iris.target)

OUT:

[0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2
 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 2 2]

# DESCR gives us description of the data set:

print (iris.DESCR)

OUT:

Iris Plants Database
=====

Notes
-----
Data Set Characteristics:
: Number of Instances: 150 (50 in each of three classes)
: Number of Attributes: 4 numeric, predictive attributes and the class
: Attribute Information:
  - sepal length in cm
  - sepal width in cm
  - petal length in cm
  - petal width in cm
  - class:
    - Iris-Setosa
    - Iris-Versicolour
    - Iris-Virginica
: Summary Statistics:

=====  =====  =====  =====  =====
              Min   Max    Mean     SD    Class Correlation
=====  =====  =====  =====  =====
sepal length:  4.3   7.9    5.84    0.83     0.7826
sepal width:   2.0   4.4    3.05    0.43    -0.4194
petal length:  1.0   6.9    3.76    1.76     0.9490 (high!)
petal width:   0.1   2.5    1.20    0.76     0.9565 (high!)
=====  =====  =====  =====  =====

: Missing Attribute Values: None
: Class Distribution: 33.3% for each of 3 classes.
: Creator: R.A. Fisher

```

:Donor: Michael Marshall (MARSHALL%PLU@io.arc.nasa.gov)
:Date: July, 1988

This is a copy of UCI ML iris datasets.
<http://archive.ics.uci.edu/ml/datasets/Iris>

The famous Iris database, first used by Sir R.A Fisher

This is perhaps the best known database to be found in the pattern recognition literature. Fisher's paper is a classic in the field and is referenced frequently to this day. (See Duda & Hart, for example.) The data set contains 3 classes of 50 instances each, where each class refers to a type of iris plant. One class is linearly separable from the other 2; the latter are NOT linearly separable from each other.

References

-
- Fisher, R.A. "The use of multiple measurements in taxonomic problems" Annual Eugenics, 7, Part II, 179-188 (1936); also in "Contributions to Mathematical Statistics" (John Wiley, NY, 1950).
 - Duda, R.O., & Hart, P.E. (1973) Pattern Classification and Scene Analysis. (Q327.D83) John Wiley & Sons. ISBN 0-471-22361-1. See page 218.
 - Dasarathy, B.V. (1980) "Nosing Around the Neighborhood: A New System Structure and Classification Rule for Recognition in Partially Exposed Environments". IEEE Transactions on Pattern Analysis and Machine Intelligence, Vol. PAMI-2, No. 1, 67-71.
 - Gates, G.W. (1972) "The Reduced Nearest Neighbor Rule". IEEE Transactions on Information Theory, May 1972, 431-433.
 - See also: 1988 MLC Proceedings, 54-64. Cheeseman et al's AUTOCLASS II conceptual clustering system finds 3 classes in the data.
 - Many, many more ...

6.1.2 Data sets in scikit learn

load_boston: boston house-prices dataset (regression).
load_iris: iris dataset (classification).
load_diabetes: diabetes dataset (regression).
load_digits: digits dataset (classification).
load_linnerud: linnerud dataset (multivariate regression).
load_wine: wine dataset (classification).
load_breast_cancer: breast cancer wisconsin dataset (classification).

6.1.3 Other sources of test data sets

<https://archive.ics.uci.edu/ml/datasets.html>
<https://blog.bigml.com/list-of-public-data-sources-fit-for-machine-learning/>

6.2 Splitting data into training and test sets

To test the accuracy of a model we will test the model on data that it has not seen before. We will divide available data into two sets: a training set that the model will learn from, and a test set which will be used to test the accuracy of the model on new data. A convenient way to split the data is to use scikit-learn's `train_test_split` method. This randomly divides the data between training and test sets. We may specify what proportion to keep for the test set (0.2 - 0.3 is common).

```
import numpy as np
from sklearn import datasets
from sklearn.model_selection import train_test_split

# Load the iris data

iris=datasets.load_iris()

# Extra out the feature data (data), and the classification (target)

X=iris.data
y=iris.target

X_train,X_test,y_train,y_test=train_test_split(
    X,y,test_size=0.3,random_state=0)

# Random_state is integer seed.
# If this is omitted than a different seed will be used each time

Let's look at the size of the data sets:
```

```
print ('Shape of X:', X.shape)
print ('Shape of y:', y.shape)
print ('Shape of X_train:', X_train.shape)
print ('Shape of y_train:', y_train.shape)
print ('Shape of X_test:', X_test.shape)
print ('Shape of y_test:', y_test.shape)
```

OUT:

```
Shape of X: (150, 4)
Shape of y: (150,)
Shape of X_train: (105, 4)
Shape of y_train: (105,)
Shape of X_test: (45, 4)
Shape of y_test: (45,)
```

The data has been split randomly, 70% into the training set and 30% into the test set.

6.3 Feature scaling

Many machine learning algorithms work best when numerical data for each of the features (the characteristics such as petal length and sepal length in the iris data set) are on approximately the same scale. The conversion to a similar scale is called data normalisation or data scaling. We perform this as part of our data pre-processing before training an algorithm.

Two common methods of scaling data are 1) to scale all data between 0 and 1 when 0 and 1 are the minimum and maximum values for each feature, and 2) scale the data so that all features have a mean value of zero and a standard deviation of 1. We will perform this latter normalisation. Scikit learn will perform this for us, but the principle is simple: to normalise in this way, subtract the feature mean from all values, and then divide by the feature standard deviation.

The normalisation parameters are established using the training data set. These parameters are then applied also to the test data set.

Let's first import our packages including StandardScaler from sklearn.preprocessing:

```
import numpy as np
from sklearn import datasets
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
```

To improve readability of the results, we'll set up a function to format NumPy output, controlling the width and decimal places.

```
def set_numpy_decimal_places(places, width=0):
    set_np = '{0:.' + str(width) + '.' + str(places) + 'f}'
    np.set_printoptions(formatter={'float': lambda x: set_np.format(x)})
```

```
set_numpy_decimal_places(3,6)
```

We'll load up our iris data:

```
# Load iris data

iris = datasets.load_iris()
X=iris.data
y=iris.target

# Create training and test data sets
X_train,X_test,y_train,y_test=train_test_split(
    X,y,test_size=0.3,random_state=0)
```

We'll now apply our scalar, training it on the training data set, and applying it to both the training and test data set.

```
# Initialise a new scaling object
sc=StandardScaler()

# Set up the scaler just on the training set
sc.fit(X_train)

# Apply the scaler to the training and test sets
X_train_std=sc.transform(X_train)
X_test_std=sc.transform(X_test)
```

Let's see what it has done to our data sets. Our training data set appears not to be perfectly normalised, but it is on exactly the same scale as the training data set, which is what our machine learning algorithms will need.

```
print ('Original training set data:')
print ('Mean: ', X_train.mean(axis=0))
print ('StDev:', X_train.std(axis=0))
```

```
print ('\nScaled training set data:')
print ('Mean: ', X_train_std.mean(axis=0))
print ('StDev:', X_train_std.std(axis=0))

print ('\nOriginal test set data:')
print ('Mean: ', X_test.mean(axis=0))
print ('StDev:', X_test.std(axis=0))

print ('\nScaled test set data:')
print ('Mean: ', X_test_std.mean(axis=0))
print ('StDev:', X_test_std.std(axis=0))
```

OUT:

```
Original training set data:
Mean:  [ 5.893  3.045  3.829  1.227]
StDev: [ 0.873  0.439  1.796  0.778]
```

```
Scaled training set data:
Mean:  [ 0.000 -0.000 -0.000 -0.000]
StDev: [ 1.000  1.000  1.000  1.000]
```

```
Original test set data:
Mean:  [ 5.727  3.076  3.596  1.133]
StDev: [ 0.688  0.414  1.656  0.715]
```

```
Scaled test set data:
Mean:  [-0.191  0.070 -0.130 -0.120]
StDev: [ 0.789  0.943  0.922  0.919]
```

6.4 Using logistic regression to diagnose breast cancer

Here we will use the first of our machine learning algorithms to diagnose whether someone has a benign or malignant tumour. We are using a form of logistic regression. In common to many machine learning models it incorporates a regularisation term which sacrifices a little accuracy in predicting outcomes in the training set for improved accuracy in predicting the outcomes of patients not used in the training set.

We will use the Wisconsin Breast Cancer diagnosis data set, a classic 'toy' machine learning database. It is pre-loaded in scikit-learn, but is also available at:

[https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+\(Diagnostic\)](https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic))

The data set contains data on 562 patients, with 32 features for each patient.

Let's repeat what we've covered so far: loading data, splitting the data into training and test sets, and normalising the data. We'll print out the list of data fields and the patient classification outcomes.

Once you have had a look through this why not try changing the load data line to the iris data set we have seen before and see how the same code works there (where there are three possible outcomes).

Just replace the first line of the `# Load dataset` section with:

```
data_set = datasets.load_breast_cancer()
```

*A reminder that we are using the Anaconda distribution for scientific Python, which contains all the required packages, download from:

<https://www.anaconda.com/download/>

```
# import required modules

from sklearn import datasets
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
import pandas as pd
from sklearn.linear_model import LogisticRegression

# Load Dataset

data_set = datasets.load_breast_cancer()
X=data_set.data
y=data_set.target

# Show data fields
print ('Data fields data set:')
print (data_set.feature_names)

# Show classifications
print ('\nClassification outcomes:')
print (data_set.target_names)

# Create training and test data sets
X_train,X_test,y_train,y_test=train_test_split(
    X,y,test_size=0.25, random_state=0)

# Initialise a new scaling object for normalising input data
sc=StandardScaler()

# Set up the scaler just on the training set
sc.fit(X_train)

# Apply the scaler to the training and test sets
```

```
X_train_std=sc.transform(X_train)
X_test_std=sc.transform(X_test)
```

OUT:

Data fields data set:

```
['mean radius' 'mean texture' 'mean perimeter' 'mean area'
 'mean smoothness' 'mean compactness' 'mean concavity'
 'mean concave points' 'mean symmetry' 'mean fractal dimension'
 'radius error' 'texture error' 'perimeter error' 'area error'
 'smoothness error' 'compactness error' 'concavity error'
 'concave points error' 'symmetry error' 'fractal dimension error'
 'worst radius' 'worst texture' 'worst perimeter' 'worst area'
 'worst smoothness' 'worst compactness' 'worst concavity'
 'worst concave points' 'worst symmetry' 'worst fractal dimension']
```

Classification outcomes:

```
['malignant' 'benign']
```

Now let's see how easy it is to build and logistic regression model with scikit-learn. (We'll come back to that $C=100$ in a later section - that is the regularisation term which can help avoid over-fitting to the training data set and improve accuracy for predicting the outcomes for previously unseen data).

```
# Run logistic regression model from sklearn
from sklearn.linear_model import LogisticRegression
lr=LogisticRegression(C=100,random_state=0)
lr.fit(X_train_std,y_train)
```

That's it! We can now use the model to predict outcomes for patients not yet seen.

```
y_pred=lr.predict(X_test_std)
```

Let's calculate a simple accuracy score (in the next module we'll look at a range of accuracy scores). This is simply the percentage of test cases correctly predicted.

```
correct = (y_test == y_pred).sum()
incorrect = (y_test != y_pred).sum()
accuracy = correct / (correct + incorrect) * 100
```

```
print('\nPercent Accuracy: %0.1f' %accuracy)
```

OUT:

Percent Accuracy: 93.7

That's not bad for our first model. We can look at the individual patients in more detail:

```
# Show more detailed results
```

```
prediction = pd.DataFrame()
prediction['actual'] = data_set.target_names[y_test]
prediction['predicted'] = data_set.target_names[y_pred]
prediction['correct'] = prediction['actual'] == prediction['predicted']
```

```
print ('\nDetailed results for first 20 tests:')
print (prediction.head(20))
```

OUT:

Detailed results for first 20 tests:

	actual	predicted	correct
0	malignant	malignant	True

1	benign	benign	True
2	benign	benign	True
3	benign	benign	True
4	benign	benign	True
5	benign	benign	True
6	benign	benign	True
7	benign	benign	True
8	benign	benign	True
9	benign	benign	True
10	benign	benign	True
11	benign	benign	True
12	benign	benign	True
13	benign	malignant	False
14	benign	benign	True
15	malignant	malignant	True
16	benign	benign	True
17	malignant	malignant	True
18	malignant	malignant	True
19	malignant	malignant	True

There we have our first machine learning model!

6.5 Adding standard diagnostic performance metrics to a ml diagnosis model

Here we will repeat the logistic regression model on cancer diagnosis, but add in commonly used measures of clinical diagnostic test performance. These may be used when the predicted outcome may be classified as true or false.

In this example we'll break down our code into functions. This is good practice for longer programmes. The functions are usually presented in alphabetical order. The main code comes after all functions have been defined. This makes the flow of the programme, as defined in the main code (not by the order of the functions), easy to follow. As a general rule functions should be named by their action. Names should adequately describe everything the function does (the best functional programming has functions that do one thing).

The diagnostic measures covered are:

- 1) accuracy: proportion of test results that are correct
- 2) sensitivity: proportion of true +ve identified
- 3) specificity: proportion of true -ve identified
- 4) positive likelihood: increased probability of true +ve if test +ve
- 5) negative likelihood: reduced probability of true +ve if test -ve
- 6) false positive rate: proportion of false +ves in true -ve patients
- 7) false negative rate: proportion of false -ves in true +ve patients
- 8) positive predictive value: chance of true +ve if test +ve
- 9) negative predictive value: chance of true -ve if test -ve
- 10) precision = positive predictive value
- 11) recall = sensitivity
- 12) $f1 = (2 * \text{precision} * \text{recall}) / (\text{precision} + \text{recall})$

Let's look at the code, and run it:

```
# import required modules

from sklearn import datasets
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
import numpy as np

def calculate_diagnostic_performance(actual_predicted):
    """ Calculate diagnostic performance.

    Takes a Numpy array of 1 and zero, two columns: actual and predicted

    Note that some statistics are repeats with different names
    (precision = positive_predictive_value and recall = sensitivity).
    Both names are returned

    Returns a dictionary of results:

    1) accuracy: proportion of test results that are correct
    2) sensitivity: proportion of true +ve identified
    3) specificity: proportion of true -ve identified
    4) positive likelihood: increased probability of true +ve if test +ve
    5) negative likelihood: reduced probability of true +ve if test -ve
```

```

6) false positive rate: proportion of false +ves in true -ve patients
7) false negative rate: proportion of false -ves in true +ve patients
8) positive predictive value: chance of true +ve if test +ve
9) negative predictive value: chance of true -ve if test -ve
10) precision = positive predictive value
11) recall = sensitivity
12) f1 = (2 * precision * recall) / (precision + recall)
13) positive rate = rate of true +ve (not strictly a performance measure)
"""

# Calculate results
actual_positives = actual_predicted[:, 0] == 1
actual_negatives = actual_predicted[:, 0] == 0
test_positives = actual_predicted[:, 1] == 1
test_negatives = actual_predicted[:, 1] == 0
test_correct = actual_predicted[:, 0] == actual_predicted[:, 1]
accuracy = np.average(test_correct)
true_positives = actual_positives & test_positives
true_negatives = actual_negatives & test_negatives
sensitivity = np.sum(true_positives) / np.sum(actual_positives)
specificity = np.sum(true_negatives) / np.sum(actual_negatives)
positive_likelihood = sensitivity / (1 - specificity)
negative_likelihood = (1 - sensitivity) / specificity
false_positive_rate = 1 - specificity
false_negative_rate = 1 - sensitivity
positive_predictive_value = np.sum(true_positives) / np.sum(test_positives)
negative_predictive_value = np.sum(true_negatives) / np.sum(test_negatives)
precision = positive_predictive_value
recall = sensitivity
f1 = (2 * precision * recall) / (precision + recall)
positive_rate = np.mean(actual_predicted[:, 1])

# Add results to dictionary
performance = {}
performance['accuracy'] = accuracy
performance['sensitivity'] = sensitivity
performance['specificity'] = specificity
performance['positive_likelihood'] = positive_likelihood
performance['negative_likelihood'] = negative_likelihood
performance['false_positive_rate'] = false_positive_rate
performance['false_negative_rate'] = false_negative_rate
performance['positive_predictive_value'] = positive_predictive_value
performance['negative_predictive_value'] = negative_predictive_value
performance['precision'] = precision
performance['recall'] = recall
performance['f1'] = f1
performance['positive_rate'] = positive_rate

return performance

def load_data ():
    """Load the data set. Here we load the Breast Cancer Wisconsin (Diagnostic)
    Data Set. Data could be loaded from other sources though the structure
    should be compatible with this data set, that is an object with the
    following attributes:
        .data (holds feature data)
        .feature_names (holds feature titles)
        .target_names (holds outcome classification names)
        .target (holds classification as zero-based number)

```

```

        .DESCR (holds text-based description of data set)"""

    data_set = datasets.load_breast_cancer()
    return data_set

def normalise (X_train,X_test):
    """Normalise X data, so that training set has mean of zero and standard
    deviation of one"""

    # Initialise a new scaling object for normalising input data
    sc=StandardScaler()
    # Set up the scaler just on the training set
    sc.fit(X_train)
    # Apply the scaler to the training and test sets
    X_train_std=sc.transform(X_train)
    X_test_std=sc.transform(X_test)
    return X_train_std, X_test_std

def print_diagnostic_results (performance):
    """Iterate through, and print, the performance metrics dictionary"""

    print('\nMachine learning diagnostic performance measures:')
    print('-----')
    for key, value in performance.items():
        print (key, '= %0.3f' %value) # print 3 decimal places
    return

def split_data (data_set, split=0.25):
    """Extract X and y data from data_set object, and split into training and
    test data. Split defaults to 75% training, 25% test if not other value
    passed to function"""

    X=data_set.data
    y=data_set.target
    X_train,X_test,y_train,y_test=train_test_split(
        X,y,test_size=split, random_state=0)
    return X_train,X_test,y_train,y_test

def test_model(model, X, y):
    """Return predicted y given X (attributes)"""

    y_pred = model.predict(X)
    test_results = np.vstack((y, y_pred)).T
    return test_results

def train_model (X, y):
    """Train the model """

    from sklearn.linear_model import LogisticRegression
    model = LogisticRegression(C=100,random_state=0)
    model.fit(X, y)
    return model

##### Main code #####

# Load data
data_set = load_data()

```

```
# Split data into training and test sets
X_train,X_test,y_train,y_test = split_data(data_set, 0.25)

# Normalise data
X_train_std, X_test_std = normalise(X_train,X_test)

# Train model
model = train_model(X_train_std,y_train)

# Produce results for test set
test_results = test_model(model, X_test_std, y_test)

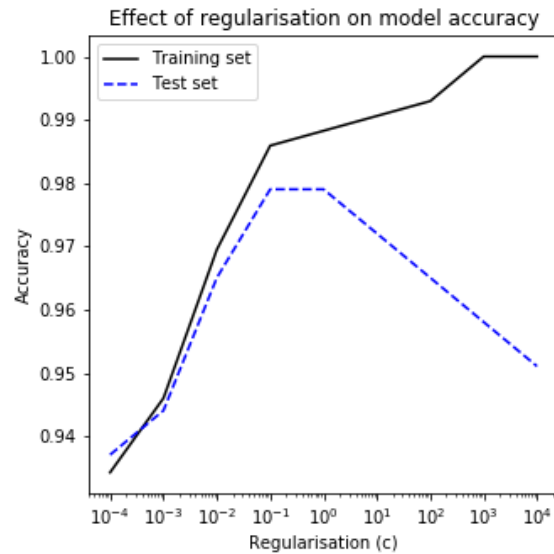
# Measure performance of test set predictions
performance = calculate_diagnostic_performance(test_results)

# Print performance metrics
print_diagnostic_results(performance)
```

OUT:

Machine learning diagnostic performance measures:

```
-----
accuracy = 0.937
sensitivity = 0.933
specificity = 0.943
positive_likelihood = 16.489
negative_likelihood = 0.071
false_positive_rate = 0.057
false_negative_rate = 0.067
positive_predictive_value = 0.966
negative_predictive_value = 0.893
precision = 0.966
recall = 0.933
f1 = 0.949
positive_rate = 0.608
```



6.6 Regularisation

Many machine learning techniques include an option to fine-tune regularisation. Regularisation helps to avoid over-fitting of the model to the training set at the cost of accuracy of predication for previously unseen samples in the test set. In the logistic regression method that we have been looking at the regularisation term in the model fit is 'c'. The lower the c value the greater the regularisation. The previous code has been amended below to loop through a series of c values. For each value of c the model fit is run 100 times with different random train/test splits, and the average results are presented.

Not that as c increases (that is regularisation is reduced) the accuracy of fitting the training set increases until it reaches a plateau. With the test set of data, increasing c first improves accuracy but then, above a certain point, accuracy starts to drop. When the model is effectively un-regularised (very high c) we have 95% accuracy in the test set. By fine-tuning c we can improve accuracy of the test set to 98%.

```
# import required modules
```

```
from sklearn import datasets
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

```
%matplotlib inline
```

```
def calculate_diagnostic_performance (actual_predicted):
    """ Calculate diagnostic performance.
```

```
    Takes a Numpy array of 1 and zero, two columns: actual and predicted
```

```
    Note that some statistics are repeats with different names
    (precision = positive_predictive_value and recall = sensitivity).
    Both names are returned
```

```
    Returns a dictionary of results:
```

- 1) accuracy: proportion of test results that are correct
- 2) sensitivity: proportion of true +ve identified

```

3) specificity: proportion of true -ve identified
4) positive likelihood: increased probability of true +ve if test +ve
5) negative likelihood: reduced probability of true +ve if test -ve
6) false positive rate: proportion of false +ves in true -ve patients
7) false negative rate: proportion of false -ves in true +ve patients
8) positive predictive value: chance of true +ve if test +ve
9) negative predictive value: chance of true -ve if test -ve
10) precision = positive predictive value
11) recall = sensitivity
12) f1 = (2 * precision * recall) / (precision + recall)
13) positive rate = rate of true +ve (not strictly a performance measure)
"""

# Calculate results
actual_positives = actual_predicted[:, 0] == 1
actual_negatives = actual_predicted[:, 0] == 0
test_positives = actual_predicted[:, 1] == 1
test_negatives = actual_predicted[:, 1] == 0
test_correct = actual_predicted[:, 0] == actual_predicted[:, 1]
accuracy = np.average(test_correct)
true_positives = actual_positives & test_positives
true_negatives = actual_negatives & test_negatives
sensitivity = np.sum(true_positives) / np.sum(actual_positives)
specificity = np.sum(true_negatives) / np.sum(actual_negatives)
positive_likelihood = sensitivity / (1 - specificity)
negative_likelihood = (1 - sensitivity) / specificity
false_positive_rate = 1 - specificity
false_negative_rate = 1 - sensitivity
positive_predictive_value = np.sum(true_positives) / np.sum(test_positives)
negative_predictive_value = np.sum(true_negatives) / np.sum(test_negatives)
precision = positive_predictive_value
recall = sensitivity
f1 = (2 * precision * recall) / (precision + recall)
positive_rate = np.mean(actual_predicted[:, 1])

# Add results to dictionary
performance = {}
performance['accuracy'] = accuracy
performance['sensitivity'] = sensitivity
performance['specificity'] = specificity
performance['positive_likelihood'] = positive_likelihood
performance['negative_likelihood'] = negative_likelihood
performance['false_positive_rate'] = false_positive_rate
performance['false_negative_rate'] = false_negative_rate
performance['positive_predictive_value'] = positive_predictive_value
performance['negative_predictive_value'] = negative_predictive_value
performance['precision'] = precision
performance['recall'] = recall
performance['f1'] = f1
performance['positive_rate'] = positive_rate

return performance

def chart_results(results):
    x = results['c']
    y1 = results['training_accuracy']
    y2 = results['test_accuracy']

    # Create figure

```

```

fig = plt.figure(figsize=(5,5))
ax = fig.add_subplot(111)
ax.plot(x,y1, color='k',linestyle='solid', label = 'Training set')
ax.plot(x,y2, color='b',linestyle='dashed', label = 'Test set')
ax.set_xscale('log')
ax.set_xlabel('Regularisation (c)')
ax.set_ylabel('Accuracy')
plt.title('Effect of regularisation on model accuracy')
plt.legend()
plt.savefig('plot_26.png')
plt.show()

def load_data ():
    """Load the data set. Here we load the Breast Cancer Wisconsin (Diagnostic)
    Data Set. Data could be loaded from other sources though the structure
    should be compatible with thi sdata set, that is an object with the
    following attribtes:
        .data (holds feature data)
        .feature_names (holds feature titles)
        .target_names (holds outcome classification names)
        .target (holds classification as zero-based number)
        .DESCR (holds text-based description of data set)"""

    data_set = datasets.load_breast_cancer()
    return data_set

def normalise (X_train,X_test):
    """Normalise X data, so that training set has mean of zero and standard
    deviation of one"""

    # Initialise a new scaling object for normalising input data
    sc=StandardScaler()
    # Set up the scaler just on the training set
    sc.fit(X_train)
    # Apply the scaler to the training and test sets
    X_train_std=sc.transform(X_train)
    X_test_std=sc.transform(X_test)
    return X_train_std, X_test_std

def print_diagnostic_results (performance):
    """Iterate through, and print, the performance metrics dictionary"""

    print('\nMachine learning diagnostic performance measures:')
    print('-----')
    for key, value in performance.items():
        print (key, '= %0.3f' %value) # print 3 decimal places
    return

def split_data (data_set, split=0.25):
    """Extract X and y data from data_set object, and split into tarining and
    test data. Split defaults to 75% training, 25% test if not other value
    passed to function"""

    X=data_set.data
    y=data_set.target
    X_train,X_test,y_train,y_test=train_test_split(

```

```

        X,y,test_size=split)
    return X_train,X_test,y_train,y_test

def test_model(model, X, y):
    """Return predicted y given X (attributes)"""

    y_pred = model.predict(X)
    test_results = np.vstack((y, y_pred)).T
    return test_results

def train_model (X, y, c):
    """Train the model """

    from sklearn.linear_model import LogisticRegression
    model = LogisticRegression(C=c)
    model.fit(X, y)
    return model

##### Main code #####

# Load data
data_set = load_data()

# List of regularisation values
c_list = [0.0001, 0.001, 0.01, 0.1, 1, 10, 100, 1000, 10000]
training_accuracy = []
test_accuracy = []
c_results = [] # record c

for c in c_list:
    # observe progress
    print('c = ',c)

    for i in range(1000):

        # Split data into trainign and test sets
        X_train,X_test,y_train,y_test = split_data(data_set, 0.25)

        # Normalise data
        X_train_std, X_test_std = normalise(X_train,X_test)
        # Repeat test 1000x per level of c
        c_results.append(c)

        # Train model
        model = train_model(X_train_std,y_train, c)

        # Produce results for training set
        test_results = test_model(model, X_train_std, y_train)
        performance = calculate_diagnostic_performance(test_results)
        training_accuracy.append(performance['accuracy'])

        # Produce results for test set
        test_results = test_model(model, X_test_std, y_test)
        performance = calculate_diagnostic_performance(test_results)
        test_accuracy.append(performance['accuracy'])

```

```

results = pd.DataFrame()
results['c'] = c_results
results['training_accuracy'] = training_accuracy
results['test_accuracy'] = test_accuracy
summary = results.groupby('c').median()
summary['c'] = list(summary.index)

print ()
print (summary)
chart_results (summary)

```

OUT:

	training_accuracy	test_accuracy	c
c			
0.0001	0.934272	0.937063	0.0001
0.0010	0.946009	0.944056	0.0010
0.0100	0.969484	0.972028	0.0100
0.1000	0.985915	0.979021	0.1000
1.0000	0.988263	0.979021	1.0000
10.0000	0.990610	0.972028	10.0000
100.0000	0.992958	0.965035	100.0000
1000.0000	1.000000	0.958042	1000.0000
10000.0000	1.000000	0.951049	10000.0000

6.7 Learning rates: How much data do you need?

Do you have enough data samples to build a good machine learning model? Examining the learning rate of your model will help you decide whether it could be improved by having more data.

Here we repeat the logistic regression model on the Wisconsin Breast Cancer Diagnostic data set. We set out regularisation parameter (c) to 1, from our previous experiment, and then look at the effect of restricting our training set to varying sizes (the test set remains the same size, at 25% of our data).

We can see that as we increase our training set size the accuracy of fitting the training set reduces (it is easier to over-fit smaller data sets), and increase the accuracy of the test set. When we reach the most data we have there has not yet been a plateau in the accuracy of our test set, and the test set accuracy is significantly poorer than the training set accuracy (at our optimum regularisation for this amount of data). These two observations suggest that we would benefit from having more data for the model. If we did have more data then we should the experiment to find the optimum regularisation: generally as data set size increases, the need for regularisation reduces.

Different types of machine learning model may have different learning rates. This may influence your choice of model.

```
# import required modules

from sklearn import datasets
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

def calculate_diagnostic_performance (actual_predicted):
    """Here we truncate calculation of results just to accuracy measurement"""

    # Calculate results

    test_correct = actual_predicted[:, 0] == actual_predicted[:, 1]
    accuracy = np.average(test_correct)

    # Add results to dictionary
    performance = {}
    performance['accuracy'] = accuracy
    return performance

def chart_results(results):
    x = results['n']
    y1 = results['training_accuracy']
    y2 = results['test_accuracy']

    # Create figure
    fig = plt.figure(figsize=(5,5))
    ax = fig.add_subplot(111)
    ax.plot(x,y1, color='k',linestyle='solid', label = 'Training set')
    ax.plot(x,y2, color='b',linestyle='dashed', label = 'Test set')
    ax.set_xlabel('training set size (cases)')
    ax.set_ylabel('Accuracy')
    plt.title('Effect of training set size on model accuracy')
    plt.legend()
    plt.show()

def load_data ():
    """Load the data set. Here we load the Breast Cancer Wisconsin (Diagnostic)
```

```

Data Set. Data could be loaded from other sources though the structure
should be compatible with thi sdata set, that is an object with the
following attribtes:
    .data (holds feature data)
    .feature_names (holds feature titles)
    .target_names (holds outcome classification names)
    .target (holds classification as zero-based number)
    .DESCR (holds text-based description of data set)"""

data_set = datasets.load_breast_cancer()
return data_set

def normalise (X_train,X_test):
    """Normalise X data, so that training set has mean of zero and standard
    deviation of one"""

    # Initialise a new scaling object for normalising input data
    sc=StandardScaler()
    # Set up the scaler just on the training set
    sc.fit(X_train)
    # Apply the scaler to the training and test sets
    X_train_std=sc.transform(X_train)
    X_test_std=sc.transform(X_test)
    return X_train_std, X_test_std

def print_diagnostic_results (performance):
    """Iterate through, and print, the performance metrics dictionary"""

    print('\nMachine learning diagnostic performance measures:')
    print('-----')
    for key, value in performance.items():
        print (key, '= %0.3f' %value) # print 3 decimal places
    return

def split_data (data_set, split, n):
    """Extract X and y data from data_set object, and split into tarining and
    test data. Split defaults to 75% training, 25% test if not other value
    passed to function"""

    X=data_set.data
    y=data_set.target
    X_train,X_test,y_train,y_test=train_test_split(
        X,y,test_size=split)
    X_train = X_train[0:n]
    y_train = y_train[0:n]
    return X_train,X_test,y_train,y_test

def test_model(model, X, y):
    """Return predicted y given X (attributes)"""

    y_pred = model.predict(X)
    test_results = np.vstack((y, y_pred)).T
    return test_results

def train_model (X, y):
    """Train the model """

    from sklearn.linear_model import LogisticRegression

```

```

    model = LogisticRegression(C=1000)
    model.fit(X, y)
    return model

##### Main code #####

# Load data
data_set = load_data()

# List of regularisation values
number_of_training_points = range(25, 450, 25)

# Set up empty lists to record results
training_accuracy = []
test_accuracy = []
n_results = []

for n in number_of_training_points:
    # Repeat ml model/prediction 1000 times for each different number of runs
    for i in range(1000):

        # Split data into training and test sets
        X_train,X_test,y_train,y_test = split_data(data_set, 0.25, n)

        # Normalise data
        X_train_std, X_test_std = normalise(X_train,X_test)
        # Repeat test 1000x per level of c
        n_results.append(n)

        # Train model
        model = train_model(X_train_std,y_train)

        # Produce results for training set
        test_results = test_model(model, X_train_std, y_train)
        performance = calculate_diagnostic_performance(test_results)
        training_accuracy.append(performance['accuracy'])

        # Produce results for test set
        test_results = test_model(model, X_test_std, y_test)
        performance = calculate_diagnostic_performance(test_results)
        test_accuracy.append(performance['accuracy'])

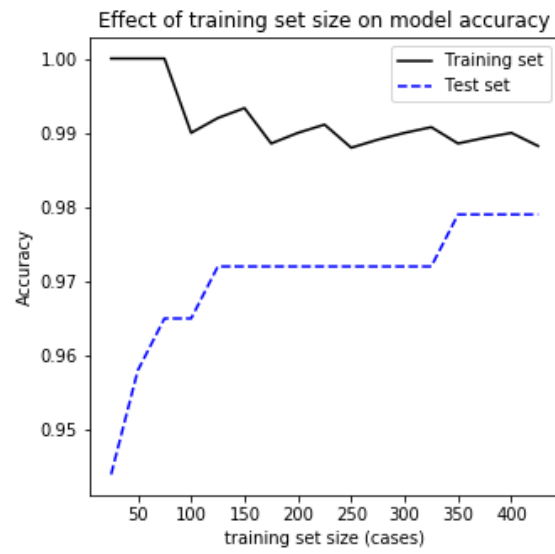
results = pd.DataFrame()
results['n'] = n_results
results['training_accuracy'] = training_accuracy
results['test_accuracy'] = test_accuracy
summary = results.groupby('n').median()
summary['n'] = list(summary.index)

print (summary)
chart_results (summary)

```

OUT:

	training_accuracy	test_accuracy	n
n			
25	1.0	0.930070	25
50	1.0	0.944056	50



75	1.0	0.951049	75
100	1.0	0.951049	100
125	1.0	0.958042	125
150	1.0	0.958042	150
175	1.0	0.958042	175
200	1.0	0.958042	200
225	1.0	0.958042	225
250	1.0	0.958042	250
275	1.0	0.958042	275
300	1.0	0.958042	300
325	1.0	0.958042	325
350	1.0	0.958042	350
375	1.0	0.958042	375
400	1.0	0.951049	400
425	1.0	0.958042	425

6.8 Working with ordinal and categorical data

Some data sets may have ordinal data, which are descriptions with a natural order, such as small, medium large. There may also be categorical data which has no obvious order like green, blue, red. We'll usually want to convert both of these into numbers for use by machine learning models.

Let's look at an example:

```
import pandas as pd

colour = ['green', 'green', 'red', 'blue', 'green', 'red', 'red']
size = ['small', 'small', 'large', 'medium', 'medium', 'x large', 'x small']

df = pd.DataFrame()
df['colour'] = colour
df['size'] = size

print (df)
```

OUT:

	colour	size
0	green	small
1	green	small
2	red	large
3	blue	medium
4	green	medium
5	red	x large
6	red	x small

6.8.1 Working with ordinal data

One of our columns is obviously ordinal data: size has a natural order to it. We can convert this text to a number by mapping a dictionary to the column. We will create a new column (size_number) which replaces the text with a number.

Define mapping dictionary:

```
size_classes = {'x small': 1,
                'small': 2,
                'medium': 3,
                'large': 4,
                'x large': 5}
```

Map to dataframe and put results in a new column:

```
df['size_number'] = df['size'].map(size_classes)
```

Display the new dataframe:

```
print (df)
```

OUT:

	colour	size	size_number
0	green	small	2
1	green	small	2
2	red	large	4
3	blue	medium	3

4	green	medium	3
5	red	x large	5
6	red	x small	1

6.8.2 Working with categorical data

There is no obvious sensible mapping of colour to a number. So in this case we create an extra column for each colour and put a one in the relevant column. For this we use pandas *get_dummies* method.

```
colours_df = pd.get_dummies(df['colour'])
```

```
print (colours_df)
```

OUT:

	blue	green	red
0	0	1	0
1	0	1	0
2	0	0	1
3	1	0	0
4	0	1	0
5	0	0	1
6	0	0	1

We then combine the new dataframe with the original one, and we can delete the temporary one we made:

```
df = pd.concat([df, colours_df], axis=1, join='inner')
```

```
del colours_df
```

```
print (df)
```

OUT:

	colour	size	size_number	blue	green	red
0	green	small	2	0	1	0
1	green	small	2	0	1	0
2	red	large	4	0	0	1
3	blue	medium	3	1	0	0
4	green	medium	3	0	1	0
5	red	x large	5	0	0	1
6	red	x small	1	0	0	1

6.8.3 Selecting just our new columns

At the moment we have both the original data and the transformed data. For use in the model we would just keep the new columns. Here we'll use the pandas *loc* method to select column slices from *size_number* onwards:

```
df1 = (df.loc[:, 'size_number':])
```

```
print (df1)
```

OUT:

	size_number	blue	green	red
0	2	0	1	0
1	2	0	1	0

2	4	0	0	1
3	3	1	0	0
4	3	0	1	0
5	5	0	0	1
6	1	0	0	1

6.9 Support Vector Machines (SVMs)

So far we have used logistic regression to create our machine learning model. We will now cover some alternative methods, starting with Support Vector Machines. We can keep nearly of our code. In fact we only have to change the three lines in the 'train mode' function.

We'll re-use the logistic regression code for looking for appropriate regularisation of the model (to avoid over-fitting of the model to the training data). Our three lines of code which define the model are now:

```
from sklearn.svm import SVC
model=SVC(kernel='linear',C=c)
model.fit(X_train_std,y_train)
```

(C is the regularisation term which we will vary in order to find the optimum).

SVMs can use a variety of methods to fit. Two common methods are linear (as used here) where data may

For more background on SVMs see: https://en.wikipedia.org/wiki/Support_vector_machine

```
\verbatim{Support Vector Machines (SVMs)}
# import required modules

from sklearn import datasets
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

def calculate_diagnostic_performance (actual_predicted):
    """ We will calculated only accuracy in this model """

    performance = {}
    test_correct = actual_predicted[:, 0] == actual_predicted[:, 1]
    performance['accuracy'] = np.average(test_correct)

    return performance

def chart_results(results):
    x = results['c']
    y1 = results['training_accuracy']
    y2 = results['test_accuracy']

    # Create figure
    fig = plt.figure(figsize=(5,5))
    ax = fig.add_subplot(111)
    ax.plot(x,y1, color='k',linestyle='solid', label = 'Training set')
    ax.plot(x,y2, color='b',linestyle='dashed', label = 'Test set')
    ax.set_xscale('log')
    ax.set_xlabel('Regularisation (c)')
    ax.set_ylabel('Accuracy')
    plt.title('Effect of regularisation on model accuracy')
    plt.legend()
    plt.show()

def load_data ():
```

```

        """Load the data set. Here we load the Breast Cancer Wisconsin (Diagnostic)
        Data Set. Data could be loaded from other sources though the structure
        should be compatible with this data set, that is an object with the
        following attributes:
            .data (holds feature data)
            .feature_names (holds feature titles)
            .target_names (holds outcome classification names)
            .target (holds classification as zero-based number)
            .DESCR (holds text-based description of data set)"""

    data_set = datasets.load_breast_cancer()
    return data_set

def normalise (X_train,X_test):
    """Normalise X data, so that training set has mean of zero and standard
    deviation of one"""

    # Initialise a new scaling object for normalising input data
    sc=StandardScaler()
    # Set up the scaler just on the training set
    sc.fit(X_train)
    # Apply the scaler to the training and test sets
    X_train_std=sc.transform(X_train)
    X_test_std=sc.transform(X_test)
    return X_train_std, X_test_std

def print_diagnostic_results (performance):
    """Iterate through, and print, the performance metrics dictionary"""

    print('\nMachine learning diagnostic performance measures:')
    print('-----')
    for key, value in performance.items():
        print (key, '= %0.3f' %value) # print 3 decimal places
    return

def split_data (data_set, split=0.25):
    """Extract X and y data from data_set object, and split into training and
    test data. Split defaults to 75% training, 25% test if not other value
    passed to function"""

    X=data_set.data
    y=data_set.target
    X_train,X_test,y_train,y_test=train_test_split(
        X,y,test_size=split)
    return X_train,X_test,y_train,y_test

def test_model(model, X, y):
    """Return predicted y given X (attributes)"""

    y_pred = model.predict(X)
    test_results = np.vstack((y, y_pred)).T
    return test_results

def train_model (X, y, c):
    """Train the model """

    from sklearn.svm import SVC
    model=SVC(kernel='rbf',C=c)

```

```

    model.fit(X_train_std,y_train)
    return model

##### Main code #####

# Load data
data_set = load_data()

# List of regularisation values
c_list = [0.0001, 0.001, 0.01, 0.1, 1, 10, 100, 1000, 10000]
training_accuracy = []
test_accuracy = []
c_results = [] # record c

for c in c_list:
    for i in range(1000): # repeat model for better estimation of optimal C

        # Split data into trainign and test sets
        X_train,X_test,y_train,y_test = split_data(data_set, 0.25)

        # Normalise data
        X_train_std, X_test_std = normalise(X_train,X_test)
        # Repeat test 1000x per level of c
        c_results.append(c)

        # Train model
        model = train_model(X_train_std,y_train, c)

        # Produce results for training set
        test_results = test_model(model, X_train_std, y_train)
        performance = calculate_diagnostic_performance(test_results)
        training_accuracy.append(performance['accuracy'])

        # Produce results for test set
        test_results = test_model(model, X_test_std, y_test)
        performance = calculate_diagnostic_performance(test_results)
        test_accuracy.append(performance['accuracy'])

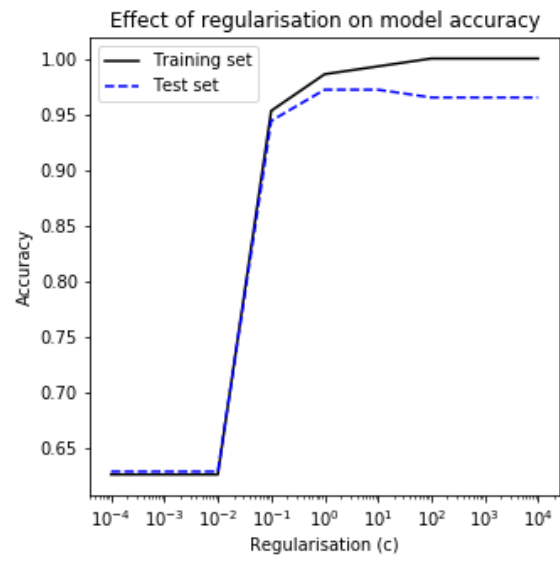
results = pd.DataFrame()
results['c'] = c_results
results['training_accuracy'] = training_accuracy
results['test_accuracy'] = test_accuracy
summary = results.groupby('c').median()
summary['c'] = list(summary.index)

print (summary)
chart_results (summary)

```

OUT:

	training_accuracy	test_accuracy	c
c			
0.0001	0.626761	0.629371	0.0001
0.0010	0.626761	0.629371	0.0010
0.0100	0.626761	0.629371	0.0100
0.1000	0.953052	0.944056	0.1000
1.0000	0.985915	0.972028	1.0000



10.0000	0.992958	0.972028	10.0000
100.0000	1.000000	0.965035	100.0000
1000.0000	1.000000	0.965035	1000.0000