An introduction to Python Programming for Research

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Chapter 1

Introduction to Python

1.1 Introduction

1.1.1 Why teach Python?

- In this first session, we will introduce Python.
- This course is about programming for data analysis and visualisation in research.
- It's not mainly about Python.
- But we have to use some language.

1.1.2 Why Python?

- Python is quick to program in
- Python is popular in research, and has lots of libraries for science
- Python interfaces well with faster languages
- Python is free, so you'll never have a problem getting hold of it, wherever you go.

1.1.3 Why write programs for research?

- Not just labour saving
- Scripted research can be tested and reproduced

1.1.4 Sensible Input - Reasonable Output

Programs are a rigorous way of describing data analysis for other researchers, as well as for computers.

Computational research suffers from people assuming each other's data manipulation is correct. By sharing codes, which are much more easy for a non-author to understand than spreadsheets, we can avoid the "SIRO" problem. The old saw "Garbage in Garbage out" is not the real problem for science:

- Sensible input
- Reasonable output

1.2 Many kinds of Python

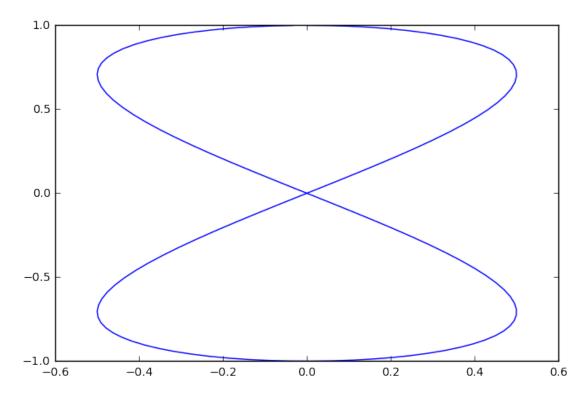
1.2.1 The Jupyter Notebook

The easiest way to get started using Python, and one of the best for research data work, is the Jupyter Notebook.

In the notebook, you can easily mix code with discussion and commentary, and mix code with the results of that code; including graphs and other data visualisations.

/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment

Out[1]: [<matplotlib.lines.Line2D at 0x2b40563e61d0>]



We're going to be mainly working in the IPython notebook in this course. To get hold of a copy of the notebook, follow the setup instructions shown on the course website, or use the installation in UCL teaching cluster rooms.

IPython notebooks consist of discussion cells, referred to as "markdown cells", and "code cells", which contain Python. This document has been created using IPython notebook, and this very cell is a **Markdown Cell**.

Code cell inputs are numbered, and show the output below.

Markdown cells contain text which uses a simple format to achive pretty layout, for example, to obtain: **bold**, *italic*

• Bullet

Quote

We write:

```
**bold**, *italic*

* Bullet

> Ouote
```

See the Markdown documentation at This Hyperlink

1.2.2 Typing code in the notebook

When working with the notebook, you can either be in a cell, typing its contents, or outside cells, moving around the notebook.

- When in a cell, press escape to leave it. When moving around outside cells, press return to enter.
- Outside a cell:
- Use arrow keys to move around.
- Press b to add a new cell below the cursor.
- Press m to turn a cell from code mode to markdown mode.
- Press shift+enter to calculate the code in the block.
- Press h to see a list of useful keys in the notebook.
- Inside a cell:
- Press tab to suggest completions of variables. (Try it!)

Supplementary material: Learn more about the notebook here. Try these videos

1.2.3 Python at the command line

Data science experts tend to use a "command line environment" to work. You'll be able to learn this at our "Software Carpentry" workshops, which cover other skills for computationally based research.

```
In [3]: %%bash
    # Above line tells Python to execute this cell as *shell code*
    # not Python, as if we were in a command line
    # This is called a 'cell magic'
    python -c "print 2*4"
```

1.2.4 Python scripts

Once you get good at programming, you'll want to be able to write your own full programs in Python, which work just like any other program on your computer. We'll not cover this in this course, you can learn more about this in MPHYG001. Here are some examples:

1.2.5 Python Libraries

We can write our own python libraries, called modules which we can import into the notebook and invoke:

```
In [6]: %%writefile draw_eight.py
    # Above line tells the notebook to treat the rest of this
    # cell as content for a file on disk.

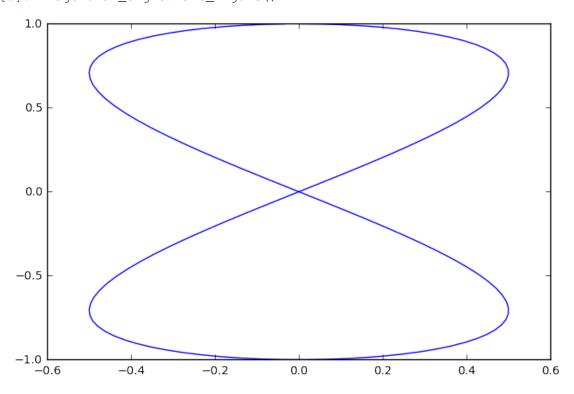
import numpy as np
import math
import matplotlib.pyplot as plt

def make_figure():
    theta=np.arange(0,4*math.pi,0.1)
    eight=plt.figure()
    axes=eight.add_axes([0,0,1,1])
    axes.plot(0.5*np.sin(theta),np.cos(theta/2))
    return eight

Writing draw_eight.py
```

In a real example, we could edit the file on disk using a program such as Notepad++ for windows or Atom for Mac.

In [7]: import draw_eight # Load the library file we just wrote to disk
In [8]: image=draw_eight.make_figure()



In [9]:

1.3 An example Python data analysis notebook

1.3.1 Why write software to manage your data and plots?

We can use programs for our entire research pipeline. Not just big scientific simulation codes, but also the small scripts which we use to tidy up data and produce plots. This should be code, so that the whole research pipeline is recorded for reproducibility. Data manipulation in spreadsheets is much harder to share or check.

You can see another similar demonstration on the software carpentry site at http://swcarpentry.github.io/python-novice-inflammation/01-numpy.html We'll try to give links to other sources of Python training along the way. Part of our approach is that we assume you know how to use the internet! If you find something confusing out there, please bring it along to the next session. In this course, we'll always try to draw your attention to other sources of information about what we're learning. Paying attention to as many of these as you need to, is just as important as these core notes.

1.3.2 Importing Libraries

Research programming is all about using libraries: tools other people have provided programs that do many cool things. By combining them we can feel really powerful but doing minimum work ourselves. The python syntax to import someone else's library is "import".

```
In [1]: import geopy # A python library for investigating geographic information.
# https://pypi.python.org/pypi/geopy
```

Now, if you try to follow along on this example in an IPython notebook, you'll probably find that you just got an error message.

You'll need to wait until we've covered installation of additional python libraries later in the course, then come back to this and try again. For now, just follow along and try get the feel for how programming for data-focused research works.

The results come out as a list inside a list: [Name, [Latitude, Longitude]]. Programs represent data in a variety of different containers like this.

1.3.3 Comments

Code after a # symbol doesn't get run.

1.3.4 Functions

We can wrap code up in a **function**, so that we can repeatedly get just the information we want.

```
In [4]: def geolocate(place):
    return geocoder.geocode(place, exactly_one = False)[0][1]
```

Defining **functions** which put together code to make a more complex task seem simple from the outside is the most important thing in programming. The output of the function is stated by "return"; the input comes in in brackets after the function name:

```
In [5]: geolocate('Cambridge')
Out[5]: (52.205337, 0.121817)
```

1.3.5 Variables

We can store a result in a variable:

1.3.6 More complex functions

The google maps API allows us to fetch a map of a place, given a latitude and longitude. The URLs look like: http://maps.googleapis.com/maps/api/staticmap?size=400x400¢er=51.51,-0.1275&zoom=12 We'll probably end up working out these URLS quite a bit. So we'll make ourselves another function to build up a URL given our parameters.

1.3.7 Checking our work

Let's see what URL we ended up with:

We can write automated tests so that if we change our code later, we can check the results are still valid.

Our previous function comes back with an Object representing the web request. In object oriented programming, we use the . operator to get access to a particular **property** of the object, in this case, the actual image at that URL is in the content property. It's a big file, so I'll just get the first few chars:

```
In [11]: map_response.content[0:20]
Out[11]: b'\x89PNG\r\n\x1a\n\x00\x00\x00\rIHDR\x00\x00\x01\x90'
```

1.3.8 Displaying results

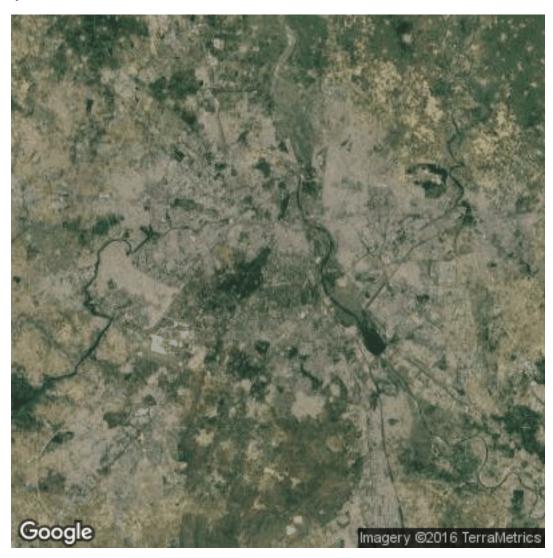
I'll need to do this a lot, so I'll wrap up our previous function in another function, to save on typing.

```
In [12]: def map_at(*args, **kwargs):
    return request_map_at(*args, **kwargs).content
```

I can use a library that comes with IPython notebook to display the image. Being able to work with variables which contain images, or documents, or any other weird kind of data, just as easily as we can with numbers or letters, is one of the really powerful things about modern programming languages like Python.



```
In [16]: IPython.core.display.Image(map_at(*geolocate("New Delhi")))
Out[16]:
```



1.3.9 Manipulating Numbers

Now we get to our research project: we want to find out how urbanised the world is, based on satellite imagery, along a line between two cites. We expect the satellite image to be greener in the countryside. We'll use lots more libraries to count how much green there is in an image.

```
In [17]: from io import BytesIO # A library to convert between files and strings
    import numpy as np # A library to deal with matrices
    from matplotlib import image as img # A library to deal with images
```

Let's define what we count as green:

This code has assumed we have our pixel data for the image as a $400 \times 400 \times 3$ 3-d matrix, with each of the three layers being red, green, and blue pixels.

We find out which pixels are green by comparing, element-by-element, the middle (green, number 1) layer to the top (red, zero) and bottom (blue, 2)

Now we just need to parse in our data, which is a PNG image, and turn it into our matrix format:

We'll also need a function to get an evenly spaced set of places between two endpoints:

1.3.10 Creating Images

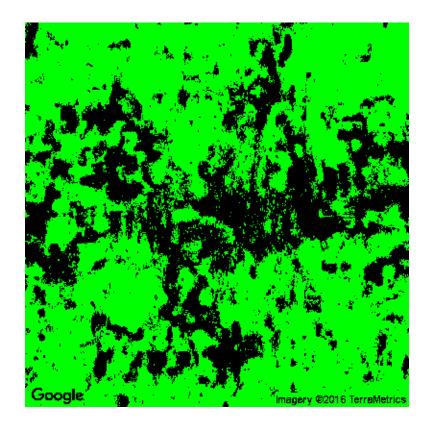
We should display the green content to check our work:

Out [24]:



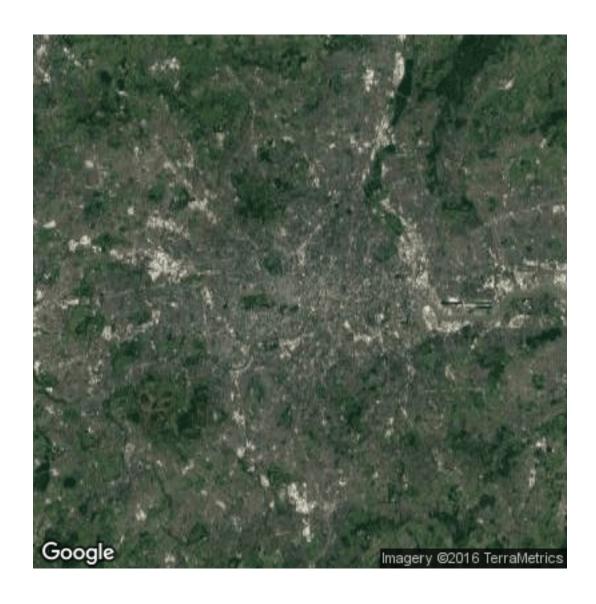
/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a momes/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a momes

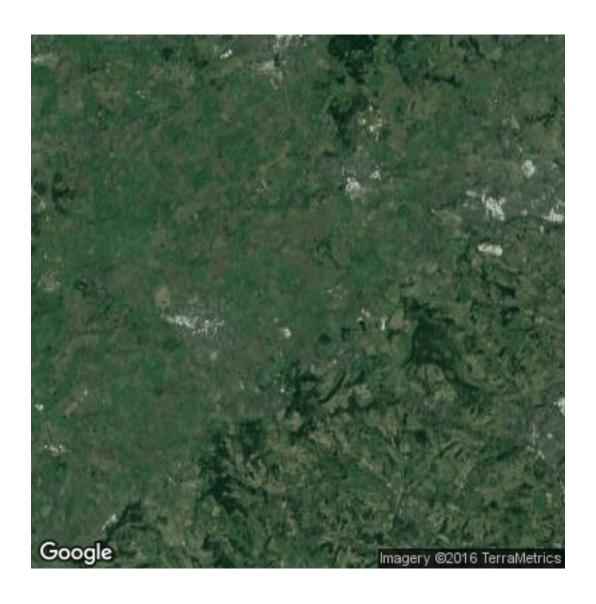
Out [25]:



1.3.11 Looping

We can loop over each element in out list of coordinates, and get a map for that place:







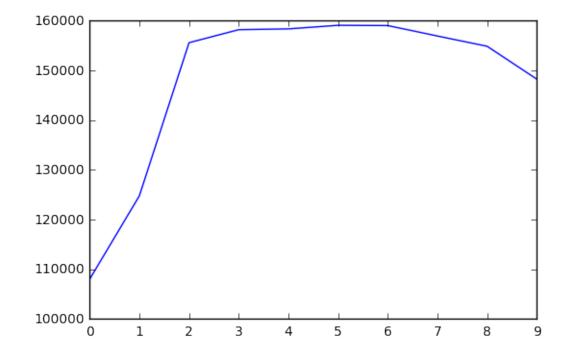


So now we can count the green from London to Birmingham!

1.3.12 Plotting graphs

Let's plot a graph.

Out[29]: [<matplotlib.lines.Line2D at 0x2adf0ba606a0>]



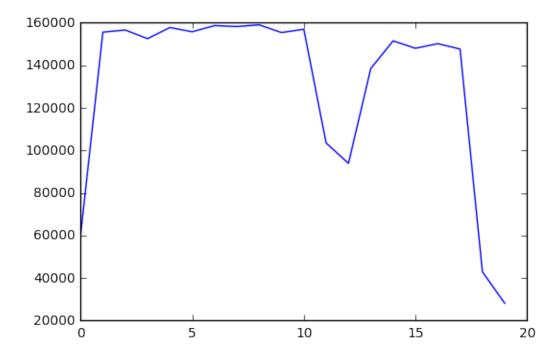
From a research perspective, of course, this code needs a lot of work. But I hope the power of using programming is clear.

1.3.13 Composing Program Elements

We built little pieces of useful code, to:

- Find latitude and longitude of a place
- Get a map at a given latitude and longitude
- Decide whether a (red, green, blue) triple is mainly green
- Decide whether each pixel is mainly green
- Plot a new image showing the green places
- Find evenly spaced points between two places

By putting these together, we can make a function which can plot this graph automatically for any two places:



And that's it! We've covered, very very quickly, the majority of the python language, and much of the theory of software engineering.

Now we'll go back, carefully, through all the concepts we touched on, and learn how to use them properly ourselves.

1.4 Variables

1.4.1 Variable Assignment

When we generate a result, the answer is displayed, but not kept anywhere.

```
In [1]: 2*3
Out[1]: 6
```

If we want to get back to that result, we have to store it. We put it in a box, with a name on the box. This is a **variable**.

```
In [2]: six = 2*3
```

```
In [3]: print six
           File "<ipython-input-3-f528ed3f7e71>", line 1
        print six
    SyntaxError: Missing parentheses in call to 'print'
  If we look for a variable that hasn't ever been defined, we get an error.
In [4]: print(seven)
        NameError
                                                        Traceback (most recent call last)
         <ipython-input-4-37b67c799511> in <module>()
    ---> 1 print(seven)
        NameError: name 'seven' is not defined
  That's not the same as an empty box, well labeled:
In [5]: nothing = None
In [6]: print(nothing)
None
In [7]: type(None)
Out[7]: NoneType
  (None is the special python value for a no-value variable.)
  Supplementary Materials: There's more on variables at http://swcarpentry.github.io/python-novice-
inflammation/01-numpy.html
  Anywhere we could put a raw number, we can put a variable label, and that works fine:
In [8]: print(5*six)
30
In [9]: scary = six*six*six
In [10]: print scary
           File "<ipython-input-10-0b56d395c7ae>", line 1
        print scary
    SyntaxError: Missing parentheses in call to 'print'
```

1.4.2 Reassignment and multiple labels

But here's the real scary thing: it seems like we can put something else in that box:

Note that the data that was there before has been lost.

No labels refer to it any more - so it has been "Garbage Collected"! We might imagine something pulled out of the box, and thrown on the floor, to make way for the next occupant.

In fact, though, it is the **label** that has moved. We can see this because we have more than one label referring to the same box:

```
In [13]: name = "James"
In [14]: nom = name
In [15]: print(nom)
James
In [16]: print(name)
```

And we can move just one of those labels:

```
In [17]: nom = "Hetherington"
In [18]: print(name)
James
In [19]: print(nom)
Hetherington
```

So we can now develop a better understanding of our labels and boxes: each box is a piece of space (an *address*) in computer memory. Each label (variable) is a reference to such a place.

When the number of labels on a box ("variables referencing an address") gets down to zero, then the data in the box cannot be found any more.

After a while, the language's "Garbage collector" will wander by, notice a box with no labels, and throw the data away, **making that box available for more data**.

Old fashioned languages like C and Fortran don't have Garbage collectors. So a memory address with no references to it still takes up memory, and the computer can more easily run out.

So when I write:

```
In [20]: name = "Jim"
```

The following things happen:

- 1. A new text **object** is created, and an address in memory is found for it.
- 2. The variable "name" is moved to refer to that address.
- 3. The old address, containing "James", now has no labels.
- 4. The garbage collector frees the memory at the old address.

Supplementary materials: There's an online python tutor which is great for visualising memory and references. Try the scenario we just looked at

Labels are contained in groups called "frames": our frame contains two labels, 'nom' and 'name'.

1.4.3 Objects and types

An object, like name, has a type. In the online python tutor example, we see that the objects have type "str". str means a text object: Programmers call these 'strings'.

```
In [21]: type(name)
Out[21]: str
```

Depending on its type, an object can have different *properties*: data fields Inside the object. Consider a Python complex number for example:

```
In [22]: z=3+1j
In [23]: dir(z)
Out[23]: ['__abs___',
            __add__',
           '_bool__',
           '__class__',
           '__delattr__',
           '__dir__',
           '__divmod__',
            __doc__',
            '___eq___',
            '___float___',
            __floordiv__',
            '__format__',
            ___ge__',
             __getattribute___',
            '__getnewargs___',
            __gt__',
             __hash___',
             __init___',
            __int__',
            '__le__',
             __lt___',
             __mod___',
            ___mul___',
             _ne__',
             _neg__',
             _new__',
            __pos__',
```

```
'__pow__',
            '___radd___',
           '__rdivmod___',
           '__reduce__',
           '__reduce_ex__',
           '__repr__',
           '__rfloordiv__',
           '__rmod__',
           '___rmul___',
           '__rpow__',
           '__rsub__',
           '__rtruediv__',
           '__setattr__',
           '__sizeof__',
           '__str__',
           '__sub__',
           '__subclasshook___',
           '__truediv__',
           'conjugate',
           'imag',
           'real']
In [24]: type(z)
Out[24]: complex
In [25]: z.real
Out[25]: 3.0
In [26]: z.imag
Out [26]: 1.0
  A property of an object is accessed with a dot.
  The jargon is that the "dot operator" is used to obtain a property of an object.
  When we try to access a property that doesn't exist, we get an error:
In [27]: z.wrong
         AttributeError
                                                        Traceback (most recent call last)
         <ipython-input-27-76215e50e85b> in <module>()
    ---> 1 z.wrong
         AttributeError: 'complex' object has no attribute 'wrong'
```

1.4.4 Reading error messages.

It's important, when learning to program, to develop an ability to read an error message and find, from in amongst all the confusing noise, the bit of the error message which tells you what to change!

We don't yet know what is meant by AttributeError, or "Traceback".

But in the above, we can see that the error happens on the **third** line of our code cell. We can also see that the error message: > 'complex' object has no attribute 'wrong' ... tells us something important. Even if we don't understand the rest, this is useful for debugging!

1.4.5 Variables and the notebook kernel

When I type code in the notebook, the objects live in memory between cells.

```
In [29]: number = 0
In [30]: print(number)
0

If I change a variable:
In [31]: number = number +1
In [32]: print(number)
```

It keeps its new value for the next cell.

But cells are **not** always evaluated in order.

If I now go back to Input 22, reading number = number + 1, and run it again, with shift-enter. Number will change from 2 to 3, then from 3 to 4. Try it!

So it's important to remember that if you move your cursor around in the notebook, it doesn't always run top to bottom.

Supplementary material: (1) https://ipython.org/ipython-doc/3/notebook/index.html (2) http://ipython.org/videos.html

1.5 Using Functions

1.5.1 Calling functions

We often want to do thing to our objects that are more complicated than just assigning them to variables.

```
In [1]: len("pneumonoultramicroscopicsilicovolcanoconiosis")
Out[1]: 45
```

Here we have "called a function".

The function len takes one input, and has one output. The output is the length of whatever the input was.

Programmers also call function inputs "parameters" or, confusingly, "arguments". Here's another example:

```
In [2]: sorted("Python")
Out[2]: ['P', 'h', 'n', 'o', 't', 'y']
```

Which gives us back a *list* of the letters in Python, sorted alphabetically.

The input goes in brackets after the function name, and the output emerges wherever the function is used.

So we can put a function call anywhere we could put a "literal" object or a variable.

1.5.2 Using methods

Objects come associated with a bunch of functions designed for working on objects of that type. We access these with a dot, just as we do for data attributes:

```
In [6]: "shout".upper()
Out[6]: 'SHOUT'
```

These are called methods. If you try to use a method defined for a different type, you get an error:

```
In [7]: x = 5
In [8]: type(x)
Out[8]: int
In [9]: x.upper()
```

```
AttributeError Traceback (most recent call last)

<ipython-input-9-2262f8ba8d84> in <module>()
----> 1 x.upper()

AttributeError: 'int' object has no attribute 'upper'
```

If you try to use a method that doesn't exist, you get an error:

Methods and properties are both kinds of **attribute**, so both are accessed with the dot operator. Objects can have both properties and methods:

```
In [11]: z = 1+5j
In [12]: z.real
Out[12]: 1.0
In [13]: z.conjugate()
Out[13]: (1-5j)
In [14]: z.conjugate
Out[14]: <function complex.conjugate>
```

1.5.3 Functions are just a type of object!

Now for something that will take a while to understand: don't worry if you don't get this yet, we'll look again at this in much more depth later in the course.

If we forget the (), we realise that a method is just a property which is a function!

```
In [15]: z.conjugate
Out[15]: <function complex.conjugate>
In [16]: type(z.conjugate)
```

```
Out[16]: builtin_function_or_method
In [17]: somefunc=z.conjugate
In [18]: somefunc()
Out[18]: (1-5j)
```

Functions are just a kind of variable, and we can assign new labels to them:

```
In [19]: sorted([1,5,3,4])
Out[19]: [1, 3, 4, 5]
In [20]: magic = sorted
In [21]: type(magic)
Out[21]: builtin_function_or_method
In [22]: magic(["Technology", "Advanced"])
Out[22]: ['Advanced', 'Technology']
```

1.5.4 Getting help on functions and methods

The 'help' function, when applied to a function, gives help on it!

```
In [23]: help(sorted)
Help on built-in function sorted in module builtins:
sorted(...)
    sorted(iterable, key=None, reverse=False) --> new sorted list
```

The 'dir' function, when applied to an object, lists all its attributes (properties and methods):

```
In [24]: dir("Hexxo")
Out [24]: ['__add__',
            '__class__',
'__contains__',
            '__delattr__',
            '__dir__',
            '__doc__',
            '___eq___',
            '__format__',
            '___ge___',
            '__getattribute__',
            '__getitem__',
            '__getnewargs___',
            '___gt___',
            ____hash___',
            '__init__',
            '__iter__',
            '__le__',
```

```
'__len__',
'__lt__',
'__mod__',
'__mul__',
'__ne__',
'__new__',
'__reduce__',
'__reduce_ex__',
'__repr__',
'__rmod__',
'__rmul__',
___setattr___',
'__str__',
'__subclasshook__',
'capitalize',
'casefold',
'center',
'count',
'encode',
'endswith',
'expandtabs',
'find',
'format',
'format_map',
'index',
'isalnum',
'isalpha',
'isdecimal',
'isdigit',
'isidentifier',
'islower',
'isnumeric',
'isprintable',
'isspace',
'istitle',
'isupper',
'join',
'ljust',
'lower',
'lstrip',
'maketrans',
'partition',
'replace',
'rfind',
'rindex',
'rjust',
'rpartition',
'rsplit',
'rstrip',
'split',
'splitlines',
'startswith',
'strip',
```

```
'swapcase',
'title',
'translate',
'upper',
'zfill']
```

Most of these are confusing methods beginning and ending with __, part of the internals of python. Again, just as with error messages, we have to learn to read past the bits that are confusing, to the bit we want:

```
In [25]: "Hexxo".replace("x", "l")
Out[25]: 'Hello'
In [26]: help("FIsh".replace)
Help on built-in function replace:
replace(...) method of builtins.str instance
    S.replace(old, new[, count]) -> str

    Return a copy of S with all occurrences of substring old replaced by new. If the optional argument count is given, only the first count occurrences are replaced.
```

1.5.5 Operators

Now that we know that functions are a way of taking a number of inputs and producing an output, we should look again at what happens when we write:

This is just a pretty way of calling an "add" function. Things would be more symmetrical if add were actually written

```
x = +(2,3)
```

Where '+' is just the name of the name of the adding function.

In python, these functions **do** exist, but they're actually **methods** of the first input: they're the mysterious ___ functions we saw earlier (Two underscores.)

```
In [29]: x.__add__(7)
Out[29]: 12
```

We call these symbols, +, - etc, "operators". The meaning of an operator varies for different types:

```
In [30]: "Hello" + "Goodbye"
Out[30]: 'HelloGoodbye'
In [31]: [2, 3, 4] + [5, 6]
Out[31]: [2, 3, 4, 5, 6]
```

Sometimes we get an error when a type doesn't have an operator:

The word "operand" means "thing that an operator operates on"! Or when two types can't work together with an operator:

To do this, put:

```
In [35]: [2, 3, 4] + [5]
Out[35]: [2, 3, 4, 5]
```

Just as in Mathematics, operators have a built-in precedence, with brackets used to force an order of operations:

```
In [36]: print 2+3*4
```

```
File "<ipython-input-36-47a4b786a9a6>", line 1
print 2+3*4

SyntaxError: Missing parentheses in call to 'print'

In [37]: print (2+3)*4

5

TypeError Traceback (most recent call last)

<ipython-input-37-f21a6482567b> in <module>()
----> 1 print (2+3)*4

TypeError: unsupported operand type(s) for *: 'NoneType' and 'int'
```

Supplementary material: http://www.mathcs.emory.edu/~valerie/courses/fall10/155/resources/op_precedence.html

1.6 Types

We have seen that Python objects have a 'type':

```
In [1]: type(5)
Out[1]: int
```

1.6.1 Floats and integers

Python has two core numeric types, int for integer, and float for real number.

```
Out[6]: float
```

The meaning of an operator varies depending on the type it is applied to! (And on the python version.)

```
In [7]: print(one//ten)
0
In [8]: one_float/ten_float
Out[8]: 0.1
In [9]: print(type(one/ten))
<class 'float'>
In [10]: type(tenth)
Out[10]: float
```

The divided by operator when applied to floats, means divide by for real numbers. But when applied to integers, it means divide then round down:

So if I have two integer variables, and I want the float division, I need to change the type first. There is a function for every type name, which is used to convert the input to an output of the desired type.

I lied when I said that the float type was a real number. It's actually a computer representation of a real number called a "floating point number". Representing $\sqrt{2}$ or $\frac{1}{3}$ perfectly would be impossible in a computer, so we use a finite amount of memory to do it.

Supplementary material:

- https://docs.python.org/2/tutorial/floatingpoint.html
- http://floating-point-gui.de/formats/fp/
- Advanced: http://docs.oracle.com/cd/E19957-01/806-3568/ncg_goldberg.html

1.6.2 Strings

Python has a built in string type, supporting many useful methods.

So + for strings means "join them together" - concatenate.

```
In [18]: print(full.upper())
JAMES HETHERNGTON
```

As for float and int, the name of a type can be used as a function to convert between types:

```
In [19]: ten, one
Out[19]: (10, 1)
In [20]: print(ten + one)

In [21]: print(float( str(ten)+str(one) ))
101.0
```

We can remove extraneous material from the start and end of a string:

```
In [22]: " Hello ".strip()
Out[22]: 'Hello'
```

1.6.3 Lists

Python's basic **container** type is the list

We can define our own list with square brackets:

```
In [23]: [1, 3, 7]
Out[23]: [1, 3, 7]
In [24]: type([1, 3, 7])
Out[24]: list
```

Lists *do not* have to contain just one type:

```
In [25]: various_things = [1, 2, "banana", 3.4, [1,2] ]
```

We access an **element** of a list with an int in square brackets:

```
In [26]: various_things[2]
Out[26]: 'banana'
```

```
In [27]: index = 0
          various_things[index]
Out[27]: 1
  Note that list indices start from zero.
  We can quickly make a list with numbers counted up:
In [28]: count_to_five = range(5)
          print(list(count to five))
[0, 1, 2, 3, 4]
  We can use a string to join together a list of strings:
In [29]: name = ["James", "Philip", "John", "Hetherington"]
          print("==".join(name))
James==Philip==John==Hetherington
  And we can split up a string into a list:
In [30]: "Ernst Stavro Blofeld".split(" ")
Out[30]: ['Ernst', 'Stavro', 'Blofeld']
In [31]: "Ernst Stavro Blofeld".split("o")
Out[31]: ['Ernst Stavr', ' Bl', 'feld']
  And combine these:
In [32]: "->".join("John Ronald Reuel Tolkein".split(" "))
Out[32]: 'John->Ronald->Reuel->Tolkein'
  A matrix can be represented by nesting lists – putting lists inside other lists.
In [33]: identity = [[1, 0], [0, 1]]
In [34]: identity[0][0]
Out[34]: 1
  ... but later we will learn about a better way of representing matrices.
```

1.6.4 Sequences

Many other things can be treated like lists. Python calls things that can be treated like lists sequences. A string is one such *sequence type*

```
In [35]: print(count_to_five[1])
1
In [36]: print("James"[2])
```

```
In [37]: count_to_five = list(range(5))
In [38]: count_to_five[1:3]
Out[38]: [1, 2]
In [39]: "Hello World"[4:8]
Out[39]: 'o Wo'
In [40]: len(various_things)
Out[40]: 5
In [41]: len("Python")
Out[41]: 6
In [42]: name
Out[42]: ['James', 'Philip', 'John', 'Hetherington']
In [43]: "John" in name
Out[43]: True
In [44]: 3 in count_to_five
Out[44]: True
In [45]: "James's Class"
Out[45]: "James's Class"
In [46]: '"Wow!", said Bob.'
Out[46]: '"Wow!", said Bob.'
```

1.6.5 Unpacking

Multiple values can be **unpacked** when assigning from sequences, like dealing out decks of cards.

1.7 Containers

In [53]:

1.7.1 Checking for containment.

The list we saw is a container type: its purpose is to hold other objects. We can ask python whether or not a container contains a particular item:

ValueError: need more than 2 values to unpack

```
In [1]: 'Dog' in ['Cat', 'Dog', 'Horse']
Out[1]: True
In [2]: 'Bird' in ['Cat', 'Dog', 'Horse']
Out[2]: False
In [3]: 2 in range(5)
Out[3]: True
In [4]: 99 in range(5)
Out[4]: False
```

1.7.2 Mutability

A list can be modified:

1.7.3 Tuples

A tuple is an immutable sequence. It is like a list, execpt it cannot be changed. It is defined with round brackets.

```
In [7]: x = 0,
        type(x)
Out[7]: tuple
In [8]: my_tuple = ("Hello", "World")
        my_tuple[0]="Goodbye"
        TypeError
                                                   Traceback (most recent call last)
        <ipython-input-8-d3ad0c7e33f1> in <module>()
          1 my_tuple = ("Hello", "World")
    ----> 2 my_tuple[0]="Goodbye"
        TypeError: 'tuple' object does not support item assignment
In [9]: type(my_tuple)
Out[9]: tuple
  str is immutable too:
In [10]: fish = "Hake"
         fish[0] = 'R'
```

But note that container reassignment is moving a label, **not** changing an element:

```
In [11]: fish = "Rake" ## OK!
```

Supplementary material: Try the online memory visualiser for this one.

1.7.4 Memory and containers

The way memory works with containers can be important:

```
In [12]: x = list(range(3))
         Х
Out[12]: [0, 1, 2]
In [13]: y = x
         У
Out[13]: [0, 1, 2]
In [14]: z = x[0:3]
        y[1] = "Gotcha!"
In [15]: x
Out[15]: [0, 'Gotcha!', 2]
In [16]: y
Out[16]: [0, 'Gotcha!', 2]
In [17]: z
Out[17]: [0, 1, 2]
In [18]: z[2] = "Really?"
In [19]: x
Out[19]: [0, 'Gotcha!', 2]
In [20]: y
Out[20]: [0, 'Gotcha!', 2]
In [21]: z
Out[21]: [0, 1, 'Really?']
```

Supplementary material: This one works well at the [memory visualiser](http://www.pythontutor.com/visualize.html#cofrontend.js&cumulative=false&heapPrimitives=true&textReferences=false&py=2&rawInputLstJSON=%5B%5D&curInstr=The explanation: While y is a second label on the same object, z is a separate object with the same data.

The difference between y=x and z=x[:] is important. (Remember [:] is equivalent to [0:<last>])

```
In [22]: x
Out[22]: [0, 'Gotcha!', 2]
In [23]: y = x
In [24]: y = x[:]
```

Nested objects make it even more complicated:

 $Try\ the\ [visualiser] (http://www.pythontutor.com/visualize.html\#code=x\%3D\%5B\%5B'a','b'\%5D,'c'\%5D\%0Ay\%3Dx\%0frontend.js\&cumulative=false\&heapPrimitives=true\&textReferences=false\&py=2\&rawInputLstJSON=\%5B\%5D\&curInstr=again.$

1.7.5 Identity vs Equality

Having the same data is different from being the same actual object in memory:

The == operator checks, element by element, that two containers have the same data. The is operator checks that they are actually the same object.

But, and this point is really subtle, for immutables, the python language might save memory by reusing a single instantiated copy. This will always be safe.

This can be useful in understanding problems like the one above:

```
In [32]: x = range(3)
         \lambda = X
         z=x[:]
In [33]: x == y
Out[33]: True
In [34]: x is y
Out[34]: True
In [35]: x == z
Out[35]: True
In [36]: x is z
Out[36]: False
In [37]: {
              'a': 2,
             'b': 3
          }
Out[37]: {'a': 2, 'b': 3}
In [38]:
In [38]:
In [38]:
In [38]:
In [38]:
In [38]:
```

1.8 Dictionaries

1.8.1 The Python Dictionary

Python supports a container type called a dictionary.

This is also known as an "associative array", "map" or "hash" in other languages.

In a list, we use a number to look up an element:

```
In [1]: names="Martin Luther King".split(" ")
```

```
In [2]: names[1]
Out[2]: 'Luther'
```

In a dictionary, we look up an element using another object of our choice:

1.8.2 Keys and Values

The things we can use to look up with are called keys:

```
In [8]: me.keys()
Out[8]: dict_keys(['Jobs', 'name', 'age'])
```

The things we can look up are called **values**:

```
In [9]: me.values()
Out[9]: dict_values([['Programmer', 'Teacher'], 'James', 39])
```

When we test for containment on a dict we test on the **keys**:

```
In [10]: 'Jobs' in me
Out[10]: True
In [11]: 'James' in me
Out[11]: False
In [12]: 'James' in me.values()
Out[12]: True
```

1.8.3 Immutable Keys Only

The way in which dictionaries work is one of the coolest things in computer science: the "hash table". The details of this are beyond the scope of this course, but we will consider some aspects in the section on performance programming.

One consequence of this implementation is that you can only use **immutable** things as keys.

Remember – square brackets denote lists, round brackets denote tuples.

1.8.4 No guarantee of order

Another consequence of the way dictionaries work is that there's no guaranteed order among the elements:

1.8.5 Sets

A set is a list which cannot contain the same element twice. We make one by calling set () on any sequence, e.g. a list or string.

```
In [17]: unique_letters
Out[17]: {' ', 'H', 'J', 'a', 'e', 'q', 'h', 'i', 'm', 'n', 'o', 'r', 's', 't'}
  Or by defining a literal like a dictionary, but without the colons:
In [18]: primes_below_ten = { 2, 3, 5, 7}
In [19]: type(unique_letters)
Out[19]: set
In [20]: type(primes_below_ten)
Out[20]: set
In [21]: unique letters
Out[21]: {' ', 'H', 'J', 'a', 'e', 'g', 'h', 'i', 'm', 'n', 'o', 'r', 's', 't'}
  This will be easier to read if we turn the set of letters back into a string, with join:
In [22]: "".join(unique_letters)
Out[22]: 'JarnotgmeH hsi'
  A set has no particular order, but is really useful for checking or storing unique values.
  Set operations work as in mathematics:
In [23]: x = set("Hello")
          y = set("Goodbye")
In [24]: x & y # Intersection
Out[24]: {'e', 'o'}
In [25]: x | y # Union
```

In [16]: name = "James Hetherington"

unique letters = set(name)

Out[25]: {'G', 'H', 'b', 'd', 'e', 'l', 'o', 'y'}

Out[26]: {'G', 'b', 'd', 'y'}

Your programs will be faster and more readable if you use the appropriate container type for your data's meaning. Always use a set for lists which can't in principle contain the same data twice, always use a dictionary for anything which feels like a mapping from keys to values.

In [26]: y - x # y intersection with complement of x: letters in Goodbye but not in Hello

1.9 Data structures

1.9.1 Nested Lists and Dictionaries

In research programming, one of our most common tasks is building an appropriate *structure* to model our complicated data. Later in the course, we'll see how we can define our own types, with their own attributes, properties, and methods. But probably the most common approach is to use nested structures of lists, dictionaries, and sets to model our data. For example, an address might be modelled as a dictionary with appropriately named fields:

A collection of people's addresses is then a list of dictionaries:

A more complicated data structure, for example for a census database, might have a list of residents or employees at each address:

Which is then a list of dictionaries, with keys which are strings or lists. We can go further, e.g.:

```
In [8]: UCL['Residential']=False
```

And we can write code against our structures:

This was an example of a 'list comprehension', which have used to get data of this structure, and which we'll see more of in a moment...

1.9.2 Exercise: a Maze Model.

Work with a partner to design a data structure to represent a maze using dictionaries and lists.

- Each place in the maze has a name, which is a string.
- Each place in the maze has one or more people currently standing at it, by name.
- Each place in the maze has a maximum capacity of people that can fit in it.
- From each place in the maze, you can go from that place to a few other places, using a direction like 'up', 'north', or 'sideways'

Create an example instance, in a notebook, of a simple structure for your maze:

- The front room can hold 2 people. James is currently there. You can go outside to the garden, or upstairs to the bedroom, or north to the kitchen.
- From the kitchen, you can go south to the front room. It fits 1 person.
- From the garden you can go inside to front room. It fits 3 people. Sue is currently there.
- From the bedroom, you can go downstairs to the front room. You can also jump out of the window to the garden. It fits 2 people.

Make sure that your model:

- Allows empty rooms
- Allows you to jump out of the upstairs window, but not to fly back up.
- Allows rooms which people can't fit in.

myhouse = ["Your answer here"]

1.9.3 Solution: my Maze Model

Here's one possible solution to the Maze model. Yours will probably be different, and might be just as good. That's the artistry of software engineering: some solutions will be faster, others use less memory, while others will be easier for other people to understand. Optimising and balancing these factors is fun!

```
'exits': {
            'south' : 'living'
        'people' : [],
        'capacity': 1
    },
    'garden' : {
        'exits': {
             'inside' : 'living'
        'people' : ['Sue'],
        'capacity' : 3
    },
    'bedroom' : {
        'exits': {
             'downstairs' : 'living',
            'jump' : 'garden'
        },
        'people' : [],
        'capacity' : 1
    }
}
```

Some important points:

```
In [2]: house['living']['capacity']
Out[2]: 2
```

- The whole solution is a complete nested structure.
- I used indenting to make the structure easier to read.
- Python allows code to continue over multiple lines, so long as sets of brackets are not finished.
- There is an **Empty** person list in empty rooms, so the type structure is robust to potential movements of people.
- We are nesting dictionaries and lists, with string and integer data.

1.10 Control and Flow

1.10.1 Turing completeness

Now that we understand how we can use objects to store and model our data, we only need to be able to control the flow of our program in order to have a program that can, in principle, do anything! Specifically we need to be able to:

 Control whether a program statement should be executed or not, based on a variable. "Conditionality" • Jump back to an earlier point in the program, and run some statements again. "Branching"

Once we have these, we can write computer programs to process information in arbitrary ways: we are *Turing Complete*!

1.10.2 Conditionality

Conditionality is achieved through Python's if statement:

```
In [1]: x = 5
    if x < 0:
        print(x, " is negative")</pre>
```

The absence of output here means the if clause prevented the print statement from running.

```
In [2]: x=-10
    if x < 0:
        print(x, " is negative")
-10 is negative</pre>
```

The first time through, the print statement never happened.

The **controlled** statements are indented. Once we remove the indent, the statements will once again happen regardless.

1.10.3 Else and Elif

Python's if statement has optional elif (else-if) and else clauses:

```
In [3]: x = 5
        if x < 0:
           print("x is negative")
        else:
            print("x is positive")
x is positive
In [4]: x = 5
        if x < 0:
           print "x is negative"
        elif x == 0:
           print "x is zero"
        else:
            print "x is positive"
          File "<ipython-input-4-ba8f73cfb017>", line 3
        print "x is negative"
    SyntaxError: Missing parentheses in call to 'print'
```

Try editing the value of x here, and note that other sections are found.

1.10.4 Comparison

True and False are used to represent boolean (true or false) values.

```
In [6]: 1 > 2
Out[6]: False
```

Comparison on strings is alphabetical.

```
In [7]: "UCL" > "KCL"
Out[7]: True
But case sensitive:
```

```
In [8]: "UCL" > "kcl"
Out[8]: False
```

There's no automatic conversion of the **string** True to true:

```
In [9]: True == "True"
Out[9]: False
```

There are subtle implied order comparisons between types, but it would be bad style to rely on these, because most human readers of your code won't remember them, so the code is not understandable.

Any statement that evaluates to True or False can be used to control an if Statement.

1.10.5 Automatic Falsehood

Various other things automatically count as true or false, which can make life easier when coding:

```
SyntaxError: Missing parentheses in call to 'print'
```

We can use logical not and logical and to combine true and false:

not also understands magic conversion from false-like things to True or False.

```
In [18]: not not "Who's there!" # Thanks to Mysterious Student
Out[18]: True
In [19]: bool("")
Out[19]: False
In [20]: bool("James")
Out[20]: True
In [21]: bool([])
Out[21]: False
In [22]: bool(['a'])
Out[22]: True
In [23]: bool({})
Out[23]: False
In [24]: bool({'name': 'James'})
Out[24]: True
In [25]: bool(0)
Out[25]: False
In [26]: bool(1)
Out[26]: True
```

But subtly, although these quantities evaluate True or False in an if statement, they're not themselves actually True or False under ==:

```
In [27]: [] == False
Out[27]: False
In [28]: bool([]) == False
Out[28]: True
```

1.10.6 Indentation

In Python, indentation is semantically significant. You can choose how much indentation to use, so long as you are consistent, but four spaces is conventional. Please do not use tabs.

In the notebook, and most good editors, when you press <tab>, you get four spaces. No indentation when it is expected, results in an error:

1.10.7 Pass

A statement expecting identation must have some indented code. This can be annoying when commenting things out. (With #)

So the pass statement is used to do nothing.

1.10.8 Iteration

Our other aspect of control is looping back on ourselves.

We use for ... in to "iterate" over lists:

Each time through the loop, the variable in the value slot is updated to the **next** element of the sequence.

1.10.9 Iterables

Any sequence type is iterable:

```
In [3]: vowels="aeiou"
    sarcasm = []

for letter in "Okay":
    if letter.lower() in vowels:
        repetition = 3
    else:
        repetition = 1
        sarcasm.append(letter*repetition)

"".join(sarcasm)
Out[3]: 'OOOkaaay'
```

The above is a little puzzle, work through it to understand why it does what it does.

1.10.10 Dictionaries are Iterables

All sequences are iterables. Some iterables (things you can for loop over) are not sequences (things with you can do x[5] to), for example sets and dictionaries.

```
In [4]: import datetime
    now = datetime.datetime.now()

founded = {"James": 1976, "UCL": 1826, "Cambridge": 1209}
```

1.10.11 Unpacking and Iteration

Unpacking can be useful with iteration:

UCL is 190 years old.

```
In [5]: triples=[
            [4,11,15],
            [39, 4, 18]
In [6]: for whatever in triples:
            print(whatever)
[4, 11, 15]
[39, 4, 18]
In [7]: for first, middle, last in triples:
            print(middle)
11
In [8]: # A reminder that the words you use for variable names are arbitrary:
        for hedgehog, badger, fox in triples:
            print (badger)
11
4
  for example, to iterate over the items in a dictionary as pairs:
In [9]: things = {"James": [1976, 'Kendal'],
                   "UCL": [1826, 'Bloomsbury'],
                   "Cambridge": [1209, 'Cambridge']}
        print(things.items())
dict_items([('Cambridge', [1209, 'Cambridge']), ('James', [1976, 'Kendal']), ('UCL', [1826
In [10]: for name, year in founded.items():
             print (name, " is ", current_year - year, "years old.")
Cambridge is 807 years old.
James is 40 years old.
```

1.10.12 Break, Continue

- Continue skips to the next turn of a loop
- Break stops the loop early

```
In [11]: for n in range(50):
              if n==20:
                  break
              if n % 2 == 0:
                  continue
              print(n)
1
3
5
7
9
11
13
15
17
19
```

These aren't useful that often, but are worth knowing about. There's also an optional else clause on loops, executed only if you don't break, but I've never found that useful.

1.10.13 Classroom exercise: the Maze Population

Take your maze data structure. Write a program to count the total number of people in the maze, and also determine the total possible occupants.

1.10.14 Solution: counting people in the maze

With this maze structure:

```
In [1]: house = {
             'living' : {
                 'exits': {
                     'north' : 'kitchen',
                     'outside' : 'garden',
                     'upstairs' : 'bedroom'
                 },
                 'people' : ['James'],
                 'capacity' : 2
            },
             'kitchen' : {
                 'exits': {
                     'south' : 'living'
                 'people' : [],
                 'capacity' : 1
             },
             'garden' : {
                 'exits': {
```

```
'inside' : 'living'
},
'people' : ['Sue'],
'capacity' : 3
},
'bedroom' : {
    'exits': {
        'downstairs' : 'living',
        'jump' : 'garden'
    },
    'people' : [],
    'capacity' : 1
}
```

We can count the occupants and capacity like this:

1.11 Comprehensions

1.11.1 The list comprehension

If you write a for loop **inside** a pair of square brackets for a list, you magic up a list as defined. This can make for concise but hard to read code, so be careful.

```
In [1]: [2**x for x in range(10)]
Out[1]: [1, 2, 4, 8, 16, 32, 64, 128, 256, 512]
```

Which is equivalent to the following code without using comprehensions:

You can do quite weird and cool things with comprehensions:

```
In [3]: [len(str(2**x)) for x in range(10)]
Out[3]: [1, 1, 1, 1, 2, 2, 2, 3, 3, 3]
```

1.11.2 Selection in comprehensions

You can write an if statement in comprehensions too:

1.11.3 Comprehensions versus building lists with append:

This code:

```
In [6]: result=[]
    for x in range(30):
        if x%3 == 0:
            result.append(2**x)
    result
Out[6]: [1, 8, 64, 512, 4096, 32768, 262144, 2097152, 16777216, 134217728]
```

Does the same as the comprehension above. The comprehension is generally considered more readable. Comprehensions are therefore an example of what we call 'syntactic sugar': they do not increase the capabilities of the language.

Instead, they make it possible to write the same thing in a more readable way.

Almost everything we learn from now on will be either syntactic sugar or interaction with something other than idealised memory, such as a storage device or the internet. Once you have variables, conditionality, and branching, your language can do anything. (And this can be proved.)

1.11.4 Nested comprehensions

If you write two for statements in a comprehension, you get a single array generated over all the pairs:

```
In [7]: [x - y for x in range(4) for y in range(4)]
Out[7]: [0, -1, -2, -3, 1, 0, -1, -2, 2, 1, 0, -1, 3, 2, 1, 0]
```

You can select on either, or on some combination:

```
In [8]: [x - y for x in range(4) for y in range(4) if x>=y]
Out[8]: [0, 1, 0, 2, 1, 0, 3, 2, 1, 0]
```

If you want something more like a matrix, you need to do two nested comprehensions!

```
In [9]: [[x - y for x in range(4)] for y in range(4)]
Out[9]: [[0, 1, 2, 3], [-1, 0, 1, 2], [-2, -1, 0, 1], [-3, -2, -1, 0]]
```

Note the subtly different square brackets.

Note that the list order for multiple or nested comprehensions can be confusing:

```
In [10]: [x+y for x in ['a','b','c'] for y in ['1','2','3']]
Out[10]: ['a1', 'a2', 'a3', 'b1', 'b2', 'b3', 'c1', 'c2', 'c3']
In [11]: [[x+y for x in ['a','b','c']] for y in ['1','2','3']]
Out[11]: [['a1', 'b1', 'c1'], ['a2', 'b2', 'c2'], ['a3', 'b3', 'c3']]
```

1.11.5 Dictionary Comprehensions

You can automatically build dictionaries, by using a list comprehension syntax, but with curly brackets and a colon:

```
In [12]: { (str(x))*3: x for x in range(3) }
Out[12]: {'000': 0, '111': 1, '222': 2}
```

1.11.6 List-based thinking

Once you start to get comfortable with comprehensions, you find yourself working with containers, nested groups of lists and dictionaries, as the 'things' in your program, not individual variables.

Given a way to analyse some dataset, we'll find ourselves writing stuff like:

```
analysed_data = [analyze(datum) for datum in data]
```

There are lots of built-in methods that provide actions on lists as a whole:

```
In [13]: any([True, False, True])
Out[13]: True
In [14]: all([True, False, True])
Out[14]: False
In [15]: max([1, 2, 3])
Out[15]: 3
In [16]: sum([1, 2, 3])
Out[16]: 6
```

My favourite is map, which is syntactic sugar for a simple list comprehension that applies one function to every member of a list:

```
In [17]: [str(x) for x in range(10)]
Out[17]: ['0', '1', '2', '3', '4', '5', '6', '7', '8', '9']
In [18]: list(map(str, range(10)))
Out[18]: ['0', '1', '2', '3', '4', '5', '6', '7', '8', '9']
    So I can write:
analysed_data = map(analyse, data)
```

1.11.7 Classroom Exercise: Occupancy Dictionary

Take your maze data structure. Write a program to print out a new dictionary, which gives, for each room's name, the number of people in it. Don't add in a zero value in the dictionary for empty rooms.

The output should look similar to:

```
In [19]: {'bedroom': 1, 'garden': 3, 'kitchen': 1, 'living': 2}
Out[19]: {'bedroom': 1, 'garden': 3, 'kitchen': 1, 'living': 2}
```

1.11.8 Solution

With this maze structure:

```
In [1]: house = {
            'living' : {
                 'exits': {
                     'north' : 'kitchen',
                     'outside' : 'garden',
                     'upstairs' : 'bedroom'
                 },
                 'people' : ['James'],
                 'capacity' : 2
            },
            'kitchen' : {
                 'exits': {
                     'south' : 'living'
                 'people' : [],
                 'capacity' : 1
            },
             'garden' : {
                 'exits': {
                     'inside' : 'living'
                 'people' : ['Sue'],
                 'capacity' : 3
            },
             'bedroom' : {
                 'exits': {
                     'downstairs' : 'living',
                     'jump' : 'garden'
                 },
                 'people' : [],
                 'capacity': 1
            }
```

We can get a simpler dictionary with just capacities like this:

```
In [2]: {name : room['capacity'] for name, room in house.items()}
Out[2]: {'bedroom': 1, 'garden': 3, 'kitchen': 1, 'living': 2}
```

1.12 Functions

1.12.1 Definition

We use def to define a function, and return to pass back a value:

1.12.2 Default Parameters

We can specify default values for parameters:

If you have some parameters with defaults, and some without, those with defaults **must** go later. If you have multiple default arguments, you can specify neither, one or both:

1.12.3 Side effects

Functions can do things to change their **mutable** arguments, so return is optional. This is pretty awful style, in general, functions should normally be side-effect free. Here is a contrived example of a function that makes plausible use of a side-effect

In this example, we're using [:] to access into the same list, and write it's data.

```
vec = [element*2 for element in vec]
```

would just move a local label, not change the input.

But I'd usually just write this as a function which **returned** the output:

Let's remind ourselves of the behaviour for modifying lists in-place using [:] with a simple array:

1.12.4 Early Return

Return without arguments can be used to exit early from a function

Here's a slightly more plausibly useful function-with-side-effects to extend a list with a specified padding datum.

1.12.5 Unpacking arguments

If a vector is supplied to a function with a '*', its elements are used to fill each of a function's arguments.

1.12.6 Sequence Arguments

Similarly, if a * is used in the **definition** of a function, multiple arguments are absorbed into a list **inside** the function:

1.12.7 Keyword Arguments

If two asterisks are used, named arguments are supplied inside the function as a dictionary:

These different approaches can be mixed:

1.13 Using Libraries

'__name__',

1.13.1 Import

To use a function or type from a python library, rather than a **built-in** function or type, we have to import the library.

```
In [1]: math.sin(1.6)
       ______
       NameError
                                                Traceback (most recent call last)
       <ipython-input-1-ecc9cee3d19a> in <module>()
   ----> 1 math.sin(1.6)
       NameError: name 'math' is not defined
In [2]: import math
In [3]: math.sin(1.6)
Out[3]: 0.9995736030415051
  We call these libraries modules:
In [4]: type(math)
Out[4]: module
  The tools supplied by a module are attributes of the module, and as such, are accessed with a dot.
In [5]: dir(math)
Out[5]: ['__doc__',
         '___file__',
        '__loader__',
```

```
'__package__',
'__spec__',
'acos',
'acosh',
'asin',
'asinh',
'atan',
'atan2',
'atanh',
'ceil',
'copysign',
'cos',
'cosh',
'degrees',
'e',
'erf',
'erfc',
'exp',
'expm1',
'fabs',
'factorial',
'floor',
'fmod',
'frexp',
'fsum',
'gamma',
'hypot',
'isfinite',
'isinf',
'isnan',
'ldexp',
'lgamma',
'log',
'log10',
'log1p',
'log2',
'modf',
'pi',
'pow',
'radians',
'sin',
'sinh',
'sqrt',
'tan',
'tanh',
'trunc']
```

They include properties as well as functions:

```
In [6]: math.pi
Out[6]: 3.141592653589793
```

You can always find out where on your storage medium a library has been imported from:

Note that import does *not* install libraries from PyPI. It just makes them available to your current notebook session, assuming they are already installed. Installing libraries is harder, and we'll cover it later. So what libraries are available? Until you install more, you might have just the modules that come with Python, the *standard library*

Supplementary Materials: Review the list of standard library modules: https://docs.python.org/2/library/

If you installed via Anaconda, then you also have access to a bunch of modules that are commonly used in research.

Supplementary Materials: Review the list of modules that are packaged with Anaconda by default: http://docs.continuum.io/anaconda/pkg-docs.html (The green ticks)

We'll see later how to add more libraries to our setup.

1.13.2 Why bother?

Why bother with modules? Why not just have everything available all the time?

The answer is that there are only so many names available! Without a module system, every time I made a variable whose name matched a function in a library, I'd lose access to it. In the olden days, people ended up having to make really long variable names, thinking their names would be unique, and they still ended up with "name clashes". The module mechanism avoids this.

1.13.3 Importing from modules

Still, it can be annoying to have to write math.sin(math.pi) instead of sin(pi). Things can be imported *from* modules to become part of the current module:

Importing one-by-one like this is a nice compromise between typing and risk of name clashes. It *is* possible to import **everything** from a module, but you risk name clashes.

1.13.4 Import and rename

You can rename things as you import them to avoid clashes or for typing convenience

1.14 Defining your own classes

1.14.1 User Defined Types

A **class** is a user-programmed Python type.

It is defined like this:

```
In [1]: class Room(object):
     pass
```

Just as with other python types, you use the name of the type as a function to make a variable of that type:

In the jargon, we say that an **object** is an **instance** of a particular **class**.

Once we have an object with a type of our own devising, we can add properties at will:

```
In [4]: myroom.name = "Living"
In [5]: myroom.name
Out[5]: 'Living'
```

The most common use of a class is to allow us to group data into an object in a way that is easier to read and understand than organising data into lists and dictionaries.

```
In [6]: myroom.capacity = 3
          myroom.occupants = ["James", "Sue"]
```

1.14.2 Methods

So far, our class doesn't do much!

We define functions **inside** the definition of a class, in order to give them capabilities, just like the methods on built-in types.

When we write methods, we always write the first function argument as self, to refer to the object instance itself, the argument that goes "before the dot".

This is just a convention for this variable name, not a keyword. You could call it something else if you wanted.

1.14.3 Constructors

Normally, though, we don't want to add data to the class attributes on the fly like that. Instead, we define a **constructor** that converts input data into an object.

Methods which begin and end with **two underscores** in their names fulfil special capabilities in Python, such as constructors.

1.14.4 Object-oriented design

In building a computer system to model a problem, therefore, we often want to make:

- classes for each *kind of thing* in our system
- methods for each capability of that kind
- properties (defined in a constructor) for each piece of information describing that kind

For example, the below program might describe our "Maze of Rooms" system: We define a "Maze" class which can hold rooms:

```
In [16]: class Maze(object):
             def __init__(self, name):
                 self.name = name
                 self.rooms = {}
             def add_room(self, room):
                 room.maze = self # The Room needs to know which Maze it is a part of
                 self.rooms[room.name] = room
             def occupants(self):
                 return [occupant for room in self.rooms.values()
                          for occupant in room.occupants.values()]
             def wander(self):
                 "Move all the people in a random direction"
                 for occupant in self.occupants():
                     occupant.wander()
             def describe(self):
                 for room in self.rooms.values():
                     room.describe()
             def step(self):
                 house.describe()
                 print("")
                 house.wander()
                 print("")
             def simulate(self, steps):
                 for _ in range(steps):
                     self.step()
  And a "Room" class with exits, and people:
In [17]: class Room(object):
             def __init__(self, name, exits, capacity, maze = None):
                 self.maze = maze
                 self.name = name
                 self.occupants = {} # Note the default argument, occupants start empty
                 self.exits = exits # Should be a dictionary from directions to room names
                 self.capacity = capacity
             def has_space(self):
                 return len(self.occupants) < self.capacity</pre>
             def available_exits(self):
                 return [exit for exit, target in self.exits.items()
                         if self.maze.rooms[target].has_space() ]
             def random_valid_exit(self):
                 import random
                 if not self.available_exits():
                     return None
                 return random.choice(self.available exits())
```

```
def destination(self, exit):
                 return self.maze.rooms[ self.exits[exit] ]
             def add_occupant(self, occupant):
                 occupant.room = self # The person needs to know which room it is in
                 self.occupants[occupant.name] = occupant
             def delete_occupant(self, occupant):
                 del self.occupants[occupant.name]
             def describe(self):
                 if self.occupants:
                     print(self.name, ": ", " ".join(self.occupants.keys()))
  We define a "Person" class for room occupants:
In [18]: class Person(object):
             def __init__(self, name, room = None):
                 self.name=name
             def use(self, exit):
                 self.room.delete_occupant(self)
                 destination=self.room.destination(exit)
                 destination.add_occupant(self)
                 print(self.name, "goes", exit, "to the", destination.name)
             def wander(self):
                 exit = self.room.random_valid_exit()
                 if exit:
                      self.use(exit)
  And we use these classes to define our people, rooms, and their relationships:
In [19]: james=Person('James')
         sue=Person('Sue')
         bob=Person('Bob')
         clare=Person('Clare')
In [20]: living=Room('livingroom', {'outside':'garden', 'upstairs':'bedroom', 'north':'kite
         kitchen=Room('kitchen', {'south':'livingroom'}, 1)
         garden=Room('garden', {'inside':'livingroom'}, 3)
         bedroom=Room('bedroom', {'jump':'garden', 'downstairs': 'livingroom'}, 1)
In [21]: house=Maze('My House')
In [22]: for room in [living, kitchen, garden, bedroom]:
             house.add room(room)
In [23]: living.add_occupant(james)
In [24]: garden.add_occupant(sue)
         garden.add_occupant(clare)
In [25]: bedroom.add_occupant(bob)
```

And we can run a "simulation" of our model:

```
In [26]: house.simulate(3)
bedroom : Bob
livingroom : James
garden : Clare Sue
Bob goes downstairs to the livingroom
James goes outside to the garden
Clare goes inside to the livingroom
livingroom : Clare Bob
garden : James Sue
Clare goes north to the kitchen
Bob goes upstairs to the bedroom
James goes inside to the livingroom
Sue goes inside to the livingroom
bedroom : Bob
livingroom : James Sue
kitchen : Clare
Bob goes jump to the garden
James goes outside to the garden
Sue goes upstairs to the bedroom
Clare goes south to the livingroom
```

1.14.5 Object oriented design

There are many choices for how to design programs to do this. Another choice would be to separately define exits as a different class from rooms. This way, we can use arrays instead of dictionaries, but we have to first define all our rooms, then define all our exits.

```
In [27]: class Maze(object):
             def __init__(self, name):
                 self.name = name
                 self.rooms = []
                 self.occupants = []
             def add_room(self, name, capacity):
                 result = Room(name, capacity)
                 self.rooms.append(result)
                 return result
             def add_exit(self, name, source, target, reverse= None):
                 source.add_exit(name, target)
                 if reverse:
                     target.add_exit(reverse, source)
             def add_occupant(self, name, room):
                 self.occupants.append(Person(name, room))
                 room.occupancy += 1
```

```
def wander(self):
                 "Move all the people in a random direction"
                 for occupant in self.occupants:
                     occupant.wander()
             def describe(self):
                 for occupant in self.occupants:
                     occupant.describe()
             def step(self):
                 house.describe()
                 print("")
                 house.wander()
                 print("")
             def simulate(self, steps):
                 for _ in range(steps):
                     self.step()
In [28]: class Room(object):
             def __init__(self, name, capacity):
                 self.name = name
                 self.capacity = capacity
                 self.occupancy = 0
                 self.exits = []
             def has_space(self):
                 return self.occupancy < self.capacity</pre>
             def available_exits(self):
                 return [exit for exit in self.exits if exit.valid() ]
             def random_valid_exit(self):
                 import random
                 if not self.available_exits():
                     return None
                 return random.choice(self.available_exits())
             def add_exit(self, name, target):
                 self.exits.append(Exit(name, target))
In [29]: class Person(object):
             def __init__(self, name, room = None):
                 self.name=name
                 self.room=room
             def use(self, exit):
                 self.room.occupancy -= 1
                 destination=exit.target
                 destination.occupancy +=1
                 self.room=destination
                 print(self.name, "goes", exit.name, "to the", destination.name)
             def wander(self):
```

```
exit = self.room.random valid exit()
                 if exit:
                     self.use(exit)
             def describe(self):
                 print(self.name, "is in the", self.room.name)
In [30]: class Exit(object):
             def __init__(self, name, target):
                 self.name = name
                 self.target = target
             def valid(self):
                 return self.target.has space()
In [31]: house=Maze('My New House')
In [32]: living=house.add_room('livingroom', 2)
         bed = house.add room('bedroom', 1)
         garden = house.add_room('garden', 3)
         kitchen = house.add_room('kitchen', 1)
In [33]: house.add_exit('north', living, kitchen, 'south')
In [34]: house.add_exit('upstairs', living, bed, 'downstairs')
In [35]: house.add_exit('outside', living, garden, 'inside')
In [36]: house.add_exit('jump',bed, garden)
In [37]: house.add_occupant('James', living)
         house.add_occupant('Sue', garden)
         house.add_occupant('Bob', bed)
         house.add_occupant('Clare', garden)
In [38]: house.simulate(3)
James is in the livingroom
Sue is in the garden
Bob is in the bedroom
Clare is in the garden
James goes north to the kitchen
Sue goes inside to the livingroom
Bob goes jump to the garden
Clare goes inside to the livingroom
James is in the kitchen
Sue is in the livingroom
Bob is in the garden
Clare is in the livingroom
Sue goes upstairs to the bedroom
Bob goes inside to the livingroom
Clare goes outside to the garden
```

James is in the kitchen Sue is in the bedroom Bob is in the livingroom Clare is in the garden

James goes south to the livingroom Sue goes jump to the garden Bob goes outside to the garden Clare goes inside to the livingroom

This is a huge topic, about which many books have been written. The differences between these two designs are important, and will have long-term consequences for the project. That is the how we start to think about **software engineering**, as opposed to learning to program, and is an important part of this course.

1.14.6 Exercise: Your own solution

Compare the two solutions above. Discuss with a partner which you like better, and why. Then, starting from scratch, design your own. What choices did you make that are different from mine?

Chapter 2

Working with Data

2.1 Loading data from files

2.1.1 Loading data

An important part of this course is about using Python to analyse and visualise data. Most data, of course, is supplied to us in various *formats*: spreadsheets, database dumps, or text files in various formats (csv, tsv, json, yaml, hdf5, netcdf) It is also stored in some *medium*: on a local disk, a network drive, or on the internet in various ways. It is important to distinguish the data format, how the data is structured into a file, from the data's storage, where it is put.

We'll look first at the question of data *transport*: loading data from a disk, and at downloading data from the internet. Then we'll look at data *parsing*: building Python structures from the data. These are related, but separate questions.

2.1.2 An example datafile

Let's write an example datafile to disk so we can investigate it. We'll just use a plain-text file. IPython notebook provides a way to do this: if we put %%writefile at the top of a cell, instead of being interpreted as python, the cell contents are saved to disk.

```
In [1]: %%writefile mydata.txt
        A poet once said, 'The whole universe is in a glass of wine.'
        We will probably never know in what sense he meant it,
        for poets do not write to be understood.
        But it is true that if we look at a glass of wine closely enough we see the entire
        There are the things of physics: the twisting liquid which evaporates depending
        on the wind and weather, the reflection in the glass;
        and our imagination adds atoms.
        The glass is a distillation of the earth's rocks,
        and in its composition we see the secrets of the universe's age, and the evolution
        What strange array of chemicals are in the wine? How did they come to be?
        There are the ferments, the enzymes, the substrates, and the products.
        There in wine is found the great generalization; all life is fermentation.
        Nobody can discover the chemistry of wine without discovering,
        as did Louis Pasteur, the cause of much disease.
        How vivid is the claret, pressing its existence into the consciousness that watches
        If our small minds, for some convenience, divide this glass of wine, this universe
        into parts --
        physics, biology, geology, astronomy, psychology, and so on --
        remember that nature does not know it!
```

```
So let us put it all back together, not forgetting ultimately what it is for.

Let it give us one more final pleasure; drink it and forget it all!

- Richard Feynman

Writing mydata.txt
```

Where did that go? It went to the current folder, which for a notebook, by default, is where the notebook is on disk

Can we see it is there?

Yep! Note how we used a list comprehension to filter all the extraneous files.

2.1.3 Path independence and os

We can use dirname to get the parent folder for a folder, in a platform independent-way.

```
In [4]: os.path.dirname(os.getcwd())
Out[4]: '/home/travis/build/UCL/rsd-engineeringcourse'
We could do this manually using split:
In [5]: "/".join(os.getcwd().split("/")[:-1])
Out[5]: '/home/travis/build/UCL/rsd-engineeringcourse'
```

But this would not work on windows, where path elements are separated with a \setminus instead of a /. So it's important to use os . path for this stuff.

Supplementary Materials: If you're not already comfortable with how files fit into folders, and folders form a tree, with folders containing subfolders, then look at http://swcarpentry.github.io/shell-novice/01-filedir.html.

Satisfy yourself that after using %%writedir, you can then find the file on disk with Windows Explorer, OSX Finder, or the Linux Shell.

We can see how in Python we can investigate the file system with functions in the os module, using just the same programming approaches as for anything else.

We'll gradually learn more features of the os module as we go, allowing us to move around the disk, walk around the disk looking for relevant files, and so on. These will be important to master for automating our data analyses.

2.1.4 The python file type

In [6]: myfile=open('mydata.txt')

So, let's read our file:

In [7]: type(myfile)

```
Out[7]: _io.TextIOWrapper
  We can go line-by-line, by treating the file as an iterable:
In [8]: [x for x in myfile]
Out[8]: ["A poet once said, 'The whole universe is in a glass of wine.'\n",
         'We will probably never know in what sense he meant it, n',
         'for poets do not write to be understood. \n',
         'But it is true that if we look at a glass of wine closely enough we see the enti-
         'There are the things of physics: the twisting liquid which evaporates depending \
         'on the wind and weather, the reflection in the glass; \n',
         'and our imagination adds atoms.\n',
         "The glass is a distillation of the earth's rocks, \n",
         "and in its composition we see the secrets of the universe's age, and the evolution
         'What strange array of chemicals are in the wine? How did they come to be? \n',
         'There are the ferments, the enzymes, the substrates, and the products.\n',
         'There in wine is found the great generalization; all life is fermentation.\n',
         'Nobody can discover the chemistry of wine without discovering, \n',
         'as did Louis Pasteur, the cause of much disease.\n',
         'How vivid is the claret, pressing its existence into the consciousness that watch
         'If our small minds, for some convenience, divide this glass of wine, this university
         'into parts -- \n',
         'physics, biology, geology, astronomy, psychology, and so on -- \n',
         'remember that nature does not know it!\n',
         'So let us put it all back together, not forgetting ultimately what it is for.\n'
         'Let it give us one more final pleasure; drink it and forget it all!\n',
         ' - Richard Feynman']
```

If we do that again, the file has already finished, there is no more data.

It's really important to remember that a file is a different built in type than a string.

2.1.5 Working with files.

```
We can read one line at a time with readline:
```

```
In [11]: myfile.seek(0)
         first = myfile.readline()
In [12]: first
Out[12]: "A poet once said, 'The whole universe is in a glass of wine.'\n"
In [13]: second=myfile.readline()
In [14]: second
Out[14]: 'We will probably never know in what sense he meant it, \n'
  We can read the whole remaining file with read:
In [15]: rest=myfile.read()
In [16]: rest
Out[16]: "for poets do not write to be understood. \nBut it is true that if we look at a g.
  Which means that when a file is first opened, read is useful to just get the whole thing as a string:
In [17]: open('mydata.txt').read()
Out[17]: "A poet once said, 'The whole universe is in a glass of wine.'\nWe will probably
  You can also read just a few characters:
In [18]: myfile.seek(1335)
```

```
In [18]: myfile.seek(1335)
Out[18]: 1335
In [19]: myfile.read(15)
```

Out [19]: '\n - Richard F'

2.1.6 Converting Strings to Files

Because files and strings are different types, we CANNOT just treat strings as if they were files:

This is important, because some file format parsers expect input from a file and not a string. We can convert between them using the StringIO module in the standard library:

```
In [23]: from io import StringIO
In [24]: mystringasafile=StringIO(mystring)
In [25]: mystringasafile.readline()
Out[25]: 'Hello World\n'
In [26]: mystringasafile.readline()
Out[26]: ' My name is James'
```

Note that in a string, \n is used to represent a newline.

2.1.7 Closing files

We really ought to close files when we've finished with them, as it makes the computer more efficient. (On a shared computer, this is particularly important)

```
In [27]: myfile.close()
```

Because it's so easy to forget this, python provides a **context manager** to open a file, then close it automatically at the end of an indented block:

```
In [28]: with open('mydata.txt') as somefile:
             content = somefile.read()
         content
Out[28]: "A poet once said, 'The whole universe is in a glass of wine.'\nWe will probably
```

The code to be done while the file is open is indented, just like for an if statement.

You should pretty much always use this syntax for working with files.

2.1.8 Writing files

We might want to create a file from a string in memory. We can't do this with the notebook's %%writefile – this is just a notebook convenience, and isn't very programmable.

When we open a file, we can specify a 'mode', in this case, 'w' for writing. ('r' for reading is the default.)

```
In [29]: with open('mywrittenfile', 'w') as target:
             target.write('Hello')
             target.write('World')
In [30]: with open('mywrittenfile','r') as source:
             print(source.read())
HelloWorld
  And we can "append" to a file with mode 'a':
```

```
In [31]: with open('mywrittenfile', 'a') as target:
             target.write('Hello')
             target.write('James')
In [32]: with open('mywrittenfile','r') as source:
             print(source.read())
```

HelloWorldHelloJames

If a file already exists, mode 'w' will overwrite it.

2.2 Getting data from the Internet

We've seen about obtaining data from our local file system.

The other common place today that we might want to obtain data is from the internet.

It's very common today to treat the web as a source and store of information; we need to be able to programmatically download data, and place it in python objects.

We may also want to be able to programmatically *upload* data, for example, to automatically fill in forms.

This can be really powerful if we want to, for example, do automated metaanalysis across a selection of research papers.

2.2.1 URLs

All internet resources are defined by a Uniform Resource Locator.

```
In [1]: "http://maps.googleapis.com:80/maps/api/staticmap?size=400x400&center=51.51,-0.127.
Out[1]: 'http://maps.googleapis.com:80/maps/api/staticmap?size=400x400&center=51.51,-0.127.
```

A url consists of:

- A *scheme* (http, https, ssh, ...)
- A *host* (maps.googleapis.com, the name of the remote computer you want to talk to)
- A port (optional, most protocols have a typical port associated with them, e.g. 80 for http)
- A *path* (Like a file path on the machine, here it is maps/api/staticmap)
- A *query* part after a ?, (optional, usually ampersand-separated *parameters* e.g. size=400x400, or zoom=12)

Supplementary materials: These can actually be different for different protocols, the above is a simplification, you can see more, for example, at https://en.wikipedia.org/wiki/URI_scheme

URLs are not allowed to include all characters; we need to, for example, "escape" a space that appears inside the URL, replacing it with %20, so e.g. a request of http://some example.com/ would need to be http://some%20example.com/

Supplementary materials: The code used to replace each character is the ASCII code for it.

Supplementary materials: The escaping rules a are quite subtle. See https://en.wikipedia.org/wiki/Percent-encoding

2.2.2 Requests

The python requests library can help us manage and manipulate URLs. It is easier to use than the 'urllib' library that is part of the standard library, and is included with anaconda and canopy. It sorts out escaping, parameter encoding, and so on for us.

To request the above URL, for example, we write:

When we do a request, the result comes back as text. For the png image in the above, this isn't very readable:

Just as for file access, therefore, we will need to send the text we get to a python module which understands that file format.

Again, it is important to separate the *transport* model, (e.g. a file system, or an "http request" for the web, from the data model of the data that is returned.)

2.2.3 Example: Sunspots

Let's try to get something scientific: the sunspot cycle data from http://sidc.be/silso/home:

```
In [5]: spots=requests.get('http://www.sidc.be/silso/INFO/snmtotcsv.php').text
In [6]: spots[0:80]
Out[6]: '1749;01;1749.042; 96.7; -1.0; -1;1\n1749;02;1749.123; 104.3; -1.0; -1;1\n174
```

This looks like semicolon-separated data, with different records on different lines. (Line separators come out as \n)

There are many many scientific datasets which can now be downloaded like this - integrating the download into your data pipeline can help to keep your data flows organised.

2.2.4 Writing our own Parser

We'll need a python library to handle semicolon-separated data like the sunspot data. You might be thinking: "But I can do that myself!":

```
In [7]: lines=spots.split("\n")
        lines[0:5]
Out[7]: ['1749;01;1749.042; 96.7; -1.0;
                                             -1;1',
         '1749;02;1749.123; 104.3; -1.0;
                                             -1;1',
         '1749;03;1749.204; 116.7; -1.0;
                                             -1;1',
         '1749;04;1749.288; 92.8; -1.0;
                                             -1;1',
         '1749;05;1749.371; 141.7; -1.0;
                                             -1;1']
In [8]: years=[line.split(";")[0] for line in lines]
In [9]: years[0:15]
Out[9]: ['1749',
         '1749',
         '1749',
         '1749',
         '1749',
         '1749',
         '1749',
         '1749',
         '1749',
         '1749',
         '1749',
         '1749',
         '1750',
         '1750',
         '1750']
```

But **don't**: what if, for example, one of the records contains a separator inside it; most computers will put the content in quotes, so that, for example,

```
"something; something"; something; something
```

has three fields, the first of which is

```
something; something
```

The naive code above would give four fields, of which the first is

"Something

You'll never manage to get all that right; so you'll be better off using a library to do it.

2.2.5 Writing data to the internet

Note that we're using requests.get.get is used to receive data from the web. You can also use post to fill in a web-form programmatically.

Supplementary material: Learn about using post with requests.

Supplementary material: Learn about the different kinds of http request: Get, Post, Put, Delete...

This can be used for all kinds of things, for example, to programmatically add data to a web resource. It's all well beyond our scope for this course, but it's important to know it's possible, and start to think about the scientific possibilities.

2.3 Field and Record Data

2.3.1 Separated Value Files

Let's carry on with our sunspots example:

We want to work programmatically with Separated Value files.

These are files which have:

- Each record on a line
- Each record has multiple *fields*
- Fields are separated by some *separator*

Typical separators are the space, tab, comma, and semicolon separated values files, e.g.:

- Space separated value (e.g. field1, "field two", field3)
- Comma separated value (e.g. 'field1, another field, "wow, another field")

Comma-separated-value is abbreviated CSV, and tab separated value TSV.

CSV is also used to refer to all the different sub-kinds of separated value files, i.e. some people use csv to refer to tab, space and semicolon separated files.

CSV is not a particularly superb data format, because it forces your data model to be a list of lists. Richer file formats describe "serialisations" for dictionaries and for deeper-than-two nested list structures as well.

Nevertheless, because you can always export *spreadsheets* as CSV files, (each cell is a field, each row is a record) CSV files are very popular.

2.3.2 CSV variants.

Some CSV formats define a comment character, so that rows beginning with, e.g., a #, are not treated as data, but give a human comment.

Some CSV formats define a three-deep list structure, where a double-newline separates records into blocks.

Some CSV formats assume that the first line defines the names of the fields, e.g.:

```
name, age
James, 39
Will, 2
```

2.3.3 Python CSV readers

The Python standard library has a csv module. However, it's less powerful than the CSV capabilities in numpy, the main scientific python library for handling data. Numpy is destributed with Anaconda and Canopy, so we recommend you just use that.

Numpy has powerful capabilities for handling matrices, and other fun stuff, and we'll learn about these later in the course, but for now, we'll just use numpy's CSV reader, and assume it makes us lists and dictionaries, rather than it's more exciting array type.

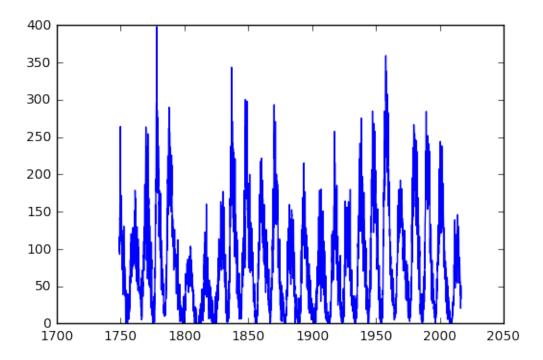
genfromtxt is a powerful CSV reader. I used the delimiter optional argument to specify the delimeter. I could also specify names=True if I had a first line naming fields, and comments=# if I had comment lines.

```
In [5]: sunspots[0][3]
Out[5]: 96.700000000000003
```

We can now plot the "Sunspot cycle":

/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a momes/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a momes

```
Out[6]: [<matplotlib.lines.Line2D at 0x2b60c31fb940>]
```



The plot command accepted an array of 'X' values and an array of 'Y' values. We used a special NumPy ":" syntax, which we'll learn more about later.

2.3.4 Naming Columns

I happen to know that the columns here are defined as follows: From http://www.sidc.be/silso/infosnmtot:

CSV

Filename: SN_m_tot_V2.0.csv Format: Comma Separated values (adapted for import in spreadsheets) The separator is the semicolon ';'.

Contents: * Column 1-2: Gregorian calendar date - Year - Month * Column 3: Date in fraction of year. * Column 4: Monthly mean total sunspot number. * Column 5: Monthly mean standard deviation of the input sunspot numbers. * Column 6: Number of observations used to compute the monthly mean total sunspot number. * Column 7: Definitive/provisional marker. '1' indicates that the value is definitive. '0' indicates that the value is still provisional.

I can actually specify this to the formatter:

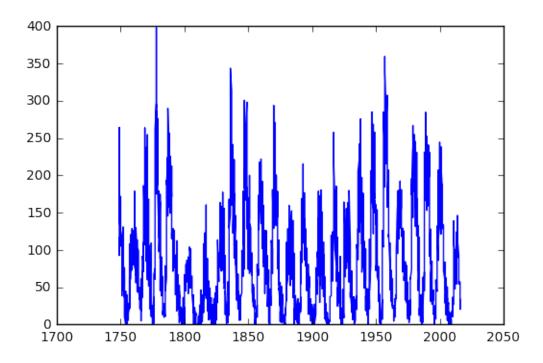
```
----> 1 sunspots= np.genfromtxt(StringIO(spots), delimiter=';',
                                   names=['year','month','date',
         2
         3
                                   'mean','deviation','observations','definitive'])
       NameError: name 'StringIO' is not defined
In [8]: sunspots
Out[8]: array([[ 1.74900000e+03,  1.00000000e+00,
                                                    1.74904200e+03, ...,
                -1.00000000e+00, -1.0000000e+00,
                                                    1.00000000e+00],
              [ 1.74900000e+03, 2.00000000e+00,
                                                    1.74912300e+03, ...,
                -1.00000000e+00, -1.0000000e+00,
                                                    1.00000000e+00],
              [ 1.74900000e+03, 3.00000000e+00,
                                                    1.74920400e+03, ...,
                -1.00000000e+00, -1.0000000e+00,
                                                    1.00000000e+00],
              [ 2.01600000e+03, 8.00000000e+00,
                                                    2.01662400e+03, ...,
                 4.40000000e+00, 8.79000000e+02,
                                                    0.00000000e+00],
              [ 2.01600000e+03, 9.00000000e+00,
                                                    2.01670600e+03, ...,
                 3.80000000e+00, 7.42000000e+02, 0.00000000e+00],
              [ 2.01600000e+03, 1.00000000e+01,
                                                    2.01679100e+03, ...,
                 3.20000000e+00, 6.95000000e+02,
                                                   0.00000000e+0011)
```

2.3.5 Typed Fields

It's also often good to specify the datatype of each field.

Now, NumPy understands the names of the columns, so our plot command is more readable:

```
In [11]: sunspots['year']
Out[11]: array([1749, 1749, 1749, ..., 2016, 2016, 2016])
In [12]: plt.plot(sunspots['year'], sunspots['mean'])
Out[12]: [<matplotlib.lines.Line2D at 0x2b60c3336b00>]
```



2.4 Structured Data

2.4.1 Structured data

CSV files can only model data where each record has several fields, and each field is a simple datatype, a string or number.

We often want to store data which is more complicated than this, with nested structures of lists and dictionaries. Structured data formats like Json, YAML, and XML are designed for this.

2.4.2 **Json**

A very common structured data format is JSON.

This allows us to represent data which is combinations of lists and dictionaries as a text file which looks a bit like a Javascript (or Python) data literal.

```
In [1]: import json
```

Any nested group of dictionaries and lists can be saved:

Loading data is also really easy:

```
In [4]: %%writefile myfile.json
{
          "somekey": ["a list", "with values"]
}
Writing myfile.json

In [5]: mydataasstring=open('myfile.json').read()
In [6]: mydataasstring
Out[6]: '{\n          "somekey": ["a list", "with values"]\n}'
In [7]: mydata = json.loads(mydataasstring)
In [8]: mydata['somekey']
Out[8]: ['a list', 'with values']
```

This is a very nice solution for loading and saving python datastructures. It's a very common way of transferring data on the internet, and of saving datasets to disk.

There's good support in most languages, so it's a nice inter-language file interchange format.

2.4.3 Yaml

Yaml is a very similar dataformat to Json, with some nice additions:

- You don't need to quote strings if they don't have funny characters in
- You can have comment lines, beginning with a #
- You can write dictionaries without the curly brackets: it just notices the colons.
- You can write lists like this:

```
NameError Traceback (most recent call last)

<ipython-input-11-b8f576d14459> in <module>()
----> 1 yaml.load(open('myfile.yaml'))

NameError: name 'yaml' is not defined
```

Yaml is my favourite format for ad-hoc datafiles, but the library doesn't ship with default Python, (though it is part of Anaconda and Canopy) so some people still prefer Json for it's university.

Because Yaml gives the **option** of serialising a list either as newlines with dashes, *or* with square brackets, you can control this choice:

2.4.4 XML

Supplementary material: XML is another popular choice when saving nested data structures. It's very careful, but verbose. If your field uses XML data, you'll need to learn a python XML parser, (there are a few), and about how XML works.

2.4.5 Exercise: Saving and loading data

Use YAML or JSON to save your maze datastructure to disk and load it again.

```
In [1]: house = {
             'living' : {
                 'exits': {
                     'north' : 'kitchen',
                     'outside' : 'garden',
                     'upstairs' : 'bedroom'
                 'people' : ['James'],
                 'capacity' : 2
             'kitchen' : {
                 'exits': {
                     'south' : 'living'
                 'people' : [],
                 'capacity' : 1
            },
             'garden' : {
                 'exits': {
                     'inside' : 'living'
                 'people' : ['Sue'],
                 'capacity' : 3
            },
             'bedroom' : {
                 'exits': {
                     'downstairs' : 'living',
                     'jump' : 'garden'
                 'people' : [],
                 'capacity' : 1
            }
  Save the maze with json:
In [2]: import json
In [3]: with open('maze.json','w') as json_maze_out:
             json_maze_out.write(json.dumps(house))
  Consider the file on the disk:
In [4]: %%bash
        cat 'maze.json'
{"garden": {"capacity": 3, "people": ["Sue"], "exits": {"inside": "living"}}, "living": {"d
  and now load it into a different variable:
In [5]: with open('maze.json') as json_maze_in:
            maze_again = json.load(json_maze_in)
In [6]: maze_again
```

```
Out[6]: {'bedroom': {'capacity': 1,
          'exits': {'downstairs': 'living', 'jump': 'garden'},
          'people': []},
         'garden': {'capacity': 3, 'exits': {'inside': 'living'}, 'people': ['Sue']},
         'kitchen': {'capacity': 1, 'exits': {'south': 'living'}, 'people': []},
         'living': {'capacity': 2,
          'exits': {'north': 'kitchen', 'outside': 'garden', 'upstairs': 'bedroom'},
          'people': ['James']}}
  Or with YAML:
In [7]: import yaml
                                                  Traceback (most recent call last)
        ImportError
        <ipython-input-7-fc3d1333bd52> in <module>()
    ---> 1 import yaml
        ImportError: No module named 'yaml'
In [8]: with open('maze.yaml','w') as yaml_maze_out:
            yaml_maze_out.write(yaml.dump(house))
        NameError
                                                  Traceback (most recent call last)
        <ipython-input-8-b8434d9d24a8> in <module>()
         1 with open('maze.yaml','w') as yaml_maze_out:
              yaml maze out.write(yaml.dump(house))
        NameError: name 'yaml' is not defined
In [9]: %%bash
        cat 'maze.yaml'
In [10]: with open('maze.yaml') as yaml_maze_in:
            maze_again = yaml.load(yaml_maze_in)
        NameError
                                                 Traceback (most recent call last)
        <ipython-input-10-f770eea227cc> in <module>()
         1 with open('maze.yaml') as yaml_maze_in:
              maze_again = yaml.load(yaml_maze_in)
```

2.5 Exercise/Example: the biggest Earthquake in the UK this Century

2.5.1 The Problem

GeoJSON is a json-based file format for sharing geographic data. One example dataset is the USGS earthquake data:

Your exercise: determine the location of the largest magnitude earthquake in the UK this century.

You'll need to: * Get the text of the web result * Parse the data as JSON * Understand how the data is structured into dictionaries and lists * Where is the magnitude? * Where is the place description or coordinates? * Program a search through all the quakes to find the biggest quake. * Find the place of the biggest quake * Form a URL for Google Maps at that latitude and longitude: look back at the introductory example * Display that image

2.5.2 Download the data

```
"minlongitude":"-9.756",
"minmagnitude":"1",
"endtime":"2015-07-13",
"orderby":"time-asc"}
```

2.5.3 Parse the data as JSON

```
In [2]: import json
In [3]: requests_json = json.loads(quakes_response.text)
```

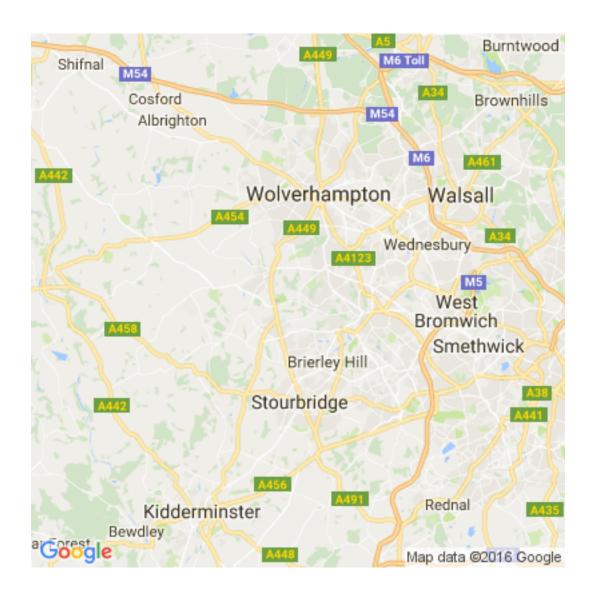
2.5.4 Investigate the data to discover how it is structured.

```
In [4]: type(requests_json)
Out[4]: dict
In [5]: requests_json.keys()
Out[5]: dict_keys(['type', 'features', 'metadata', 'bbox'])
In [6]: len(requests_json['features'])
Out[6]: 110
In [7]: requests_json['features'][0].keys()
Out[7]: dict_keys(['type', 'geometry', 'id', 'properties'])
In [8]: requests_json['features'][0]['properties']['mag']
Out[8]: 2.6
In [9]: requests_json['features'][0]['geometry']
Out[9]: {'coordinates': [-2.81, 54.77, 14], 'type': 'Point'}
```

2.5.5 Find the largest quake

2.5.6 Get a map at the point of the quake

```
In [13]: import requests
         def request_map_at(lat,long, satellite=False,zoom=12,size=(400,400),sensor=False)
           base="http://maps.googleapis.com/maps/api/staticmap?"
           params=dict(
             sensor= str(sensor).lower(),
             zoom= zoom,
             size= "x".join(map(str, size)),
             center= ",".join(map(str,(lat,long)))
           if satellite:
             params["maptype"]="satellite"
           return requests.get(base,params=params)
In [14]: import IPython
         map_png=request_map_at(lat, long,zoom=10)
2.5.7 Display the map
In [15]: IPython.core.display.Image(map_png.content)
Out[15]:
```



2.6 Plotting with Matplotlib

2.6.1 Importing Matplotlib

We import the 'pyplot' object from Matplotlib, which provides us with an interface for making figures. We usually abbreviate it.

In [1]: from matplotlib import pyplot as plt

/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment

2.6.2 Notebook magics

When we write:

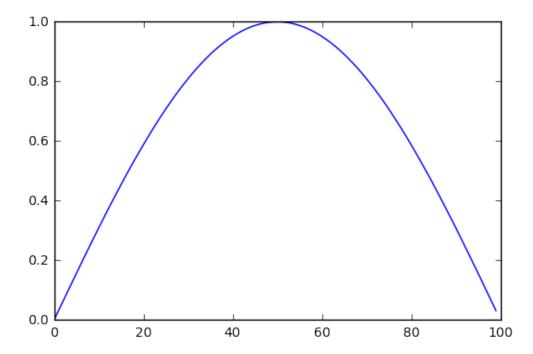
```
In [2]: %matplotlib inline
```

We tell the IPython notebook to show figures we generate alongside the code that created it, rather than in a separate window. Lines beginning with a single percent are not python code: they control how the notebook deals with python code.

Lines beginning with two percents are "cell magics", that tell IPython notebook how to interpret the particular cell; we've seen %%writefile, for example.

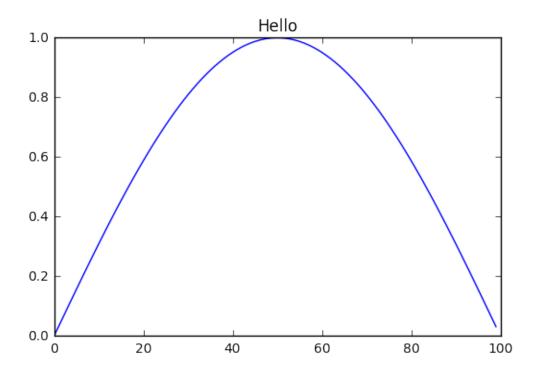
2.6.3 A basic plot

When we write:



The plot command *returns* a figure, just like the return value of any function. The notebook then displays this.

To add a title, axis labels etc, we need to get that figure object, and manipulate it. For convenience, matplotlib allows us to do this just by issuing commands to change the "current figure":



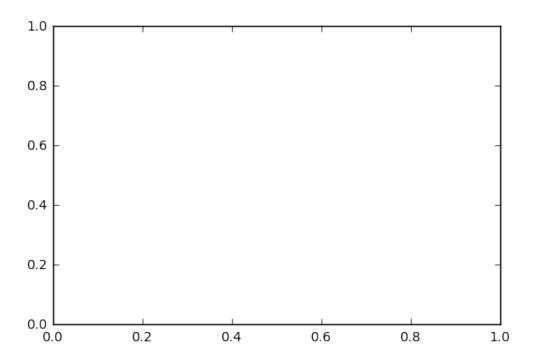
But this requires us to keep all our commands together in a single cell, and makes use of a "global" single "current plot", which, while convenient for quick exploratory sketches, is a bit cumbersome. To produce from our notebook proper plots to use in papers, Python's plotting library, matplotlib, defines some types we can use to treat individual figures as variables, and manipulate these.

2.6.4 Figures and Axes

We often want multiple graphs in a single figure (e.g. for figures which display a matrix of graphs of different variables for comparison).

So Matplotlib divides a figure object up into axes: each pair of axes is one 'subplot'. To make a boring figure with just one pair of axes, however, we can just ask for a default new figure, with brand new axes. The relevant function returns an (figure, axis) pair, which we can deal out with parallel assignment.

```
In [5]: sine_graph, sine_graph_axes=plt.subplots();
```



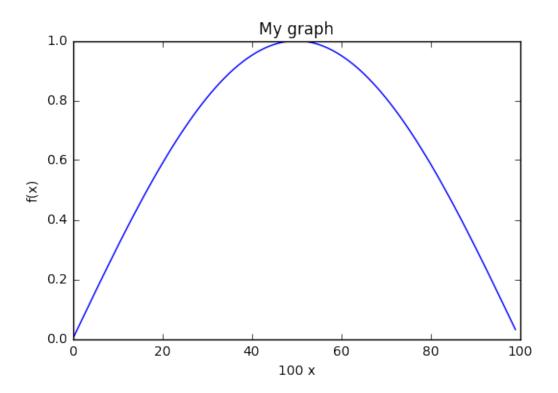
Once we have some axes, we can plot a graph on them:

```
In [6]: sine_graph_axes.plot([sin(pi*x/100.0) for x in range(100)], label='sin(x)')
Out[6]: [<matplotlib.lines.Line2D at 0x2b05899a13c8>]
We can add a title to a pair of axes:
```

```
In [7]: sine_graph_axes.set_title("My graph")
Out[7]: <matplotlib.text.Text at 0x2b05899a55c0>
In [8]: sine_graph_axes.set_ylabel("f(x)")
Out[8]: <matplotlib.text.Text at 0x2b0589a5cc50>
In [9]: sine_graph_axes.set_xlabel("100 x")
Out[9]: <matplotlib.text.Text at 0x2b0589a3c470>
```

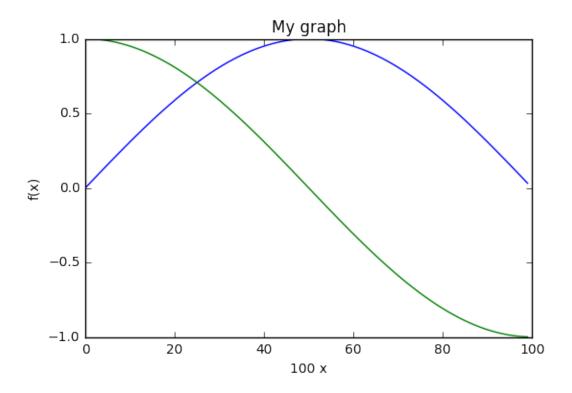
Now we need to actually display the figure. As always with the notebook, if we make a variable be returned by the last line of a code cell, it gets displayed:

```
In [10]: sine_graph
Out[10]:
```



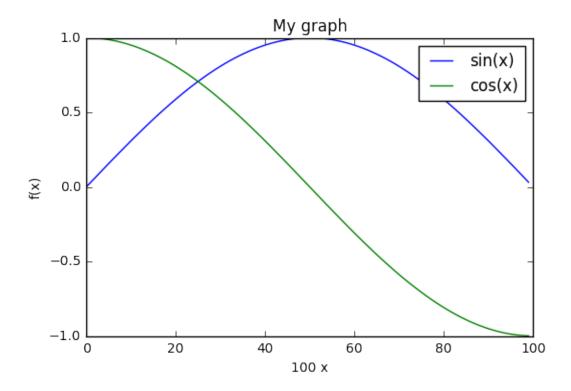
We can add another curve:

```
In [11]: sine_graph_axes.plot([cos(pi*x/100.0) for x in range(100)], label='cos(x)')
Out[11]: [<matplotlib.lines.Line2D at 0x2b05898d1f28>]
In [12]: sine_graph
Out[12]:
```



A legend will help us distinguish the curves:

```
In [13]: sine_graph_axes.legend()
Out[13]: <matplotlib.legend.Legend at 0x2b05899dc5f8>
In [14]: sine_graph
Out[14]:
```



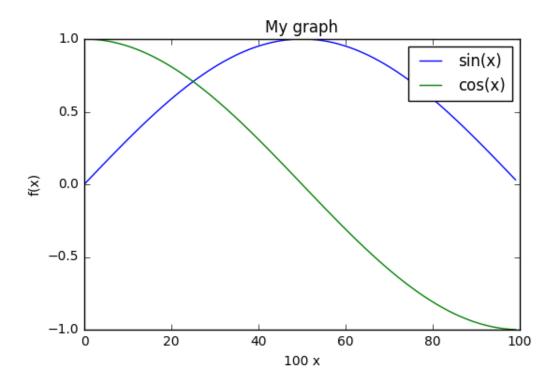
2.6.5 Saving figures.

We must be able to save figures to disk, in order to use them in papers. This is really easy:

```
In [15]: sine_graph.savefig('my_graph.png')
```

In order to be able to check that it worked, we need to know how to display an arbitrary image in the notebook.

The programmatic way is like this:

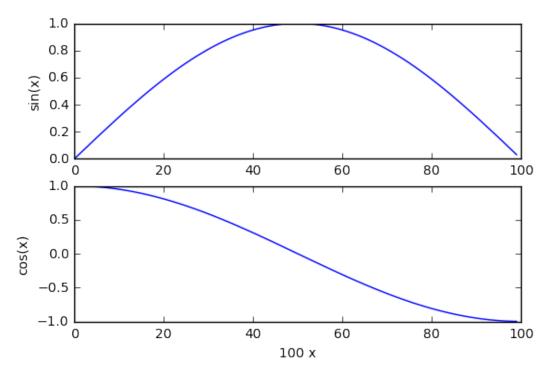


2.6.6 Subplots

We might have wanted the sin and cos graphs on separate axes:

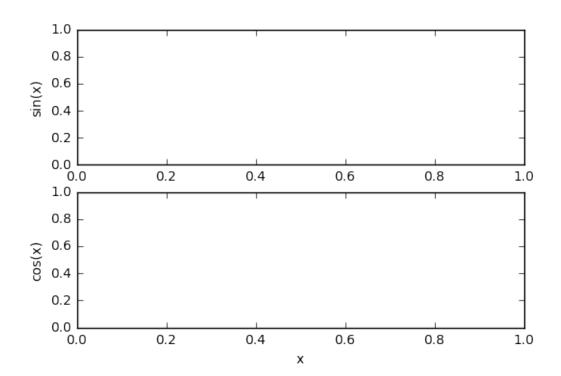
```
In [17]: double_graph=plt.figure()
<matplotlib.figure.Figure at 0x2b05899e5358>
In [18]: sin_axes=double_graph.add_subplot(2,1,1)
In [19]: cos_axes=double_graph.add_subplot(2,1,2)
In [20]: sin_axes.plot([sin(pi*x/100.0) for x in range(100)])
Out[20]: [<matplotlib.lines.Line2D at 0x2b0589af4630>]
In [21]: sin_axes.set_ylabel("sin(x)")
Out[21]: <matplotlib.text.Text at 0x2b05899ffd30>
In [22]: cos_axes.plot([cos(pi*x/100.0) for x in range(100)])
Out[22]: [<matplotlib.lines.Line2D at 0x2b0589afa128>]
In [23]: cos_axes.set_ylabel("cos(x)")
Out[23]: <matplotlib.text.Text at 0x2b0589ab4358>
In [24]: cos_axes.set_xlabel("100 x")
```

```
Out[24]: <matplotlib.text.Text at 0x2b05899f0c18>
In [25]: double_graph
Out[25]:
```

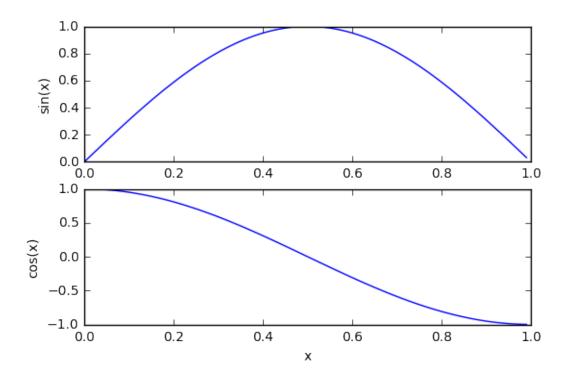


2.6.7 Versus plots

When we specify a single list to plot, the x-values are just the array index number. We usually want to plot something more meaningful:



Out[28]:



2.6.8 Learning More

There's so much more to learn about matplotlib: pie charts, bar charts, heat maps, 3-d plotting, animated plots, and so on. You can learn all this via the Matplotlib Website. You should try to get comfortable with all this, so please use some time in class, or at home, to work your way through a bunch of the examples.

2.7 NumPy

2.7.1 The Scientific Python Trilogy

Why is Python so popular for research work?

MATLAB has typically been the most popular "language of technical computing", with strong built-in support for efficient numerical analysis with matrices (the *mat* in MATLAB is for Matrix, not Maths), and plotting.

Other dynamic languages have cleaner, more logical syntax (Ruby, Haskell)
But Python users developed three critical libraries, matching the power of MATLAB for scientific work:

- Matplotlib, the plotting library created by John D. Hunter
- NumPy, a fast matrix maths library created by Travis Oliphant
- IPython, the precursor of the notebook, created by Fernando Perez

By combining a plotting library, a matrix maths library, and an easy-to-use interface allowing live plotting commands in a persistent environment, the powerful capabilities of MATLAB were matched by a free and open toolchain.

We've learned about Matplotlib and IPython in this course already. NumPy is the last part of the trilogy.

2.7.2 Limitations of Python Lists

The normal Python List is just one dimensional. To make a matrix, we have to nest Python arrays:

```
In [1]: x=[list(range(5)) for N in range(5)]
In [2]: x
Out[2]: [[0, 1, 2, 3, 4],
         [0, 1, 2, 3, 4],
         [0, 1, 2, 3, 4],
         [0, 1, 2, 3, 4],
         [0, 1, 2, 3, 4]]
In [3]: x[2][2]
Out[3]: 2
  Applying an operation to every element is a pain:
In [4]: x + 5
                                                    Traceback (most recent call last)
        TypeError
        <ipython-input-4-057023a07318> in <module>()
    ----> 1 x + 5
        TypeError: can only concatenate list (not "int") to list
In [5]: [[elem +5 for elem in row] for row in x]
Out[5]: [[5, 6, 7, 8, 9],
         [5, 6, 7, 8, 9],
         [5, 6, 7, 8, 9],
         [5, 6, 7, 8, 9],
         [5, 6, 7, 8, 9]]
```

Common useful operations like transposing a matrix or reshaping a 10 by 10 matrix into a 20 by 5 matrix are not easy to code in raw Python lists.

2.7.3 The NumPy array

NumPy's array type represents a multidimensional matrix $M_{i,j,k...n}$ The NumPy array seems at first to be just like a list:

We can also see our first weakness of NumPy arrays versus Python lists:

For NumPy arrays, you typically don't change the data size once you've defined your array, whereas for Python lists, you can do this efficiently. However, you get back lots of goodies in return...

2.7.4 Elementwise Operations

But most operations can be applied element-wise automatically!

The slowest run took 6.36 times longer than the fastest. This could mean that an intermediation 100000 loops, best of 3: 7.95 μs per loop

2.7.5 Arange and linspace

NumPy has two easy methods for defining floating-point evenly spaced arrays:

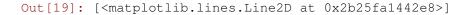
```
In [15]: x=np.arange(0,10,0.1)
        Х
Out[15]: array([ 0. , 0.1, 0.2,
                                  0.3,
                                       0.4, 0.5,
                                                    0.6,
                                                         0.7,
                                                                0.8,
                                                                      0.9,
                                                                            1.,
                                        1.5,
                      1.2,
                           1.3,
                                                    1.7,
                                                                1.9,
                                                                            2.1,
                1.1,
                                 1.4,
                                              1.6,
                                                          1.8,
                                                                      2.,
                                                          2.9,
                2.2,
                      2.3,
                            2.4, 2.5,
                                        2.6, 2.7,
                                                    2.8,
                                                                3.,
                                                                      3.1.
                                                                            3.2,
                                       3.7,
                3.3,
                      3.4,
                            3.5,
                                  3.6,
                                              3.8,
                                                    3.9,
                                                          4.,
                                                                4.1,
                                                                      4.2,
                                                                            4.3,
                                                    5.,
                                                          5.1,
                                                                           5.4,
                4.4,
                      4.5,
                            4.6,
                                  4.7,
                                       4.8,
                                              4.9,
                                                               5.2,
                                                                      5.3,
                5.5,
                      5.6,
                            5.7,
                                  5.8,
                                        5.9,
                                              6.,
                                                    6.1,
                                                          6.2,
                                                               6.3,
                                                                      6.4, 6.5,
                6.6,
                      6.7,
                            6.8,
                                 6.9,
                                        7.,
                                              7.1,
                                                    7.2,
                                                          7.3,
                                                               7.4,
                                                                      7.5,
                                                                            7.6,
                                 8.,
                      7.8,
                            7.9,
                                                               8.5, 8.6,
                7.7,
                                       8.1,
                                              8.2,
                                                    8.3,
                                                          8.4,
                                                                           8.7,
                                       9.2,
                           9., 9.1,
                                                          9.5, 9.6, 9.7, 9.8,
                8.8,
                      8.9,
                                              9.3,
                                                    9.4,
                9.91)
```

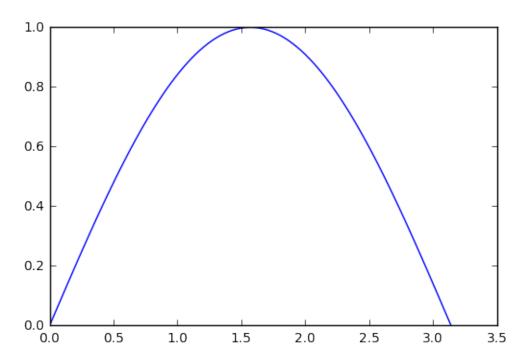
We can quickly define non-integer ranges of numbers for graph plotting:

```
In [16]: import math
In [17]: values=np.linspace(0, math.pi, 100) # Start, stop, number of steps
In [18]: values
Out[18]: array([ 0.
                                                        0.09519978,
                                                                     0.12693304,
                              0.03173326,
                                           0.06346652,
                 0.1586663 ,
                              0.19039955,
                                                        0.25386607,
                                                                     0.28559933,
                                           0.22213281,
                 0.31733259,
                              0.34906585,
                                           0.38079911,
                                                        0.41253237,
                                                                     0.44426563,
                             0.50773215,
                 0.47599889,
                                          0.53946541,
                                                        0.57119866,
                                                                     0.60293192,
                 0.63466518, 0.66639844,
                                          0.6981317 ,
                                                        0.72986496, 0.76159822,
                 0.79333148, 0.82506474, 0.856798 ,
                                                        0.88853126,
                                                                     0.92026451,
                 0.95199777, 0.98373103, 1.01546429,
                                                        1.04719755, 1.07893081,
                 1.11066407,
                             1.14239733,
                                          1.17413059,
                                                        1.20586385,
                                                                    1.23759711,
                 1.26933037,
                             1.30106362,
                                          1.33279688,
                                                        1.36453014, 1.3962634,
                 1.42799666, 1.45972992, 1.49146318,
                                                        1.52319644, 1.5549297,
                 1.58666296,
                             1.61839622,
                                          1.65012947,
                                                        1.68186273,
                                                                     1.71359599,
                 1.74532925,
                             1.77706251,
                                                                    1.87226229,
                                          1.80879577,
                                                        1.84052903,
                 1.90399555,
                             1.93572881,
                                          1.96746207,
                                                        1.99919533, 2.03092858,
                 2.06266184,
                             2.0943951 ,
                                           2.12612836,
                                                        2.15786162,
                                                                     2.18959488,
                 2.22132814,
                             2.2530614 ,
                                           2.28479466,
                                                        2.31652792,
                                                                     2.34826118,
                 2.37999443,
                             2.41172769,
                                          2.44346095,
                                                        2.47519421,
                                                                     2.50692747,
                 2.53866073,
                             2.57039399,
                                           2.60212725,
                                                        2.63386051,
                                                                     2.66559377,
                 2.69732703,
                              2.72906028,
                                           2.76079354,
                                                        2.7925268 ,
                                                                     2.82426006,
                                                        2.9511931 ,
                 2.85599332,
                             2.88772658,
                                           2.91945984,
                                                                     2.98292636,
                 3.01465962,
                             3.04639288,
                                           3.07812614,
                                                        3.10985939,
                                                                     3.14159265])
```

NumPy comes with 'vectorised' versions of common functions which work element-by-element when applied to arrays:

/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment





So we don't have to use awkward list comprehensions when using these.

2.7.6 Multi-Dimensional Arrays

NumPy's true power comes from multi-dimensional arrays:

```
In [20]: np.zeros([3,4,2])
Out[20]: array([[[ 0.,
                         0.],
                  [ 0.,
                         0.],
                  [ 0.,
                         0.],
                         0.]],
                  [ 0.,
                 [[ 0.,
                         0.],
                  [ 0.,
                         0.],
                  [ 0.,
                         0.],
                  [ 0.,
                         0.]],
                 [[ 0.,
                         0.],
                  [ 0.,
                         0.],
                  [ 0.,
                         0.],
                  [ 0.,
                         0.]])
```

Unlike a list-of-lists in Python, we can reshape arrays:

```
In [21]: x=np.array(range(40))
          y=x.reshape([4,5,2])
          У
Out[21]: array([[[ 0,
                         1],
                   [ 2,
                         3],
                   [ 4,
                         5],
                         7],
                   [ 6,
                   [ 8,
                         9]],
                  [[10, 11],
                   [12, 13],
                   [14, 15],
                   [16, 17],
                   [18, 19]],
                  [[20, 21],
                   [22, 23],
                   [24, 25],
                   [26, 27],
                   [28, 29]],
                  [[30, 31],
                   [32, 33],
                   [34, 35],
                   [36, 37],
                   [38, 39]])
  And index multiple columns at once:
```

```
In [22]: y[3,2,1]
Out[22]: 35
```

Including selecting on inner axes while taking all from the outermost:

```
In [23]: y[:,2,1]
Out[23]: array([ 5, 15, 25, 35])
```

And subselecting ranges:

```
In [24]: y[2:,:1,:]
Out[24]: array([[[20, 21]],
                [[30, 31]])
```

And transpose arrays:

```
In [25]: y.transpose()
Out[25]: array([[[ 0, 10, 20, 30],
                 [ 2, 12, 22, 32],
                 [ 4, 14, 24, 34],
```

```
[ 6, 16, 26, 36],
 [ 8, 18, 28, 38]],
 [[ 1, 11, 21, 31],
 [ 3, 13, 23, 33],
 [ 5, 15, 25, 35],
 [ 7, 17, 27, 37],
 [ 9, 19, 29, 39]]])
```

You can get the dimensions of an array with shape

```
In [26]: y.shape
Out[26]: (4, 5, 2)
In [27]: y.transpose().shape
Out[27]: (2, 5, 4)
```

Some numpy functions apply by default to the whole array, but can be chosen to act only on certain axes:

2.7.7 Array Datatypes

A Python list can contain data of mixed type:

```
In [32]: x=['hello', 2, 3.4]
In [33]: type(x[2])
Out[33]: float
In [34]: type(x[1])
Out[34]: int
```

A NumPy array always contains just one datatype:

```
In [35]: np.array(x)
```

```
Out[35]: array(['hello', '2', '3.4'], dtype='<U5')
```

NumPy will choose the least-generic-possible datatype that can contain the data:

```
In [36]: y=np.array([2, 3.4])
In [37]: y
Out[37]: array([ 2. ,  3.4])
In [38]: type(y[0])
Out[38]: numpy.float64
In [39]: z = np.array([3, 4, 5])
z
Out[39]: array([3, 4, 5])
```

2.7.8 Broadcasting

This is another really powerful feature of NumPy By default, array operations are element-by-element:

```
In [40]: np.arange(5)*np.arange(5)
Out[40]: array([ 0,  1,  4,  9, 16])
```

If we multiply arrays with non-matching shapes we get an error:

```
In [41]: np.arange(5) * np.arange(6)

ValueError Traceback (most recent call last)

<ipython-input-41-66b7c967724c> in <module>()

----> 1 np.arange(5) * np.arange(6)

ValueError: operands could not be broadcast together with shapes (5,) (6,)

In [42]: np.zeros([2,3])*np.zeros([2,4])

ValueError Traceback (most recent call last)

<ipython-input-42-4fb354a381e7> in <module>()

----> 1 np.zeros([2,3])*np.zeros([2,4])

ValueError: operands could not be broadcast together with shapes (2,3) (2,4)

ValueError: operands could not be broadcast together with shapes (2,3) (2,4)
```

```
In [43]: m1 = np.arange(100).reshape([10, 10])
In [44]: m2 = np.arange(100).reshape([10, 5, 2])
In [45]: m1+m2
        ValueError
                                                     Traceback (most recent call last)
        <ipython-input-45-e9085a7f6251> in <module>()
    ---> 1 m1+m2
        ValueError: operands could not be broadcast together with shapes (10,10) (10,5,2)
  Arrays must match in all dimensions in order to be compatible:
In [46]: np.ones([3,3])*np.ones([3,3]) # Note elementwise multiply, *not* matrix multiply.
Out[46]: array([[ 1., 1., 1.],
                 [ 1., 1., 1.],
                 [ 1., 1., 1.]])
  Except, that if one array has any Dimension 1, then the data is REPEATED to match the other.
In [47]: m1=np.arange(10).reshape([10,1])
         m1
Out[47]: array([[0],
                 [1],
                 [2],
                 [3],
                 [4],
                 [5],
                 [6],
                 [7],
                 [8],
                 [9]])
In [48]: m2=m1.transpose()
         m2
Out[48]: array([[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]])
In [49]: m1.shape # "Column Vector"
Out[49]: (10, 1)
In [50]: m2.shape # "Row Vector"
Out [50]: (1, 10)
In [51]: m1+m2
```

```
7,
Out [51]: array([[ 0,
                       1,
                           2,
                               3,
                                    4,
                                        5,
                                            6,
                           3,
                               4,
                                   5,
                                            7,
                                                     9, 10],
                 1,
                       2,
                                        6,
                                                8,
                                                 9, 10, 111,
                 [ 2,
                       3,
                           4,
                               5,
                                    6,
                                        7,
                                            8,
                 [ 3,
                           5,
                                    7,
                                            9, 10, 11, 12],
                       4,
                               6,
                                        8,
                 [ 4,
                       5,
                           6,
                               7,
                                    8,
                                        9, 10, 11, 12, 13],
                           7,
                               8,
                                    9, 10, 11, 12, 13, 14],
                 [ 5,
                       6,
                           8,
                               9, 10, 11, 12, 13, 14, 15],
                 [ 6,
                       7,
                           9, 10, 11, 12, 13, 14, 15, 16],
                 [ 7,
                       8,
                       9, 10, 11, 12, 13, 14, 15, 16, 17],
                 18,
                 [ 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]])
In [52]: 10*m1+m2
                      1, 2,
                              3, 4, 5,
                                           6, 7,
Out[52]: array([[ 0,
                                                     8,
                                                         9],
                 [10, 11, 12, 13, 14, 15, 16, 17, 18, 19],
                 [20, 21, 22, 23, 24, 25, 26, 27, 28, 29],
                 [30, 31, 32, 33, 34, 35, 36, 37, 38, 39],
                 [40, 41, 42, 43, 44, 45, 46, 47, 48, 49],
                 [50, 51, 52, 53, 54, 55, 56, 57, 58, 59],
                 [60, 61, 62, 63, 64, 65, 66, 67, 68, 69],
                 [70, 71, 72, 73, 74, 75, 76, 77, 78, 79],
                 [80, 81, 82, 83, 84, 85, 86, 87, 88, 89],
                 [90, 91, 92, 93, 94, 95, 96, 97, 98, 99]])
```

This works for arrays with more than one unit dimension.

2.7.9 Newaxis

Broadcasting is very powerful, and numpy allows indexing with np.newaxis to temporarily create new one-long dimensions on the fly.

Note that newaxis works because a $3 \times 1 \times 3$ array and a 3×3 array contain the same data, differently shaped:

2.7.10 Dot Products

NumPy multiply is element-by-element, not a dot-product:

To get a dot-product, (matrix inner product) we can use a built in function:

Though it is possible to represent this in the algebra of broadcasting and newaxis:

Or if you prefer:

We use broadcasting to generate $A_{ij}B_{jk}$ as a 3-d matrix:

Then we sum over the middle, j axis, [which is the 1-axis of three axes numbered (0,1,2)] of this 3-d matrix. Thus we generate $\Sigma_i A_{ij} B_{jk}$.

We can see that the broadcasting concept gives us a powerful and efficient way to express many linear algebra operations computationally.

2.7.11 Array DTypes

Arrays have a "dtype" which specifies their datatype:

```
In [66]: x=[2, 3.4, 7.2, 0]
In [67]: np.array(x)
Out[67]: array([ 2. , 3.4, 7.2, 0. ])
In [68]: np.array(x).dtype
Out[68]: dtype('float64')
```

These are, when you get to know them, fairly obvious string codes for datatypes: NumPy supports all kinds of datatypes beyond the python basics.

NumPy will convert python type names to dtypes:

```
In [69]: int_array= np.array(x, dtype=int)
In [70]: float_array=np.array(x, dtype=float)
In [71]: int_array
Out[71]: array([2, 3, 7, 0])
In [72]: float_array
Out[72]: array([2., 3.4, 7.2, 0.])
In [73]: int_array.dtype
Out[73]: dtype('int64')
In [74]: float_array.dtype
Out[74]: dtype('float64')
```

2.7.12 Record Arrays

These are a special array structure designed to match the CSV "Record and Field" model. It's a very different structure from the normal numPy array, and different fields *can* contain different datatypes. We saw this when we looked at CSV files:

Record arrays can be addressed with field names like they were a dictionary:

We've seen these already when we used NumPy's CSV parser.

2.7.13 Logical arrays, masking, and selection

Numpy defines operators like == and < to apply to arrays *element by element*

```
In [79]: x=np.zeros([3,4])
        Х
Out[79]: array([[ 0., 0., 0., 0.],
               [ 0., 0., 0., 0.],
               [ 0., 0., 0., 0.]])
In [80]: y=np.arange(-1,2)[:,np.newaxis]*np.arange(-2,2)[np.newaxis,:]
        У
Out[80]: array([[ 2, 1, 0, -1],
               [ 0, 0, 0, 0],
               [-2, -1, 0, 1]
In [81]: iszero = x==y
        iszero
Out[81]: array([[False, False,
                              True, False],
               [ True, True, True, True],
               [False, False, True, False]], dtype=bool)
```

A logical array can be used to select elements from an array:

```
In [82]: y[np.logical_not(iszero)]
```

```
Out [82]: array([ 2, 1, -1, -2, -1, 1])
```

Although when printed, this comes out as a flat list, if assigned to, the *selected elements of the array are changed!*

2.7.14 Numpy memory

Numpy memory management can be tricksy:

We must use np.copy to force separate memory. Otherwise NumPy tries it's hardest to make slices be

Now, this has all been very theoretical, but let's go through a practical example, and see how powerful NumPy can be.

2.8 The Boids!

2.8.1 Flocking

The aggregate motion of a flock of birds, a herd of land animals, or a school of fish is a beautiful and familiar part of the natural world... The aggregate motion of the simulated flock is created by a distributed behavioral model much like that at work in a natural flock; the birds choose their own course. Each simulated bird is implemented as an independent actor that navigates according to its local perception of the dynamic environment, the laws of simulated physics that rule its motion, and a set of behaviors programmed into it... The aggregate motion of the simulated flock is the result of the dense interaction of the relatively simple behaviors of the individual simulated birds.

– Craig W. Reynolds, "Flocks, Herds, and Schools: A Distributed Behavioral Model", *Computer Graphics* **21** 4 1987, pp 25-34 See the original paper

- Collision Avoidance: avoid collisions with nearby flockmates
- Velocity Matching: attempt to match velocity with nearby flockmates
- Flock Centering: attempt to stay close to nearby flockmates

2.8.2 Setting up the Boids

Our boids will each have an x velocity and a y velocity, and an x position and a y position.

We'll build this up in NumPy notation, and eventually, have an animated simulation of our flying boids.

```
In [1]: import numpy as np
```

Let's start with simple flying in a straight line.

Our locations, for each of our N boids, will be an array, shape $2 \times N$, with the x positions in the first row, and y positions in the second row.

```
In [2]: boid count = 10
```

We'll want to be able to seed our Boids in a random position.

We'd better define the edges of our simulation area:

We used **broadcasting** with np.newaxis to apply our upper limit to each boid. rand gives us a random number between 0 and 1. We multiply by our limits to get a number up to that limit.

But each bird will also need a starting velocity. Let's make these random too:

2.8.3 Flying in a Straight Line

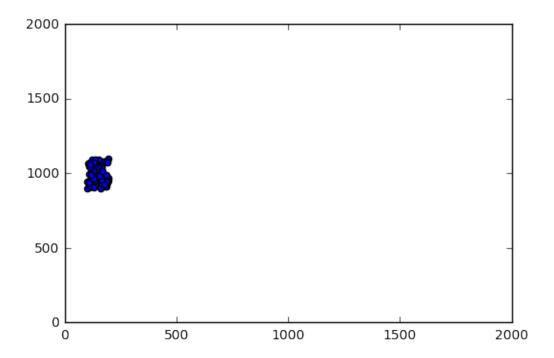
Now we see the real amazingness of NumPy: if we want to move our *whole flock* according to $\delta_x = \delta_t \cdot \frac{dv}{dt}$ We just do:

2.8.4 Matplotlib Animations

So now we can animate our Boids using the matplotlib animation tools. All we have to do is import the relevant libraries:

/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment

Then, we make a static plot, showing our first frame:



Then, we define a function which **updates** the figure for each timestep

Call FuncAnimation, and specify how many frames we want:

Save out the figure:

```
In [16]: anim.save('boids_1.mp4')
```

And download the saved animation

You can even use an external library to view the results directly in the notebook. If you're on your own computer, you can download it from https://gist.github.com/gforsyth/188c32b6efe834337d8a (See the notes on installing libraries...)

Unfortunately, if you're on the teaching cluster, you won't be able to install it there.

```
In [17]: from JSAnimation import IPython_display
    # Inline animation tool; needs manual install via
    # If you don't have this, you need to save animations as MP4.
    positions=new_flock(100, np.array([100,900]), np.array([200,1100]))
    anim
Out[17]: <matplotlib.animation.FuncAnimation at 0x2b78403b9748>
```

2.8.5 Fly towards the middle

Boids try to fly towards the middle:

```
In [18]: positions=new_flock(4, np.array([100,900]), np.array([200,1100]))
        velocities=new_flock(4, np.array([0,-20]), np.array([10,20]))
In [19]: positions
Out[19]: array([[ 174.51286306, 133.2657178, 145.39953252, 109.57643279],
                [ 966.86460366, 1081.26059289,
                                                 903.53881717, 965.45250716]])
In [20]: velocities
Out[20]: array([[ 3.71167934, 0.70904211, 7.96231575,
                                                             3.39212344],
                [-1.44749274, -18.16368322, -0.02847944, 5.49452896]])
In [21]: middle=np.mean(positions, 1)
        middle
Out[21]: array([ 140.68863654, 979.27913022])
In [22]: direction to middle = positions-middle[:, np.newaxis]
In [23]: move_to_middle_strength = 0.01
        velocities = velocities - direction_to_middle * move_to_middle_strength
  Let's update our function, and animate that:
In [24]: def update_boids(positions, velocities):
             move_to_middle_strength = 0.1
             middle=np.mean(positions, 1)
             direction_to_middle = positions - middle[:, np.newaxis]
             velocities -= direction_to_middle * move_to_middle_strength
             positions += velocities
In [25]: def animate(frame):
             update_boids(positions, velocities)
             scatter.set_offsets(positions.transpose())
In [26]: anim=animation.FuncAnimation(figure, animate,
                                 frames=50, interval=50)
In [27]: from JSAnimation import IPython_display
        positions=new_flock(100, np.array([100,900]), np.array([200,1100]))
        velocities=new_flock(100, np.array([0,-20]), np.array([10,20]))
        anim
Out[27]: <matplotlib.animation.FuncAnimation at 0x2b78403cdb70>
```

2.8.6 Avoiding collisions

We'll want to add our other flocking rules to the behaviour of the Boids. We'll need a matrix giving the distances between each bird. This should be $N \times N$.

We might think that we need to do the X-distances and Y-distances separately:

```
In [29]: xpos=positions[0,:]
In [30]: xsep_matrix = xpos[:,np.newaxis] - xpos[np.newaxis,:]
In [31]: xsep matrix.shape
Out[31]: (4, 4)
In [32]: xsep_matrix
                            , 61.27550208, 76.75290377, 1.75064368],
Out[32]: array([[ 0.
                [-61.27550208, 0. , 15.4774017 , -59.5248584 ],
                [-76.75290377, -15.4774017,
                                             0. , -75.0022601 ],
                [-1.75064368, 59.5248584, 75.0022601, 0.
                                                                       11)
  But in NumPy we can be cleverer than that, and make a 2 by N by N matrix of separations:
In [33]: separations = positions[:,np.newaxis,:] - positions[:,:,np.newaxis]
In [34]: separations.shape
Out[34]: (2, 4, 4)
  And then we can get the sum-of-squares \delta_x^2 + \delta_u^2 like this:
In [35]: squared_displacements = separations * separations
In [36]: square_distances = np.sum(squared_displacements, 0)
In [37]: square_distances
Out[37]: array([[
                               , 16999.61571187, 11364.91417818,
                   0.
                                                                      321.24148925],
                [ 16999.61571187,
                                  0. , 1928.82273902, 13000.5970045],
                [ 11364.91417818, 1928.82273902,
                                                     0. , 8777.9751443 ],
                  321.24148925, 13000.5970045, 8777.9751443,
                                                                     0.
                                                                                    ]])
  Now we need to find birds that are too close:
In [38]: alert_distance = 2000
         close_birds = square_distances < alert_distance</pre>
         close_birds
Out[38]: array([[ True, False, False, True],
                [False, True, True, False],
                [False, True, True, False],
                [ True, False, False, True]], dtype=bool)
  Find the direction distances only to those birds which are too close:
In [39]: separations_if_close = np.copy(separations)
         far_away = np.logical_not(close_birds)
In [40]: separations_if_close[0,:,:][far_away] = 0
         separations_if_close[1,:,:][far_away] = 0
         separations_if_close
```

```
, -15.4774017 , 0.
                [ 0.
                             15.4774017 , 0. ,
                                                        0.
                                                                   1,
                [ 1.75064368, 0. ,
                                                        0.
                                            0.
                                                                   ]],
               [[ 0. , 0. , 0. , -41.10076369,
                                                  , 17.83750924],
                                                        0.
                                                                  1,
                                           0.
                              41.10076369,
                [ 0.
                                                          0.
                                                                   1,
                [-17.83750924,
                              0. , 0.
                                                        0.
                                                                   111)
  And fly away from them:
In [41]: velocities = velocities + np.sum(separations if close,2)
  Now we can update our animation:
In [42]: def update_boids(positions, velocities):
            move_to_middle_strength = 0.01
            middle = np.mean(positions, 1)
            direction_to_middle = positions - middle[:,np.newaxis]
            velocities -= direction_to_middle * move_to_middle_strength
            separations = positions[:,np.newaxis,:] - positions[:,:,np.newaxis]
            squared displacements = separations * separations
            square_distances = np.sum(squared_displacements, 0)
            alert distance = 100
            far_away = square_distances > alert_distance
            separations_if_close = np.copy(separations)
            separations_if_close[0,:,:][far_away] =0
            separations_if_close[1,:,:][far_away] =0
            velocities += np.sum(separations_if_close,1)
            positions += velocities
In [43]: def animate(frame):
            update_boids(positions, velocities)
            scatter.set_offsets(positions.transpose())
        anim = animation.FuncAnimation(figure, animate,
                               frames=50, interval=50)
        from JSAnimation import IPython_display
        positions = new_flock(100, np.array([100, 900]), np.array([200, 1100]))
        velocities = new_flock(100, np.array([0,-20]), np.array([10,20]))
        anim
Out[43]: <matplotlib.animation.FuncAnimation at 0x2b78402c9f98>
2.8.7 Match speed with nearby birds
This is pretty similar:
In [44]: def update_boids(positions, velocities):
            move_to_middle_strength = 0.01
```

direction_to_middle = positions-middle[:,np.newaxis]

middle = np.mean(positions, 1)

```
velocities -= direction_to_middle*move_to_middle_strength
             separations = positions[:,np.newaxis,:] - positions[:,:,np.newaxis]
             squared_displacements = separations*separations
             square_distances = np.sum(squared_displacements, 0)
             alert distance = 100
             far_away=square_distances > alert_distance
             separations_if_close = np.copy(separations)
             separations_if_close[0,:,:][far_away] =0
             separations_if_close[1,:,:][far_away] =0
             velocities += np.sum(separations_if_close,1)
             velocity_differences = velocities[:,np.newaxis,:] - velocities[:,:,np.newaxis
             formation_flying_distance = 10000
             formation_flying_strength = 0.125
             very_far=square_distances > formation_flying_distance
             velocity_differences_if_close = np.copy(velocity_differences)
             velocity_differences_if_close[0,:,:][very_far] =0
             velocity_differences_if_close[1,:,:][very_far] =0
             velocities -= np.mean(velocity_differences_if_close, 1) * formation_flying_st
             positions += velocities
In [45]: def animate(frame):
             update_boids(positions, velocities)
             scatter.set_offsets(positions.transpose())
         anim=animation.FuncAnimation(figure, animate,
                                 frames=200, interval=50)
         from JSAnimation import IPython_display
         positions=new flock(100, np.array([100,900]), np.array([200,1100]))
         velocities=new_flock(100, np.array([0,-20]), np.array([10,20]))
         anim
Out[45]: <matplotlib.animation.FuncAnimation at 0x2b78402e0860>
```

Hopefully the power of NumPy should be pretty clear now. This would be **enormously slower** and, I think, harder to understand using traditional lists.

2.9 Recap: Understanding the "Greengraph" Example

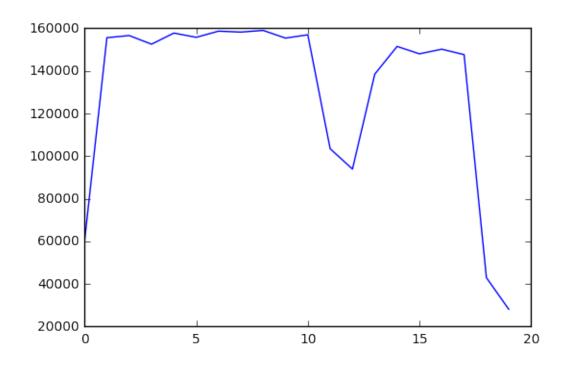
We now know enough to understand everything we did in the initial example chapter on the "Greengraph". Go back to that part of the notes, and re-read the code.

Now, we can even write it up into a class, and save it as a module.

2.9.1 Classes for Greengraph

```
import geopy
        from .map import Map
        class Greengraph(object):
            def __init__(self, start, end):
                self.start=start
                self.end=end
                self.geocoder=geopy.geocoders.GoogleV3(domain="maps.google.co.uk")
            def geolocate(self, place):
                return self.geocoder.geocode(place, exactly_one=False)[0][1]
            def location_sequence(self, start,end,steps):
              lats = np.linspace(start[0], end[0], steps)
              longs = np.linspace(start[1],end[1], steps)
              return np.vstack([lats, longs]).transpose()
            def green_between(self, steps):
                return [Map(*location).count_green()
                        for location in self.location sequence (
                            self.geolocate(self.start),
                            self.geolocate(self.end),
                            steps)]
Writing greengraph/graph.py
In [3]: %%writefile greengraph/map.py
        import numpy as np
        from io import BytesIO
        from matplotlib import image as img
        import requests
        class Map(object):
            def __init__(self, lat, long, satellite=True, zoom=10,
                         size=(400,400), sensor=False):
                base="http://maps.googleapis.com/maps/api/staticmap?"
                params=dict(
                    sensor= str(sensor).lower(),
                    zoom= zoom,
                    size= "x".join(map(str, size)),
                    center= ",".join(map(str, (lat, long))),
                    style="feature:all|element:labels|visibility:off"
                  )
                if satellite:
                    params["maptype"]="satellite"
                self.image = requests.get(base,
                            params=params).content # Fetch our PNG image data
                content = BytesIO(self.image)
                self.pixels= img.imread(content) # Parse our PNG image as a numpy array
```

```
def green (self, threshold):
                # Use NumPy to build an element-by-element logical array
                greener_than_red = self.pixels[:,:,1] > threshold* self.pixels[:,:,0]
                greener_than_blue = self.pixels[:,:,1] > threshold*self.pixels[:,:,2]
                green = np.logical_and(greener_than_red, greener_than_blue)
                return green
            def count_green(self, threshold = 1.1):
                return np.sum(self.green(threshold))
            def show_green(data, threshold = 1.1):
                green = self.green(threshold)
                out = green[:,:,np.newaxis]*array([0,1,0])[np.newaxis,np.newaxis,:]
                buffer = BytesIO()
                result = img.imsave(buffer, out, format='png')
                return buffer.getvalue()
Writing greengraph/map.py
In [4]: %%writefile greengraph/__init__.py
        from .graph import Greengraph
Writing greengraph/__init__.py
2.9.2 Invoking our code and making a plot
In [5]: from matplotlib import pyplot as plt
        from greengraph import Greengraph
        %matplotlib inline
        mygraph=Greengraph('New York','Chicago')
        data = mygraph.green_between(20)
/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py
  warnings.warn('Matplotlib is building the font cache using fc-list. This may take a momen
/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py
  warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment
In [6]: plt.plot(data)
Out[6]: [<matplotlib.lines.Line2D at 0x2b78a0a9d550>]
```



2.10 Introduction

2.10.1 What's version control?

Version control is a tool for **managing changes** to a set of files. There are many different **version control systems**:

- Git
- Mercurial (hg)
- CVS
- Subversion (svn)
- ...

2.10.2 Why use version control?

- Better kind of **backup**.
- Review **history** ("When did I introduce this bug?").
- Restore older code versions.
- Ability to undo mistakes.
- Maintain **several versions** of the code at a time.

Git is also a **collaborative** tool:

- "How can I share my code?"
- "How can I submit a change to someone else's code?"
- "How can I merge my work with Sue's?"

2.10.3 Git != GitHub

- **Git**: version control system tool to manage source code history.
- GitHub: hosting service for Git repositories.

2.10.4 How do we use version control?

Do some programming, then commit our work:

my_vcs commit Program some more. Spot a mistake: my_vcs rollback Mistake is undone.

2.10.5 What is version control? (Team version)

Sue	James
my_vcs commit	
	Join the team
	my_vcs checkout
	Do some programming
	my_vcs commit
my_vcs update	
Do some programming	Do some programming
my_vcs commit	
my_vcs update	
my_vcs merge	
my_vcs commit	

2.10.6 Scope

This course will use the git version control system, but much of what you learn will be valid with other version control tools you may encounter, including subversion (svn) and mercurial (hg).

2.11 Practising with Git

2.11.1 Example Exercise

In this course, we will use, as an example, the development of a few text files containing a description of a topic of your choice.

This could be your research, a hobby, or something else. In the end, we will show you how to display the content of these files as a very simple website.

2.11.2 Programming and documents

The purpose of this exercise is to learn how to use Git to manage program code you write, not simple text website content, but we'll just use these text files instead of code for now, so as not to confuse matters with

trying to learn version control while thinking about programming too.

In later parts of the course, you will use the version control tools you learn today with actual Python code.

2.11.3 Markdown

The text files we create will use a simple "wiki" markup style called markdown to show formatting. This is the convention used in this file, too.

You can view the content of this file in the way Markdown renders it by looking on the web, and compare the raw text.

2.11.4 Displaying Text in this Tutorial

This tutorial is based on use of the Git command line. So you'll be typing commands in the shell.

To make it easy for me to edit, I've built it using IPython notebook.

Commands you can type will look like this, using the "bash "magic" for the notebook.

with the results you should see below.

In this document, we will show the new content of an edited document like this:

But if you are following along, you should edit the file using a text editor. On windows, we recommend Notepad++. On mac, we recommend Atom

2.11.5 Setting up somewhere to work

```
In [3]: %%bash
    rm -rf learning_git/git_example # Just in case it's left over from a previous class
    mkdir -p learning_git/git_example
    cd learning_git/git_example
```

I just need to move this IPython notebook's current directory as well:

2.12 Solo work

2.12.1 Configuring Git with your name and email

First, we should configure Git to know our name and email address:

2.12.2 Initialising the repository

Now, we will tell Git to track the content of this folder as a git "repository".

```
In [9]: %%bash
    pwd # Note where we are standing-- MAKE SURE YOU INITIALISE THE RIGHT FOLDER
    qit init
```

/home/travis/build/UCL/rsd-engineeringcourse/ch02git/learning_git/git_example Initialized empty Git repository in /home/travis/build/UCL/rsd-engineeringcourse/ch02git/learning_git/git_example

As yet, this repository contains no files:

2.13 Solo work with Git

So, we're in our git working directory:

2.13.1 A first example file

So let's create an example file, and see how to start to manage a history of changes to it.

```
<my editor> index.md # Type some content into the file.
```

2.13.2 Telling Git about the File

So, let's tell Git that index.md is a file which is important, and we would like to keep track of its history:

Don't forget: Any files in repositories which you want to "track" need to be added with git add after you create them.

2.13.3 Our first commit

Now, we need to tell Git to record the first version of this file in the history of changes:

And note the confirmation from Git.

There's a lot of output there you can ignore for now.

2.13.4 Configuring Git with your editor

If you don't type in the log message directly with -m "Some message", then an editor will pop up, to allow you to edit your message on the fly.

For this to work, you have to tell git where to find your editor.

You can find out what you currently have with:

To configure Notepad++ on windows you'll need something like the below, ask a demonstrator to help for your machine.

```
git config --global core.editor "'C:/Program Files (x86)/Notepad++
    /notepad++.exe' -multiInst -nosession -noPlugin"
```

I'm going to be using vim as my editor, but you can use whatever editor you prefer. (Windows users could use "Notepad++", Mac users could use "textmate" or "sublime text", linux users could use vim, nano or emacs.)

2.13.5 Git log

Git now has one change in its history:

You can see the commit message, author, and date...

2.13.6 Hash Codes

The commit "hash code", e.g.

c438f1716b2515563e03e82231acbae7dd4f4656

is a unique identifier of that particular revision.

(This is a really long code, but whenever you need to use it, you can just use the first few characters, however many characters is long enough to make it unique, 0438 for example.)

2.13.7 Nothing to see here

Note that git will now tell us that our "working directory" is up-to-date with the repository: there are no changes to the files that aren't recorded in the repository history:

Let's edit the file again:

```
vim index.md
```

2.13.8 Unstaged changes

We can now see that there is a change to "index.md" which is currently "not staged for commit". What does this mean?

If we do a git commit now nothing will happen.

Git will only commit changes to files that you choose to include in each commit.

This is a difference from other version control systems, where committing will affect all changed files.

We can see the differences in the file with:

Deleted lines are prefixed with a minus, added lines prefixed with a plus.

2.13.9 Staging a file to be included in the next commit

To include the file in the next commit, we have a few choices. This is one of the things to be careful of with git: there are lots of ways to do similar things, and it can be hard to keep track of them all.

This says "include in the next commit, all files which have ever been included before".

Note that git add is the command we use to introduce git to a new file, but also the command we use to "stage" a file to be included in the next commit.

2.13.10 The staging area

The "staging area" or "index" is the git jargon for the place which contains the list of changes which will be included in the next commit.

You can include specific changes to specific files with git add, commit them, add some more files, and commit them. (You can even add specific changes within a file to be included in the index.)

2.13.11 Message Sequence Charts

In order to illustrate the behaviour of Git, it will be useful to be able to generate figures in Python of a "message sequence chart" flavour.

There's a nice online tool to do this, called "Message Sequence Charts".

Have a look at https://www.websequencediagrams.com

Instead of just showing you these diagrams, I'm showing you in this notebook how I make them. This is part of our "reproducible computing" approach; always generating all our figures from code.

Here's some quick code in the Notebook to download and display an MSC illustration, using the Web Sequence Diagrams API:

```
In [15]: %%writefile wsd.py
         import requests
         import re
         import IPython
         def wsd(code):
             response = requests.post("http://www.websequencediagrams.com/index.php", data-
                     'message': code,
                     'apiVersion': 1,
                 })
             expr = re.compile("(?(img|pdf|png|svg)=[a-zA-Z0-9]+)")
             m = expr.search(response.text)
             if m == None:
                 print "Invalid response from server."
                 return False
             image=requests.get("http://www.websequencediagrams.com/" + m.group(0))
             return IPython.core.display.Image(image.content)
Writing wsd.py
In [16]: from wsd import wsd
         %matplotlib inline
         wsd("Sender->Recipient: Hello\n Recipient->Sender: Message received OK")
```

```
ImportErrorTraceback (most recent call last)

<ipython-input-16-122a6b8129f8> in <module>()
----> 1 from wsd import wsd
    2 get_ipython().magic(u'matplotlib inline')
    3 wsd("Sender->Recipient: Hello\n Recipient->Sender: Message received OK")

/home/travis/build/UCL/rsd-engineeringcourse/ch02git/learning_git/git_example/wsd.]
----> 1 import requests
    2 import re
    3 import IPython
    4
    5 def wsd(code):

ImportError: No module named requests
```

2.13.12 The Levels of Git

Let's make ourselves a sequence chart to show the different aspects of Git we've seen so far:

```
In [17]: message="""
    Working Directory -> Staging Area : git add
    Staging Area -> Local Repository : git commit
    Working Directory -> Local Repository : git commit -a
    """
    wsd(message)

NameErrorTraceback (most recent call last)

<ipython-input-17-2506b1205ea1> in <module>()
    4 Working Directory -> Local Repository : git commit -a
    5 """
----> 6 wsd(message)
NameError: name 'wsd' is not defined
```

2.13.13 Review of status

```
modified:
                  index.md
Untracked files:
  (use "git add <file>..." to include in what will be committed)
        wsd.py
        wsd.pyc
In [19]: %%bash
        git commit -m "Add a lie about a mountain"
[master 197ac66] Add a lie about a mountain
1 file changed, 3 insertions(+), 1 deletion(-)
In [20]: %%bash
         git log
commit 197ac665eaa43d6dfc6e495604898a930adaf04b
Author: James Hetherington < jamespjh@gmail.com>
Date:
       Thu Nov 24 10:14:56 2016 +0000
    Add a lie about a mountain
commit 944bc260b8aba054a9c5b8ecf691f04f0f8dfdbd
Author: James Hetherington < jamespjh@gmail.com>
       Thu Nov 24 10:14:55 2016 +0000
Date:
    First commit of discourse on UK topography
```

Great, we now have a file which contains a mistake.

2.13.14 Carry on regardless

In [22]: cat index.md

In a while, we'll use Git to roll back to the last correct version: this is one of the main reasons we wanted to use version control, after all! But for now, let's do just as we would if we were writing code, not notice our mistake and keep working...

2.13.15 Commit with a built-in-add

This last command, git commit —a automatically adds changes to all tracked files to the staging area, as part of the commit command. So, if you never want to just add changes to some tracked files but not others, you can just use this and forget about the staging area!

2.13.16 Review of changes

We now have three changes in the history:

2.13.17 Git Solo Workflow

We can make a diagram that summarises the above story:

```
In [26]: message="""
    participant "Jim's repo" as R
    participant "Jim's index" as I
    participant Jim as J
```

```
note right of J: vim index.md
    note right of J: git init
    J->I: create
    J->R: create
    note right of J: git add index.md
    J->I: Add content of index.md
    note right of J: git commit
    J->R: Commit content of index.md
    note right of J: vim index.md
    note right of J: git add --update
    J->I: Add content of index.md
    note right of J: git commit -m "Add a lie"
    I->R: Commit change to index.md
    note right of J: vim index.md
    note right of J: git commit -am "Change title"
    J->I: Add content of index.md
    J->R: Commit change to index.md
    wsd(message)
   NameErrorTraceback (most recent call last)
    <ipython-input-26-42369849e02b> in <module>()
    30
    31 """
---> 32 wsd(message)
   NameError: name 'wsd' is not defined
```

2.14 Fixing mistakes

We're still in our git working directory:

2.14.1 Referring to changes with HEAD and ^

The commit we want to revert to is the one before the latest.

 $\mathtt{HEAD}^{\hat{}}$ refers to the commit before the "head", which is the latest change. That is, we want to go back to the change before the current one.

We could have used the hash code to reference this, but you can also refer to the commit before the HEAD as HEAD^, the one before that as HEAD^, the one before that as HEAD^3. We could also refer to it with the hash code, e.g. 73fbeaf

2.14.2 Reverting

Ok, so now we'd like to undo the nasty commit with the lie about Mount Fictional.

A commit may pop up, with some default text which you can accept and save.

2.14.3 Conflicted reverts

You may, depending on the changes you've tried to make, get an error message here.

If this happens, it is because git could not automagically decide how to combine the change you made after the change you want to revert, with the attempt to revert the change: this could happen, for example, if they both touch the same line.

If that happens, you need to manually edit the file to fix the problem. Skip ahead to the section on resolving conflicts, or ask a demonstrator to help.

2.14.4 Review of changes

The file should now contain the change to the title, but not the extra line with the lie. Note the log:

```
Add a lie about a mountain

commit 944bc260b8aba054a9c5b8ecf691f04f0f8dfdbd

Author: James Hetherington <jamespjh@gmail.com>
Date: 2016-11-24

First commit of discourse on UK topography
```

2.14.5 Antipatch

Notice how the mistake has stayed in the history.

There is a new commit which undoes the change: this is colloquially called an "antipatch". This is nice: you have a record of the full story, including the mistake and its correction.

2.14.6 Rewriting history

It is possible, in git, to remove the most recent change altogether, "rewriting history". Let's make another bad change, and see how to do this.

2.14.7 A new lie

```
In [4]: %%writefile index.md
       Mountains and Hills in the UK
       ================
       Engerland is not very mountainous.
       But has some tall hills, and maybe a
       mountain or two depending on your definition.
Overwriting index.md
In [5]: %%bash
       cat index.md
Mountains and Hills in the UK
Engerland is not very mountainous.
But has some tall hills, and maybe a
mountain or two depending on your definition.
In [6]: %%bash
       git diff
diff --git a/index.md b/index.md
index dd5cf9c..6f211e7 100644
--- a/index.md
+++ b/index.md
@@ -1, 4 +1, 5 @@
Mountains and Hills in the UK
===============
-England is not very mountainous.
-But has some tall hills, and maybe a mountain or two depending on your definition.
+Engerland is not very mountainous.
```

```
+But has some tall hills, and maybe a
+mountain or two depending on your definition.
\ No newline at end of file
In [7]: %%bash
        git commit -am "Add a silly spelling"
[master 256c8a5] Add a silly spelling
1 file changed, 3 insertions(+), 2 deletions(-)
In [8]: %%bash
       git log --date=short
commit 256c8a5648a150eb622212f22884c015a7102152
Author: James Hetherington < jamespjh@gmail.com>
Date: 2016-11-24
   Add a silly spelling
commit 57ceea6a8a01877cf0fb93275cf071e24783b89a
Author: James Hetherington < jamespjh@gmail.com>
Date:
       2016-11-24
    Revert "Add a lie about a mountain"
    This reverts commit 197ac665eaa43d6dfc6e495604898a930adaf04b.
commit 86e1579099f9c2a35ac123bb700eef7d3c0a142f
Author: James Hetherington < jamespjh@gmail.com>
Date: 2016-11-24
   Change title
commit 197ac665eaa43d6dfc6e495604898a930adaf04b
Author: James Hetherington < jamespjh@gmail.com>
Date: 2016-11-24
   Add a lie about a mountain
commit 944bc260b8aba054a9c5b8ecf691f04f0f8dfdbd
Author: James Hetherington < jamespjh@gmail.com>
Date: 2016-11-24
   First commit of discourse on UK topography
2.14.8 Using reset to rewrite history
In [9]: %%bash
        git reset HEAD^
Unstaged changes after reset:
```

index.md

```
In [10]: %%bash
         git log --date=short
commit 57ceea6a8a01877cf0fb93275cf071e24783b89a
Author: James Hetherington < jamespjh@gmail.com>
       2016-11-24
Date:
    Revert "Add a lie about a mountain"
    This reverts commit 197ac665eaa43d6dfc6e495604898a930adaf04b.
commit 86e1579099f9c2a35ac123bb700eef7d3c0a142f
Author: James Hetherington < jamespjh@gmail.com>
Date: 2016-11-24
    Change title
commit 197ac665eaa43d6dfc6e495604898a930adaf04b
Author: James Hetherington < jamespjh@gmail.com>
Date: 2016-11-24
    Add a lie about a mountain
commit 944bc260b8aba054a9c5b8ecf691f04f0f8dfdbd
Author: James Hetherington < jamespjh@gmail.com>
       2016-11-24
Date:
   First commit of discourse on UK topography
```

2.14.9 Covering your tracks

The silly spelling is gone, and *it isn't even in the log*. This approach to fixing mistakes, "rewriting history" with reset, instead of adding an antipatch with revert is dangerous, and we don't recommend it. But you may want to do it for small silly mistakes, such as to correct a commit message.

2.14.10 Resetting the working area

When git reset removes commits, it leaves your working directory unchanged – so you can keep the work in the bad change if you want.

If you want to lose the change from the working directory as well, you can do git reset --hard. I'm going to get rid of the silly spelling, and I didn't do --hard, so I'll reset the file from the working directory to be the same as in the index:

```
In [13]: %%bash
         cat index.md
Mountains and Hills in the UK
============
England is not very mountainous.
But has some tall hills, and maybe a mountain or two depending on your definition.
  We can add this to our diagram:
In [14]: message="""
         Working Directory -> Staging Area : git add
         Staging Area -> Local Repository : git commit
         Working Directory -> Local Repository : git commit -a
         Staging Area -> Working Directory : git checkout
         Local Repository -> Staging Area : git reset
         Local Repository -> Working Directory: git reset --hard
         from wsd import wsd
         %matplotlib inline
         wsd(message)
        ImportErrorTraceback (most recent call last)
        <ipython-input-14-9d3b538eb282> in <module>()
          7 Local Repository -> Working Directory: git reset --hard
          8 """
    ---> 9 from wsd import wsd
         10 get_ipython().magic(u'matplotlib inline')
         11 wsd (message)
        /home/travis/build/UCL/rsd-engineeringcourse/ch02git/learning_git/git_example/wsd.
    ---> 1 import requests
          2 import re
          3 import IPython
          5 def wsd(code):
        ImportError: No module named requests
  We can add it to Jim's story:
In [15]: message="""
         participant "Jim's repo" as R
         participant "Jim's index" as I
         participant Jim as J
         note right of J: git revert HEAD^
```

```
J->R: Add new commit reversing change
     R->I: update staging area to reverted version
     I->J: update file to reverted version
     note right of J: vim index.md
     note right of J: git commit -am "Add another mistake"
     J->I: Add mistake
     I->R: Add mistake
     note right of J: git reset HEAD^
     J->R: Delete mistaken commit
     R->I: Update staging area to reset commit
     note right of J: git checkout index.md
     I->J: Update file to reverted version
     . . . . .
     wsd (message)
    NameErrorTraceback (most recent call last)
    <ipython-input-15-09c73e5dba0f> in <module>()
     28
     29 """
---> 30 wsd(message)
    NameError: name 'wsd' is not defined
```

2.15 Publishing

We're still in our working directory:

2.15.1 Sharing your work

So far, all our work has been on our own computer. But a big part of the point of version control is keeping your work safe, on remote servers. Another part is making it easy to share your work with the world In this example, we'll be using the "GitHub" cloud repository to store and publish our work.

If you have not done so already, you should create an account on GitHub: go to https://github.com/, fill in a username and password, and click on "sign up for free".

2.15.2 Creating a repository

Ok, let's create a repository to store our work. Hit "new repository" on the right of the github home screen, or click here.

Fill in a short name, and a description. Choose a "public" repository. Don't choose to add a Readme.

2.15.3 Paying for GitHub

For this software carpentry course, you should use public repositories in your personal account for your example work: it's good to share! GitHub is free for open source, but in general, charges a fee if you want to keep your work private.

In the future, you might want to keep your work on GitHub private.

Students can get free private repositories on GitHub, by going to [https://github.com/edu] and filling in a form.

UCL pays for private GitHub repositories for UCL research groups: you can find the service details on our web page.

2.15.4 Adding a new remote to your repository

Instructions will appear, once you've created the repository, as to how to add this new "remote" server to your repository, in the lower box on the screen. Mine say:

2.15.5 Remotes

The first command sets up the server as a new remote, called origin.

+ 8cac8ee...57ceea6 master -> master (forced update)

Git, unlike some earlier version control systems is a "distributed" version control system, which means you can work with multiple remote servers.

Usually, commands that work with remotes allow you to specify the remote to use, but assume the origin remote if you don't.

Here, git push will push your whole history onto the server, and now you'll be able to see it on the internet! Refresh your web browser where the instructions were, and you'll see your repository!

Let's add these commands to our diagram:

```
In [4]: message="""
        Working Directory -> Staging Area : git add
        Staging Area -> Local Repository : git commit
        Working Directory -> Local Repository : git commit -a
        Staging Area -> Working Directory : git checkout
        Local Repository -> Staging Area : git reset
        Local Repository -> Working Directory: git reset --hard
        Local Repository -> Remote Repository : git push
        from wsd import wsd
        %matplotlib inline
        wsd (message)
        ImportErrorTraceback (most recent call last)
        <ipython-input-4-1d17be16dc9d> in <module>()
          8 Local Repository -> Remote Repository : git push
    ---> 10 from wsd import wsd
         11 get ipython().magic(u'matplotlib inline')
         12 wsd (message)
        /home/travis/build/UCL/rsd-engineeringcourse/ch02git/learning_git/git_example/wsd.
    ----> 1 import requests
          2 import re
          3 import IPython
          5 def wsd(code):
        ImportError: No module named requests
```

2.15.6 Playing with GitHub

Take a few moments to click around and work your way through the GitHub interface. Try clicking on 'index.md' to see the content of the file: notice how the markdown renders prettily.

Click on "commits" near the top of the screen, to see all the changes you've made. Click on the commit number next to the right of a change, to see what changes it includes: removals are shown in red, and additions in green.

2.16 Working with multiple files

2.16.1 Some new content

So far, we've only worked with one file. Let's add another:

======

Cumbria has some pretty hills, and lakes too.

Writing lakeland.md

```
In [6]: cat lakeland.md
```

Lakeland

Cumbria has some pretty hills, and lakes too.

2.16.2 Git will not by default commit your new file

nothing added to commit but untracked files present

This didn't do anything, because we've not told git to track the new file yet.

2.16.3 Tell git about the new file

Ok, now we have added the change about Cumbria to the file. Let's publish it to the origin repository.

```
git config --global push.default simple
```

When push.default is set to 'matching', git will push local branches to the remote branches that already exist with the same name.

In Git 2.0, Git will default to the more conservative 'simple' behavior, which only pushes the current branch to the corresponding remote branch that 'git pull' uses to update the current branch.

See 'git help config' and search for 'push.default' for further information. (the 'simple' mode was introduced in Git 1.7.11. Use the similar mode 'current' instead of 'simple' if you sometimes use older versions of Git)

```
To git@github.com:UCL/github-example.git 57ceea6..5a70353 master -> master
```

Visit GitHub, and notice this change is on your repository on the server. We could have said git push origin to specify the remote to use, but origin is the default.

2.17 Changing two files at once

In [10]: %%writefile lakeland.md

What if we change both files?

```
Lakeland
        Cumbria has some pretty hills, and lakes too
        Mountains:
         * Helvellyn
Overwriting lakeland.md
In [11]: %%writefile index.md
        Mountains and Lakes in the UK
         _____
        Engerland is not very mountainous.
        But has some tall hills, and maybe a
        mountain or two depending on your definition.
Overwriting index.md
In [12]: %%bash
        git status
On branch master
Your branch is up-to-date with 'origin/master'.
Changes not staged for commit:
  (use "git add <file>..." to update what will be committed)
  (use "git checkout -- <file>..." to discard changes in working directory)
```

These changes should really be separate commits. We can do this with careful use of git add, to **stage** first one commit, then the other.

Because we "staged" only index.md, the changes to lakeland.md were not included in that commit.

```
In [14]: %%bash
        git commit -am "Add Helvellyn"
[master 4d75fec] Add Helvellyn
1 file changed, 4 insertions(+), 1 deletion(-)
In [15]: %%bash
         git log --oneline
4d75fec Add Helvellyn
37f4d7c Include lakes in the scope
5a70353 Add lakeland
57ceea6 Revert "Add a lie about a mountain"
86e1579 Change title
197ac66 Add a lie about a mountain
944bc26 First commit of discourse on UK topography
In [16]: %%bash
         git push
warning: push.default is unset; its implicit value is changing in
Git 2.0 from 'matching' to 'simple'. To squelch this message
and maintain the current behavior after the default changes, use:
  git config --global push.default matching
```

To squelch this message and adopt the new behavior now, use:

```
When push.default is set to 'matching', git will push local branches
to the remote branches that already exist with the same name.
In Git 2.0, Git will default to the more conservative 'simple'
behavior, which only pushes the current branch to the corresponding
remote branch that 'git pull' uses to update the current branch.
See 'git help config' and search for 'push.default' for further information.
(the 'simple' mode was introduced in Git 1.7.11. Use the similar mode
'current' instead of 'simple' if you sometimes use older versions of Git)
To git@github.com:UCL/github-example.git
   5a70353..4d75fec master -> master
In [17]: message="""
         participant "Jim's remote" as M
         participant "Jim's repo" as R
         participant "Jim's index" as I
         participant Jim as J
         note right of J: vim index.md
         note right of J: vim lakeland.md
         note right of J: git add index.md
         J->I: Add *only* the changes to index.md to the staging area
         note right of J: git commit -m "Include lakes"
         I->R: Make a commit from currently staged changes: index.md only
         note right of J: git commit -am "Add Helvellyn"
         J->I: Stage *all remaining* changes, (lakeland.md)
         I->R: Make a commit from currently staged changes
         note right of J: git push
         R->M: Transfer commits to Github
         wsd(message)
        NameErrorTraceback (most recent call last)
        <ipython-input-17-e239c58c5cd8> in <module>()
         21 R->M: Transfer commits to Github
         22 """
    ---> 23 wsd(message)
        NameError: name 'wsd' is not defined
```

git config --global push.default simple

2.18 Collaboration

2.18.1 Form a team

Now we're going to get to the most important question of all with Git and GitHub: working with others. Organise into pairs. You're going to be working on the website of one of the two of you, together, so decide who is going to be the leader, and who the collaborator.

2.18.2 Giving permission

The leader needs to let the collaborator have the right to make changes to his code.

In GitHub, go to settings on the right, then collaborators on the left.

Add the user name of your collaborator to the box. They now have the right to push to your repository.

2.18.3 Obtaining a colleague's code

Next, the collaborator needs to get a copy of the leader's code. For this example notebook, I'm going to be collaborating with myself, swapping between my two repositories. Make yourself a space to put it your work. (I will have two)

Next, the collaborator needs to find out the URL of the repository: they should go to the leader's repository's GitHub page, and note the URL on the top of the screen. Make sure the "ssh" button is pushed, the URL should begin with git@github.com.

Copy the URL into your clipboard by clicking on the icon to the right of the URL, and then:

 $/home/travis/build/UCL/rsd-engineering course/ch02git/learning_git/partner_dirindex.md\\lakeland.md$

Note that your partner's files are now present on your disk:

2.18.4 Nonconflicting changes

Now, both of you should make some changes. To start with, make changes to *different* files. This will mean your work doesn't "conflict". Later, we'll see how to deal with changes to a shared file.

Both of you should commit, but not push, your changes to your respective files: E.g., the leader:

```
In [7]: os.chdir(working_dir)
In [8]: %%writefile Wales.md
        Mountains In Wales
        _____
        * Tryfan
        * Yr Wyddfa
Writing Wales.md
In [9]: %%bash
        ls
index.md
lakeland.md
Wales.md
wsd.py
wsd.pyc
In [10]: %%bash
         git add Wales.md
         git commit -m "Add wales"
[master 38fd3a4] Add wales
 1 file changed, 5 insertions(+)
 create mode 100644 Wales.md
```

And the partner:

```
In [11]: os.chdir(partner_dir)
In [12]: %%writefile Scotland.md
         Mountains In Scotland
         ==============
         * Ben Eighe
         * Cairngorm
Writing Scotland.md
In [13]: %%bash
         ls
index.md
lakeland.md
Scotland.md
In [14]: %%bash
        git add Scotland.md
         git commit -m "Add Scotland"
[master 1c9ad96] Add Scotland
1 file changed, 5 insertions (+)
 create mode 100644 Scotland.md
  One of you should now push with git push:
In [15]: %%bash
         git push
warning: push.default is unset; its implicit value is changing in
Git 2.0 from 'matching' to 'simple'. To squelch this message
and maintain the current behavior after the default changes, use:
  git config --global push.default matching
To squelch this message and adopt the new behavior now, use:
  git config --global push.default simple
When push.default is set to 'matching', git will push local branches
to the remote branches that already exist with the same name.
In Git 2.0, Git will default to the more conservative 'simple'
behavior, which only pushes the current branch to the corresponding
remote branch that 'git pull' uses to update the current branch.
See 'git help config' and search for 'push.default' for further information.
(the 'simple' mode was introduced in Git 1.7.11. Use the similar mode
'current' instead of 'simple' if you sometimes use older versions of Git)
To git@github.com:UCL/github-example.git
```

4d75fec..1c9ad96 master -> master

2.18.5 Rejected push

The other should then push, but should receive an error message:

```
In [16]: os.chdir(working_dir)
In [17]: %%bash
         git push
warning: push.default is unset; its implicit value is changing in
Git 2.0 from 'matching' to 'simple'. To squelch this message
and maintain the current behavior after the default changes, use:
  git config --global push.default matching
To squelch this message and adopt the new behavior now, use:
  git config --global push.default simple
When push.default is set to 'matching', git will push local branches
to the remote branches that already exist with the same name.
In Git 2.0, Git will default to the more conservative 'simple'
behavior, which only pushes the current branch to the corresponding
remote branch that 'git pull' uses to update the current branch.
See 'git help config' and search for 'push.default' for further information.
(the 'simple' mode was introduced in Git 1.7.11. Use the similar mode
'current' instead of 'simple' if you sometimes use older versions of Git)
To git@github.com:UCL/github-example.git
 ! [rejected]
                     master -> master (fetch first)
error: failed to push some refs to 'git@github.com:UCL/github-example.git'
hint: Updates were rejected because the remote contains work that you do
hint: not have locally. This is usually caused by another repository pushing
hint: to the same ref. You may want to first integrate the remote changes
hint: (e.g., 'git pull ...') before pushing again.
hint: See the 'Note about fast-forwards' in 'git push --help' for details.
  Do as it suggests:
In [18]: %%bash
         git pull
Merge made by the 'recursive' strategy.
 Scotland.md | 5 +++++
 1 file changed, 5 insertions (+)
 create mode 100644 Scotland.md
From github.com:UCL/github-example
   4d75fec..1c9ad96 master -> origin/master
 * [new branch] gh-pages -> origin/gh-pages
```

2.18.6 Merge commits

ls

A window may pop up with a suggested default commit message. This commit is special: it is a *merge* commit. It is a commit which combines your collaborator's work with your own.

Now, push again with git push. This time it works. If you look on GitHub, you'll now see that it contains both sets of changes.

```
In [19]: %%bash
         git push
warning: push.default is unset; its implicit value is changing in
Git 2.0 from 'matching' to 'simple'. To squelch this message
and maintain the current behavior after the default changes, use:
  git config --global push.default matching
To squelch this message and adopt the new behavior now, use:
  git config --global push.default simple
When push.default is set to 'matching', git will push local branches
to the remote branches that already exist with the same name.
In Git 2.0, Git will default to the more conservative 'simple'
behavior, which only pushes the current branch to the corresponding
remote branch that 'git pull' uses to update the current branch.
See 'git help config' and search for 'push.default' for further information.
(the 'simple' mode was introduced in Git 1.7.11. Use the similar mode
'current' instead of 'simple' if you sometimes use older versions of Git)
To git@github.com:UCL/github-example.git
   1c9ad96..b084e73 master -> master
  The partner now needs to pull down that commit:
In [20]: os.chdir(partner_dir)
In [21]: %%bash
         git pull
Updating 1c9ad96..b084e73
Fast-forward
Wales.md \mid 5 +++++
 1 file changed, 5 insertions(+)
 create mode 100644 Wales.md
From github.com: UCL/github-example
   1c9ad96..b084e73 master -> origin/master
In [22]: %%bash
```

```
index.md
lakeland.md
Scotland.md
Wales.md
```

2.18.7 Nonconflicted commits to the same file

Go through the whole process again, but this time, both of you should make changes to a single file, but make sure that you don't touch the same *line*. Again, the merge should work as before:

```
In [23]: %%writefile Wales.md
        Mountains In Wales
         =============
         * Tryfan
         * Snowdon
Overwriting Wales.md
In [24]: %%bash
         git diff
diff --git a/Wales.md b/Wales.md
index 3809c69..e2ca555 100644
--- a/Wales.md
+++ b/Wales.md
@@ -2,4 +2,4 @@ Mountains In Wales
============
 * Tryfan
-* Yr Wyddfa
\ No newline at end of file
+* Snowdon
\ No newline at end of file
In [25]: %%bash
         git commit -am "Translating from the Welsh"
[master 3e5a022] Translating from the Welsh
1 file changed, 1 insertion(+), 1 deletion(-)
In [26]: %%bash
         git log --oneline
3e5a022 Translating from the Welsh
b084e73 Merge branch 'master' of github.com:UCL/github-example
38fd3a4 Add wales
1c9ad96 Add Scotland
4d75fec Add Helvellyn
37f4d7c Include lakes in the scope
5a70353 Add lakeland
57ceea6 Revert "Add a lie about a mountain"
```

```
86e1579 Change title
197ac66 Add a lie about a mountain
944bc26 First commit of discourse on UK topography
In [27]: os.chdir(working_dir)
In [28]: %%writefile Wales.md
         Mountains In Wales
         ===========
         * Pen y Fan
         * Tryfan
         * Snowdon
Overwriting Wales.md
In [29]: %%bash
         git commit -am "Add a beacon"
[master fc7ee42] Add a beacon
1 file changed, 2 insertions (+), 1 deletion (-)
In [30]: %%bash
         git log --oneline
fc7ee42 Add a beacon
b084e73 Merge branch 'master' of github.com:UCL/github-example
38fd3a4 Add wales
1c9ad96 Add Scotland
4d75fec Add Helvellyn
37f4d7c Include lakes in the scope
5a70353 Add lakeland
57ceea6 Revert "Add a lie about a mountain"
86e1579 Change title
197ac66 Add a lie about a mountain
944bc26 First commit of discourse on UK topography
In [31]: %%bash
         git push
warning: push.default is unset; its implicit value is changing in
Git 2.0 from 'matching' to 'simple'. To squelch this message
and maintain the current behavior after the default changes, use:
  git config --global push.default matching
To squelch this message and adopt the new behavior now, use:
  git config --global push.default simple
When push.default is set to 'matching', git will push local branches
```

to the remote branches that already exist with the same name.

In Git 2.0, Git will default to the more conservative 'simple' behavior, which only pushes the current branch to the corresponding remote branch that 'git pull' uses to update the current branch.

See 'git help config' and search for 'push.default' for further information. (the 'simple' mode was introduced in Git 1.7.11. Use the similar mode 'current' instead of 'simple' if you sometimes use older versions of Git)

To git@github.com:UCL/github-example.git b084e73..fc7ee42 master -> master

Switching back to the other partner...

In [32]: os.chdir(partner_dir)

In [33]: %%bash git push

warning: push.default is unset; its implicit value is changing in Git 2.0 from 'matching' to 'simple'. To squelch this message and maintain the current behavior after the default changes, use:

git config --global push.default matching

To squelch this message and adopt the new behavior now, use:

git config --global push.default simple

When push.default is set to 'matching', git will push local branches to the remote branches that already exist with the same name.

In Git 2.0, Git will default to the more conservative 'simple' behavior, which only pushes the current branch to the corresponding remote branch that 'git pull' uses to update the current branch.

See 'git help config' and search for 'push.default' for further information. (the 'simple' mode was introduced in Git 1.7.11. Use the similar mode 'current' instead of 'simple' if you sometimes use older versions of Git)

To git@github.com:UCL/github-example.git

! [rejected] master -> master (fetch first)

error: failed to push some refs to 'git@github.com:UCL/github-example.git'

hint: Updates were rejected because the remote contains work that you do

hint: not have locally. This is usually caused by another repository pushing

hint: to the same ref. You may want to first integrate the remote changes

hint: (e.g., 'git pull ...') before pushing again.

hint: See the 'Note about fast-forwards' in 'git push --help' for details.

In [34]: %%bash git pull

Auto-merging Wales.md Merge made by the 'recursive' strategy.

```
Wales.md \mid 1 +
 1 file changed, 1 insertion(+)
From github.com:UCL/github-example
  b084e73..fc7ee42 master -> origin/master
In [35]: %%bash
         git push
warning: push.default is unset; its implicit value is changing in
Git 2.0 from 'matching' to 'simple'. To squelch this message
and maintain the current behavior after the default changes, use:
  git config --global push.default matching
To squelch this message and adopt the new behavior now, use:
  git config --global push.default simple
When push.default is set to 'matching', git will push local branches
to the remote branches that already exist with the same name.
In Git 2.0, Git will default to the more conservative 'simple'
behavior, which only pushes the current branch to the corresponding
remote branch that 'git pull' uses to update the current branch.
See 'git help config' and search for 'push.default' for further information.
(the 'simple' mode was introduced in Git 1.7.11. Use the similar mode
'current' instead of 'simple' if you sometimes use older versions of Git)
To git@github.com:UCL/github-example.git
   fc7ee42..d3e48a3 master -> master
In [36]: %%bash
         git log --oneline --graph
  d3e48a3 Merge branch 'master' of github.com: UCL/github-example
| * fc7ee42 Add a beacon
\star | 3e5a022 Translating from the Welsh
| /
* b084e73 Merge branch 'master' of github.com:UCL/github-example
| * 1c9ad96 Add Scotland
* | 38fd3a4 Add wales
* 4d75fec Add Helvellyn
* 37f4d7c Include lakes in the scope
* 5a70353 Add lakeland
* 57ceea6 Revert "Add a lie about a mountain"
* 86e1579 Change title
* 197ac66 Add a lie about a mountain
```

```
* 944bc26 First commit of discourse on UK topography
In [37]: os.chdir(working_dir)
In [38]: %%bash
         git pull
Updating fc7ee42..d3e48a3
Fast-forward
From github.com: UCL/github-example
   fc7ee42..d3e48a3 master -> origin/master
In [39]: %%bash
         git log --graph --oneline
    d3e48a3 Merge branch 'master' of github.com:UCL/github-example
| 
| * fc7ee42 Add a beacon
* | 3e5a022 Translating from the Welsh
   b084e73 Merge branch 'master' of github.com: UCL/github-example
1\
| * 1c9ad96 Add Scotland
* | 38fd3a4 Add wales
| / |
* 4d75fec Add Helvellyn
\star 37f4d7c Include lakes in the scope
* 5a70353 Add lakeland
* 57ceea6 Revert "Add a lie about a mountain"
* 86e1579 Change title
* 197ac66 Add a lie about a mountain
* 944bc26 First commit of discourse on UK topography
In [40]: message="""
         participant Sue as S
         participant "Sue's repo" as SR
         participant "Shared remote" as M
         participant "Jim's repo" as JR
         participant Jim as J
         note left of S: git clone
         M->SR: fetch commits
         SR->S: working directory as at latest commit
         note left of S: edit Scotland.md
         note right of J: edit Wales.md
         note left of S: git commit -am "Add scotland"
         S->SR: create commit with Scotland file
         note right of J: git commit -am "Add wales"
```

```
J->JR: create commit with Wales file
    note left of S: git push
    SR->M: update remote with changes
    note right of J: git push
    JR-->M: !Rejected change
    note right of J: git pull
    M->JR: Pull in Sue's last commit, merge histories
    JR->J: Add Scotland.md to working directory
    note right of J: git push
    JR->M: Transfer merged history to remote
     . . . .
    from wsd import wsd
    %matplotlib inline
    wsd(message)
    ImportErrorTraceback (most recent call last)
    <ipython-input-40-5a7b4bcd7c98> in <module>()
    33
    34 """
---> 35 from wsd import wsd
    36 get_ipython().magic(u'matplotlib inline')
    37 wsd (message)
    /home/travis/build/UCL/rsd-engineeringcourse/ch02git/learning_git/git_example/wsd.
---> 1 import requests
     2 import re
     3 import IPython
      5 def wsd(code):
    ImportError: No module named requests
```

2.18.8 Conflicting commits

Finally, go through the process again, but this time, make changes which touch the same line.

- * Snowdon
- * Fan y Big

Overwriting Wales.md

[master 042c980] Add another Beacon
1 file changed, 2 insertions(+), 1 deletion(-)

warning: push.default is unset; its implicit value is changing in Git 2.0 from 'matching' to 'simple'. To squelch this message and maintain the current behavior after the default changes, use:

git config --global push.default matching

To squelch this message and adopt the new behavior now, use:

git config --global push.default simple

When push.default is set to 'matching', git will push local branches to the remote branches that already exist with the same name.

In Git 2.0, Git will default to the more conservative 'simple' behavior, which only pushes the current branch to the corresponding remote branch that 'git pull' uses to update the current branch.

See 'git help config' and search for 'push.default' for further information. (the 'simple' mode was introduced in Git 1.7.11. Use the similar mode 'current' instead of 'simple' if you sometimes use older versions of Git)

To git@github.com:UCL/github-example.git d3e48a3..042c980 master -> master

In [43]: os.chdir(partner_dir)

- * Pen y Fan
- * Tryfan
- * Snowdon
- * Glyder Fawr

Overwriting Wales.md

```
[master dd2cf07] Add Glyder
1 file changed, 2 insertions(+), 1 deletion(-)
warning: push.default is unset; its implicit value is changing in
Git 2.0 from 'matching' to 'simple'. To squelch this message
and maintain the current behavior after the default changes, use:
 git config --global push.default matching
To squelch this message and adopt the new behavior now, use:
  git config --global push.default simple
When push.default is set to 'matching', git will push local branches
to the remote branches that already exist with the same name.
In Git 2.0, Git will default to the more conservative 'simple'
behavior, which only pushes the current branch to the corresponding
remote branch that 'git pull' uses to update the current branch.
See 'git help config' and search for 'push.default' for further information.
(the 'simple' mode was introduced in Git 1.7.11. Use the similar mode
'current' instead of 'simple' if you sometimes use older versions of Git)
To git@github.com:UCL/github-example.git
! [rejected]
                    master -> master (fetch first)
error: failed to push some refs to 'git@github.com:UCL/github-example.git'
hint: Updates were rejected because the remote contains work that you do
hint: not have locally. This is usually caused by another repository pushing
hint: to the same ref. You may want to first integrate the remote changes
hint: (e.g., 'git pull ...') before pushing again.
hint: See the 'Note about fast-forwards' in 'git push --help' for details.
  When you pull, instead of offering an automatic merge commit message, it says:
In [46]: %%bash
         git pull
Auto-merging Wales.md
CONFLICT (content): Merge conflict in Wales.md
Automatic merge failed; fix conflicts and then commit the result.
From github.com: UCL/github-example
```

2.18.9 Resolving conflicts

d3e48a3..042c980 master

Git couldn't work out how to merge the two different sets of changes. You now need to manually resolve the conflict.

It has marked the conflicted area:

-> origin/master

Manually edit the file, to combine the changes as seems sensible and get rid of the symbols:

Overwriting Wales.md

2.18.10 Commit the resolved file

Now commit the merged result:

```
In [49]: %%bash
git commit -a --no-edit # I added a No-edit for this non-interactive session. You

[master 3547ead] Merge branch 'master' of github.com:UCL/github-example

In [50]: %%bash
git push

warning: push.default is unset; its implicit value is changing in

Git 2.0 from 'matching' to 'simple'. To squelch this message
and maintain the current behavior after the default changes, use:

git config --global push.default matching

To squelch this message and adopt the new behavior now, use:

git config --global push.default simple

When push.default is set to 'matching', git will push local branches to the remote branches that already exist with the same name.
```

```
In Git 2.0, Git will default to the more conservative 'simple'
behavior, which only pushes the current branch to the corresponding
remote branch that 'git pull' uses to update the current branch.
See 'git help config' and search for 'push.default' for further information.
(the 'simple' mode was introduced in Git 1.7.11. Use the similar mode
'current' instead of 'simple' if you sometimes use older versions of Git)
To git@github.com:UCL/github-example.git
   042c980..3547ead master -> master
In [51]: os.chdir(working_dir)
In [52]: %%bash
        git pull
Updating 042c980..3547ead
Fast-forward
 Wales.md | 1 +
 1 file changed, 1 insertion(+)
From github.com:UCL/github-example
   042c980..3547ead master -> origin/master
In [53]: %%bash
        cat Wales.md
Mountains In Wales
===============
* Pen y Fan
* Tryfan
* Snowdon
* Glyder Fawr
* Fan y Big
In [54]: %%bash
         git log --oneline --graph
  3547ead Merge branch 'master' of github.com:UCL/github-example
| * 042c980 Add another Beacon
* | dd2cf07 Add Glyder
1/
   d3e48a3 Merge branch 'master' of github.com: UCL/github-example
1\
| * fc7ee42 Add a beacon
* | 3e5a022 Translating from the Welsh
1/
* b084e73 Merge branch 'master' of github.com:UCL/github-example
| * 1c9ad96 Add Scotland
```

```
* | 38fd3a4 Add wales
|/
* 4d75fec Add Helvellyn
* 37f4d7c Include lakes in the scope
* 5a70353 Add lakeland
* 57ceea6 Revert "Add a lie about a mountain"
* 86e1579 Change title
* 197ac66 Add a lie about a mountain
* 944bc26 First commit of discourse on UK topography
```

2.18.11 Distributed VCS in teams with conflicts

```
In [55]: message="""
        participant Sue as S
         participant "Sue's repo" as SR
         participant "Shared remote" as M
         participant "Jim's repo" as JR
        participant Jim as J
         note left of S: edit the same line in wales.md
         note right of J: edit the same line in wales.md
         note left of S: git commit -am "update wales.md"
         S->SR: add commit to local repo
         note right of J: git commit -am "update wales.md"
         J->JR: add commit to local repo
         note left of S: git push
         SR->M: transfer commit to remote
         note right of J: git push
         JR->M: !Rejected
         note right of J: git pull
         JR->J: Make confliced file with conflict markers
         note right of J: edit file to resolve conflicts
         note right of J: git add wales.md
         note right of J: git commit
         J->JR: Mark conflict as resolved
         note right of J: git push
         JR->M: Transfer merged history to remote
         note left of S: git pull
         M->SR: Download Jim's resolution of conflict.
         11 11 11
         wsd(message)
```

```
NameErrorTraceback (most recent call last)

<ipython-input-55-e385d4035beb> in <module>()
37 """
38
---> 39 wsd(message)

NameError: name 'wsd' is not defined
```

2.18.12 The Levels of Git

```
In [56]: message="""
         Working Directory -> Staging Area : git add
         Staging Area -> Local Repository : git commit
         Working Directory -> Local Repository : git commit -a
         Staging Area -> Working Directory : git checkout
         Local Repository -> Staging Area : git reset
         Local Repository -> Working Directory: git reset --hard
         Local Repository -> Remote Repository : git push
         Remote Repository -> Local Repository : git fetch
         Local Repository -> Staging Area : git merge
         Remote Repository -> Working Directory: git pull
         wsd (message)
        NameErrorTraceback (most recent call last)
        <ipython-input-56-5c43f348a040> in <module>()
        12 """
         13
    ---> 14 wsd (message)
        NameError: name 'wsd' is not defined
```

2.19 Editing directly on GitHub

2.19.1 Editing directly on GitHub

Note that you can also make changes in the GitHub website itself. Visit one of your files, and hit "edit". Make a change in the edit window, and add an appropriate commit message. That change now appears on the website, but not in your local copy. (Verify this). Now pull, and check the change is now present on your local version.

2.20 Social Coding

2.20.1 GitHub as a social network

In addition to being a repository for code, and a way to publish code, GitHub is a social network.

You can follow the public work of other coders: go to the profile of your collaborator in your browser, and hit the "follow" button.

Here's mine: if you want to you can follow me.

Using GitHub to build up a good public profile of software projects you've worked on is great for your CV!

2.21 Fork and Pull

2.21.1 Different ways of collaborating

We have just seen how we can work with others on GitHub: we add them as collaborators on our repositories and give them permissions to push changes.

Let's talk now about some other type of collaboration.

Imagine you are a user of an Open Source project like Numpy and find a bug in one of their methods.

You can inspect and clone Numpy's code in GitHub https://github.com/numpy/numpy, play around a bit and find how to fix the bug.

Numpy has done so much for you asking nothing in return, that you really want to contribute back by fixing the bug for them.

You make all of the changes but you can't push it back to Numpy's repository because you don't have permissions.

The right way to do this is **forking Numpy's repository**.

2.21.2 Forking a repository on GitHub

By forking a repository, all you do is make a copy of it in your GitHub account, where you will have write permissions as well.

If you fork Numpy's repository, you will find a new repository in your GitHub account that is an exact copy of Numpy. You can then clone it to your computer, work locally on fixing the bug and push the changes to your *fork* of Numpy.

Once you are happy with with the changes, GitHub also offers you a way to notify Numpy's developers of this changes so that they can include them in the official Numpy repository via starting a **Pull Request**.

2.21.3 Pull Request

You can create a Pull Request and select those changes that you think can be useful for fixing Numpy's bug. Numpy's developers will review your code and make comments and suggestions on your fix. Then, you can commit more improvements in the pull request for them to review and so on.

Once Numpy's developers are happy with your changes, they'll accept your Pull Request and merge the changes into their original repository, for everyone to use.

2.21.4 Practical example - Team up!

We will be working in the same repository with one of you being the leader and the other being the collaborator.

Collaborators need to go to the leader's GitHub profile and find the repository we created for that lesson. Mine is in https://github.com/jamespjh/github-example

1. Fork repository

You will see on the top right of the page a Fork button with an accompanying number indicating how many GitHub users have forked that repository.

Collaborators need to navigate to the leader's repository and click the Fork button.

Collaborators: note how GitHub has redirected you to your own GitHub page and you are now looking at an exact copy of the team leader's repository.

2. Clone your forked repo

Collaborators: go to your terminal and clone the newly created fork.

```
git clone git@github.com:jamespjh/github-example.git
```

3. Create a feature branch

It's a good practice to create a new branch that'll contain the changes we want. We'll learn more about branches later on. For now, just think of this as a separate area where our changes will be kept not to interfere with other people's work.

```
git checkout -b southwest
```

4. Make, commit and push changes to new branch

For example, let's create a new file called SouthWest.md and edit it to add this text:

- * Exmoor
- * Dartmoor
- * Bodmin Moor

Save it, and push this changes to your fork's new branch:

```
git add SouthWest.md
git commit -m "The South West is also hilly."
git push origin southwest
```

5. Create Pull Request

Go back to the collaborator's GitHub site and reload the fork. GitHub has noticed there is a new branch and is presenting us with a green button to Compare & pull request. Fantastic! Click that button.

Fill in the form with additional information about your change, as you consider necesary to make the team leader understand what this is all about.

Take some time to inspect the commits and the changes you are submitting for review. When you are ready, click on the Create Pull Request button.

Now, the leader needs to go to their GitHub site. They have been notified there is a pull request in their repo awaiting revision.

6. Feedback from team leader

Leaders can see the list of pull requests in the vertical menu of the repo, on the right hand side of the screen. Select the pull request the collaborator has done, and inspect the changes.

There are three tabs: in one you can start a conversation with the collaborator about their changes, and in the others you can have a look at the commits and changes made.

Go to the tab labeled as "Files Changed". When you hover over the changes, a small + button appears. Select one line you want to make a comment on. For example, the line that contains "Exmoor".

GitHub allows you to add a comment about that specific part of the change. Your collaborator has forgotten to add a title at the beginning of the file right before "Exmoor", so tell them so in the form presented after clicking the + button.

7. Fixes by collaborator

Collaborators will be notified of this comment by email and also in their profiles page. Click the link accompanying this notification to read the comment from the team leader.

Go back to your local repository, make the changes suggested and push them to the new branch. Add this at the beginning of your file:

```
Hills in the South West:
```

Then push the change to your fork:

```
git add .
git commit -m "Titles added as requested."
git push origin southwest
```

This change will automatically be added to the pull request you started.

8. Leader accepts pull request

The team leader will be notified of the new changes that can be reviewed in the same fashion as earlier. Let's assume the team leader is now happy with the changes.

Leaders can see in the "Conversation" tab of the pull request a green button labelled Merge pull request. Click it and confirm the decision.

The collaborator's pull request has been accepted and appears now in the original repository owned by the team leader.

Fork and Pull Request done!

2.21.5 Some Considerations

- Fork and Pull Request are things happening only on the repository's server side (GitHub in our case). Consequently, you can't do things like git fork or git pull-request from the local copy of a repository.
- You not always need to fork repositories with the intention of contributing. You can fork a library you
 use, install it manually on your computer, and add more functionality or customise the existing one,
 so that it is more useful for you and your team.
- Numpy's example is only illustrative. Normally, Open Source projects have in their Wiki a set of instructions you need to follow if you want to contribute to their software.
- Pull Requests can also be done for merging branches in a non-forked repository. It's typically used in teams to merge code from a branch into the master branch and ask team colleagues for code reviews before merging.
- It's a good practice before starting a fork and a pull request to have a look at existing forks and pull requests. You can find the list of pull requests on the vertical menu on right hand side. Try to also find the network graph displaying all existing forks of a repo, like this example in the NumpyDoc repo: https://github.com/numpy/numpydoc/network

2.22 Git Theory

2.22.1 The revision Graph

Revisions form a GRAPH

```
In [1]: import os
        top_dir = os.getcwd()
        git_dir = os.path.join(top_dir, 'learning_git')
        working_dir=os.path.join(git_dir, 'git_example')
        os.chdir(working dir)
In [2]: %%bash
        git log --graph --oneline
    3547ead Merge branch 'master' of github.com:UCL/github-example
I \setminus
| * 042c980 Add another Beacon
* | dd2cf07 Add Glyder
1/
    d3e48a3 Merge branch 'master' of github.com:UCL/github-example
| * fc7ee42 Add a beacon
* | 3e5a022 Translating from the Welsh
1/
   b084e73 Merge branch 'master' of github.com:UCL/github-example
| \ |
| * 1c9ad96 Add Scotland
* | 38fd3a4 Add wales
\perp
* 4d75fec Add Helvellyn
* 37f4d7c Include lakes in the scope
* 5a70353 Add lakeland
* 57ceea6 Revert "Add a lie about a mountain"
* 86e1579 Change title
* 197ac66 Add a lie about a mountain
* 944bc26 First commit of discourse on UK topography
```

2.22.2 Git concepts

- Each revision has a parent that it is based on
- These revisions form a graph
- Each revision has a unique hash code
- In Sue's copy, revision 43 is ab3578d6
- Jim might think that is revision 38, but it's still ab3579d6
- Branches, tags, and HEAD are labels pointing at revisions
- Some operations (like fast forward merges) just move labels.

2.22.3 The levels of Git

There are four **Separate** levels a change can reach in git:

- The Working Copy
- The index (aka staging area)
- The local repository
- The remote repository

Understanding all the things git reset can do requires a good grasp of git theory.

- git reset <commit> <filename>: Reset index and working version of that file to the version in a given commit
- git reset --soft <commit>: Move local repository branch label to that commit, leave working dir and index unchanged
- git reset <commit>: Move local repository and index to commit ("-mixed")
- git reset --hard <commit>: Move local repostiory, index, and working directory copy to that state

2.23 Branches

Branches are increadibly important to why git is cool and powerful.

They are an easy and cheap way of making a second version of your software, which you work on in parallel, and pull in your changes when you are ready.

```
In [1]: import os
        top_dir = os.getcwd()
        git_dir = os.path.join(top_dir, 'learning_git')
        working_dir=os.path.join(git_dir, 'git_example')
        os.chdir(working_dir)
In [2]: %%bash
        git branch # Tell me what branches exist
* master
In [3]: %%bash
        git checkout -b experiment # Make a new branch
Switched to a new branch 'experiment'
In [4]: %%bash
       git branch
* experiment
 master
In [5]: %%bash
        git commit -am "Add Cadair Idris"
On branch experiment
Untracked files:
       wsd.py
        wsd.pyc
nothing added to commit but untracked files present
In [6]: %%bash
        git checkout master # Switch to an existing branch
Your branch is up-to-date with 'origin/master'.
```

```
Switched to branch 'master'
In [7]: %%bash
       cat Wales.md
Mountains In Wales
================
* Pen y Fan
* Tryfan
* Snowdon
* Glyder Fawr
* Fan y Big
In [8]: %%bash
       git checkout experiment
Switched to branch 'experiment'
In [9]: cat Wales.md
Mountains In Wales
_____
* Pen y Fan
* Tryfan
* Snowdon
* Glyder Fawr
* Fan y Big
```

2.23.1 Publishing branches

To let the server know there's a new branch use:

We use --set-upstream origin (Abbreviation -u) to tell git that this branch should be pushed to and pulled from origin per default.

If you are following along, you should be able to see your branch in the list of branches in GitHub.

Once you've used git push -u once, you can push new changes to the branch with just a git push.

If others checkout your repository, they will be able to do git checkout experiment to see your branch content, and collaborate with you in the branch.

```
origin/experiment
origin/gh-pages
origin/master
```

Local branches can be, but do not have to be, connected to remote branches They are said to "track" remote branches. push -u sets up the tracking relationship.

2.23.2 Find out what is on a branch

In addition to using git diff to compare to the state of a branch, you can use git log to look at lists of commits which are in a branch and haven't been merged yet.

Git uses various symbols to refer to sets of commits. The double dot ${\tt A..B}$ means "ancestor of B and not ancestor of A"

So in a purely linear sequence, it does what you'd expect.

But in cases where a history has branches, the definition in terms of ancestors is important.

If there are changes on both sides, like this:

```
In [16]: %%bash
         git checkout master
Your branch is up-to-date with 'origin/master'.
Switched to branch 'master'
In [17]: %%writefile Scotland.md
         Mountains In Scotland
         =============
         * Ben Eighe
         * Cairngorm
         * Aonach Eagach
Overwriting Scotland.md
In [18]: %%bash
         git diff Scotland.md
diff --git a/Scotland.md b/Scotland.md
index 36f83a1..44eb7ea 100644
--- a/Scotland.md
+++ b/Scotland.md
@@ -2,4 +2,5 @@ Mountains In Scotland
=============
* Ben Eighe
-* Cairngorm
\ No newline at end of file
+* Cairngorm
+* Aonach Eagach
\ No newline at end of file
In [19]: %%bash
         git commit -am "Commit Aonach onto master branch"
[master fc4054f] Commit Aonach onto master branch
 1 file changed, 2 insertions(+), 1 deletion(-)
  Then this notation is useful to show the content of what's on what branch:
In [20]: %%bash
         git log --left-right --oneline master...experiment
< fc4054f Commit Aonach onto master branch
```

Three dots means "everything which is not a common ancestor" of the two commits, i.e. the differences between them.

2.23.3 Merging branches

We can merge branches, and just as we would pull in remote changes, there may or may not be conflicts.

2.23.4 Cleaning up after a branch

```
In [23]: %%bash
         git branch
 experiment
* master
In [24]: %%bash
         git branch -d experiment
Deleted branch experiment (was 3547ead).
In [25]: %%bash
         git branch
* master
In [26]: %%bash
         git branch --remote
  origin/experiment
  origin/gh-pages
  origin/master
In [27]: %%bash
         git push --delete origin experiment
         # Remove remote branch
         # - also can use github interface
```

```
To git@github.com:UCL/github-example.git
- [deleted] experiment

In [28]: %%bash
git branch --remote

origin/gh-pages
origin/master
```

2.23.5 A good branch strategy

- A production branch: code used for active work
- A develop branch: for general new code
- feature branches: for specific new ideas
- release branches: when you share code with others
- Useful for isolated bug fixes

2.23.6 Grab changes from a branch

Make some changes on one branch, switch back to another, and use:

```
git checkout <branch> <path>
```

To quickly grab a file from one branch into another.

Using git checkout with a path takes the content of files. To grab the content of a specific *commit* from another branch, and apply it as a patch to your branch, use:

```
git cherry-pick <commit>
```

2.24 Git Stash

If you find you want to pull, but you're not ready to commit, you can use

```
In [3]: %%bash
        git stash
        git pull
Saved working directory and index state WIP on master: fc4054f Commit Aonach onto master be
HEAD is now at fc4054f Commit Aonach onto master branch
Already up-to-date.
In [4]: %%bash
        git stash apply
On branch master
Your branch is ahead of 'origin/master' by 1 commit.
  (use "git push" to publish your local commits)
Changes not staged for commit:
  (use "git add <file>..." to update what will be committed)
  (use "git checkout -- <file>..." to discard changes in working directory)
        modified:
                   Wales.md
Untracked files:
  (use "git add <file>..." to include in what will be committed)
        wsd.py
        wsd.pyc
no changes added to commit (use "git add" and/or "git commit -a")
```

The "Stash" is a way of temporarily saving your working area, and can help out in a pinch.

2.25 Tagging

Tags are easy to read labels for revisions, and can be used anywhere we would name a commit. Produce real results *only* with tagged revisions

If .. is used without a following commit name, HEAD is assumed.

2.26 Working with generated files: gitignore

In [9]: %%writefile Makefile

Enter file name:

We often end up with files that are generated by our program. It is bad practice to keep these in Git; just keep the sources.

Examples include .o and .x files for compiled languages, .pyc files in Python. In our example, we might want to make our .md files into a PDF with pandoc:

```
MDS=$(wildcard *.md)
    PDFS=$(MDS:.md=.pdf)

    default: $(PDFS)

    %.pdf: %.md
        pandoc $< -o $@

Writing Makefile

In [10]: %%bash
    make

make[1]: Entering directory `/home/travis/build/UCL/rsd-engineeringcourse/ch02git/learning.pandoc index.md -o index.pdf
make[1]: Leaving directory `/home/travis/build/UCL/rsd-engineeringcourse/ch02git/learning.gandoc: Error producing PDF from TeX source.
! LaTeX Error: File `lmodern.sty' not found.

Type X to quit or <RETURN> to proceed,
or enter new name. (Default extension: sty)
```

```
! Emergency stop.
<read *>
1.4 \usepackage
make[1]: *** [index.pdf] Error 43
  We now have a bunch of output .pdf files corresponding to each Markdown file.
  But we don't want those to show up in git:
In [11]: %%bash
         git status
On branch master
Your branch is ahead of 'origin/master' by 2 commits.
  (use "git push" to publish your local commits)
Untracked files:
  (use "git add <file>..." to include in what will be committed)
        Makefile
        wsd.py
        wsd.pyc
nothing added to commit but untracked files present (use "git add" to track)
  Use .gitignore files to tell Git not to pay attention to files with certain paths:
In [12]: %%writefile .gitignore
         *.pdf
Writing .gitignore
In [13]: %%bash
         git status
On branch master
Your branch is ahead of 'origin/master' by 2 commits.
  (use "git push" to publish your local commits)
Untracked files:
  (use "git add <file>..." to include in what will be committed)
        .gitignore
        Makefile
        wsd.py
        wsd.pyc
nothing added to commit but untracked files present (use "git add" to track)
In [14]: %%bash
         git add Makefile
```

```
git add .gitignore
git commit -am "Add a makefile and ignore generated files"
git push
```

[master 9826500] Add a makefile and ignore generated files
2 files changed, 9 insertions(+)
create mode 100644 .gitignore
create mode 100644 Makefile

warning: push.default is unset; its implicit value is changing in Git 2.0 from 'matching' to 'simple'. To squelch this message and maintain the current behavior after the default changes, use:

```
git config --global push.default matching
```

To squelch this message and adopt the new behavior now, use:

```
git config --global push.default simple
```

When push.default is set to 'matching', git will push local branches to the remote branches that already exist with the same name.

In Git 2.0, Git will default to the more conservative 'simple' behavior, which only pushes the current branch to the corresponding remote branch that 'git pull' uses to update the current branch.

See 'git help config' and search for 'push.default' for further information. (the 'simple' mode was introduced in Git 1.7.11. Use the similar mode 'current' instead of 'simple' if you sometimes use older versions of Git)

```
To git@github.com:UCL/github-example.git 3547ead..9826500 master -> master
```

2.27 Git clean

In [16]: %%**bash** ls

index.md
lakeland.md
Makefile
Pennines.md
Scotland.md
Wales.md
wsd.py
wsd.pyc

• With -f: don't prompt

- with -d: remove directories
- with -x: Also remote .gitignored files
- with -X: Only remove .gitignore files

2.28 Hunks

2.28.1 Git Hunks

A "Hunk" is one git change. This changeset has three hunks:

2.28.2 Interactive add

git add and git reset can be used to stage/unstage a whole file, but you can use interactive mode to stage by hunk, choosing yes or no for each hunk.

```
git add -p myfile.py

+import matplotlib
+import numpy as np
#Stage this hunk [y,n,a,d,/,j,J,g,e,?]?
```

2.29 GitHub pages

2.29.1 Yaml Frontmatter

GitHub will publish repositories containing markdown as web pages, automatically. You'll need to add this content:

A pair of lines with three dashes, to the top of each markdown file. This is how GitHub knows which markdown files to make into web pages. Here's why for the curious.

```
Engerland is not very mountainous.

But has some tall hills, and maybe a mountain or two depending on your definition

Overwriting index.md

In [18]: %%bash
```

```
git commit -am "Add github pages YAML frontmatter"
[master deca6a9] Add github pages YAML frontmatter
1 file changed, 7 insertions(+), 4 deletions(-)
```

2.29.2 The gh-pages branch

GitHub creates github pages when you use a special named branch.

Mountains and Lakes in the UK

This is best used to create documentation for a program you write, but you can use it for anything.

The first time you do this, GitHub takes a few minutes to generate your pages.

The website will appear at http://username.github.io/repositoryname, for example: http://UCL.github.io/github-example/

2.29.3 UCL layout for GitHub pages

You can use GitHub pages to make HTML layouts, here's an example of how to do it, and how it looks. We won't go into the detail of this now, but after the class, you might want to try this.

2.30 Working with multiple remotes

2.30.1 Distributed versus centralised

Older version control systems (cvs, svn) were "centralised"; the history was kept only on a server, and all commits required an internet.

Centralised	Distributed
Server has history	Every user has full history

Centralised	Distributed
Your computer has one snapshot	Many local branches
To access history, need internet	History always available
You commit to remote server	Users synchronise histories
cvs, subversion(svn)	git, mercurial (hg), bazaar (bzr)

With modern distributed systems, we can add a second remote. This might be a personal *fork* on github:

```
In [1]: import os
       top_dir = os.getcwd()
       git_dir = os.path.join(top_dir, 'learning_git')
       working_dir=os.path.join(git_dir, 'git_example')
       os.chdir(working_dir)
In [2]: %%bash
       git checkout master
       git remote add jamespjh git@github.com:jamespjh/github-example.git
       git remote -v
Your branch is ahead of 'origin/master' by 1 commit.
  (use "git push" to publish your local commits)
jamespjh
              git@github.com:jamespjh/github-example.git (fetch)
jamespjh
               git@github.com:jamespjh/github-example.git (push)
origin
             git@github.com:UCL/github-example.git (fetch)
             git@github.com:UCL/github-example.git (push)
origin
Switched to branch 'master'
  We can push to a named remote:
In [3]: %%writefile Pennines.md
       Mountains In the Pennines
        ______
        * Cross Fell
        * Whernside
Overwriting Pennines.md
In [4]: %%bash
       git commit -am "Add Whernside"
[master a4b3b07] Add Whernside
 1 file changed, 2 insertions(+), 1 deletion(-)
In [5]: %%bash
       git push -uf jamespjh master
```

Branch master set up to track remote branch master from jamespjh.

2.30.2 Referencing remotes

You can always refer to commits on a remote like this:

To see the differences between remotes, for example.

To see what files you have changed that aren't updated on a particular remote, for example:

When you reference remotes like this, you're working with a cached copy of the last time you interacted with the remote. You can do git fetch to update local data with the remotes without actually pulling. You can also get useful information about whether tracking branches are ahead or behind the remote breanches they track:

2.31 Hosting Servers

2.31.1 Hosting a local server

- Any repository can be a remote for pulls
- Can pull/push over shared folders or ssh
- Pushing to someone's working copy is dangerous
- Use git init --bare to make a copy for pushing
- You don't need to create a "server" as such, any 'bare' git repo will do.

```
In [9]: bare_dir=os.path.join(git_dir, 'bare_repo')
        os.chdir(git_dir)
In [10]: %%bash
         mkdir -p bare_repo
         cd bare_repo
         git init --bare
Initialized empty Git repository in /home/travis/build/UCL/rsd-engineeringcourse/ch02git/least-
In [11]: os.chdir(working dir)
In [12]: %%bash
         git remote add local_bare ../bare_repo
         git push -u local bare master
Branch master set up to track remote branch master from local_bare.
To ../bare repo
                master -> master
 * [new branch]
In [13]: %%bash
         git remote -v
jamespjh
               git@github.com:jamespjh/github-example.git (fetch)
jamespjh
               git@github.com:jamespjh/github-example.git (push)
                  ../bare_repo (fetch)
local_bare
local_bare
                  ../bare_repo (push)
            git@github.com:UCL/github-example.git (fetch)
origin
             git@github.com:UCL/github-example.git (push)
origin
```

You can now work with this local repository, just as with any other git server. If you have a colleague on a shared file system, you can use this approach to collaborate through that file system.

2.31.2 Home-made SSH servers

Classroom exercise: Try creating a server for yourself using a machine you can SSH to:

```
ssh <mymachine>
mkdir mygitserver
cd mygitserver
git init --bare
exit
git remote add <somename> ssh://user@host/mygitserver
git push -u <somename> master
```

2.32 SSH keys and GitHub

Classroom exercise: If you haven't already, you should set things up so that you don't have to keep typing in your password whenever you interact with GitHub via the command line.

You can do this with an "ssh keypair". You may have created a keypair in the Software Carpentry shell training. Go to the ssh settings page on GitHub and upload your public key by copying the content from your computer. (Probably at .ssh/id_rsa.pub)

If you have difficulties, the instructions for this are on the GitHub website.

2.33 Rebasing

2.33.1 Rebase vs merge

A git *merge* is only one of two ways to get someone else's work into yours. The other is called a rebase. In a merge, a revision is added, which brings the branches together. Both histories are retained. In a rebase, git tries to work out

What would you need to have done, to make your changes, if your colleague had already made theirs?

Git will invent some new revisions, and the result will be a repository with an apparently linear history.

2.33.2 An example rebase

We've built a repository to help visualise the difference between a merge and a rebase, at https://github.com/UCL-RITS/wocky_rebase/blob/master/wocky.md.

The initial state of both collaborators is a text file, wocky.md:

```
It was clear and cold, and the slimy monsters
```

On the master branch, a second commit ('Dancing') has been added:

```
It was clear and cold,
and the slimy monsters
danced and spun in the waves
```

On the "Carollian" branch, a commit has been added translating the initial state into Lewis Caroll's language:

```
'Twas brillig, and the slithy toves
```

So the logs look like this:

```
git log --oneline --graph master

* 2a74d89 Dancing
* 6a4834d Initial state

git log --oneline --graph carollian

* 2232bf3 Translate into Caroll's language
* 6a4834d Initial state
```

If we now **merge** carollian into master, the final state will include both changes:

```
'Twas brillig,
and the slithy toves
danced and spun in the waves
```

But the graph shows a divergence and then a convergence:

```
git log --oneline --graph
```

```
* b41f869 Merge branch 'carollian' into master_merge_carollian
|\
| * 2232bf3 Translate into Caroll's language
* | 2a74d89 Dancing
|/
* 6a4834d Initial state
```

But if we rebase, the final content of the file is still the same, but the graph is different:

```
git log --oneline --graph master_rebase_carollian

* df618e0 Dancing

* 2232bf3 Translate into Caroll's language

* 6a4834d Initial state

To trigger the rebase, we did:

git checkout master
git rebase carollian

If this had been a remote, we would merge it with:
```

```
git pull --rebase
```

2.33.3 Fast Forwards

If we want to continue with the translation, and now want to merge the rebased branch into the carollian branch, we get:

```
Updating 2232bf3..df618e0
Fast-forward
wocky.md | 1 +
1 file changed, 1 insertion(+)
```

The rebased branch was **rebased on** the carollian branch, so this merge was just a question of updating *metadata* to redefine the branch label: a "fast forward".

2.33.4 Rebasing pros and cons

Some people like the clean, apparently linear history that rebase provides.

But rebase rewrites history.

If you've already pushed, or anyone else has got your changes, things will get screwed up.

If you know your changes are still secret, it might be better to rebase to keep the history clean. If in doubt, just merge.

2.34 Squashing

A second use of the git rebase command, is to rebase your work on top of one of *your own* earlier commits, in interactive mode, to "squash" several commits that should really be one:

```
ea15 Some good work
1154 Fix another typo
de73 Fix a typo
ab11 A great piece of work
cd27 Initial commit
```

2.34.1 Using rebase to squash

```
If we type
```

```
git rebase -i ab11 #OR HEAD^^
    an edit window pops up with:

pick cd27 Initial commit
pick ab11 A great piece of work
pick de73 Fix a typo
pick l154 Fix another typo
pick ea15 Some good work

# Rebase 60709da..30e0ccb onto 60709da
#
# Commands:
# p, pick = use commit
# e, edit = use commit, but stop for amending
# s, squash = use commit, but meld into previous commit
```

We can rewrite select commits to be merged, so that the history is neater before we push. This is a great idea if you have lots of trivial typo commits.

```
pick cd27 Initial commit
pick ab11 A great piece of work
squash de73 Fix a typo
squash 1154 Fix another typo
pick ea15 Some good work
```

save the interactive rebase config file, and rebase will build a new history:

```
git log
de82 Some good work
fc52 A great piece of work
cd27 Initial commit
```

Note the commit hash codes for 'Some good work' and 'A great piece of work' have changed, as the change they represent has changed.

2.35 Debugging With Git Bisect

You can use

```
git bisect
```

to find out which commit caused a bug.

2.35.1 An example repository

In a nice open source example, I found an arbitrary exemplar on github

This has been set up to break itself at a random commit, and leave you to use bisect to work out where it has broken:

Which will make a bunch of commits, of which one is broken, and leave you in the broken final state

2.35.2 Bisecting manually

Bisect needs one known good and one known bad commit to get started

2.35.3 Solving Manually

```
python squares.py 2 # 4
git bisect good
python squares.py 2 # 4
git bisect good
python squares.py 2 # 4
git bisect good
python squares.py 2 # Crash
git bisect bad
python squares.py 2 # Crash
git bisect bad
python squares.py 2 # Crash
git bisect bad
python squares.py 2 #Crash
git bisect bad
python squares.py 2 # 4
git bisect good
python squares.py 2 # 4
git bisect good
python squares.py 2 # 4
git bisect good
  And eventually:
git bisect good
    Bisecting: 0 revisions left to test after this (roughly 0 steps)
python squares.py 2
git bisect good
2777975a2334c2396ccb9faf98ab149824ec465b is the first bad commit
commit 2777975a2334c2396ccb9faf98ab149824ec465b
Author: Shawn Siefkas <shawn.siefkas@meredith.com>
Date:
       Thu Nov 14 09:23:55 2013 -0600
    Breaking argument type
git bisect end
```

2.35.4 Solving automatically

If we have an appropriate unit test, we can do all this automatically:

```
[687e95c658e9fe81b6548a29f7c0853d09dc9d6c] Comment 749
running python squares.py 2
Bisecting: 124 revisions left to test after this (roughly 7 steps)
[da9f6c0f81564657bb43263ba17714821fd73bd5] Comment 625
running python squares.py 2
Bisecting: 62 revisions left to test after this (roughly 6 steps)
[0a69abf3c8439a4194f103613d61b144e64a4ae7] Comment 686
running python squares.py 2
Bisecting: 30 revisions left to test after this (roughly 5 steps)
[93991efe0085bd1a13b644dd8f3677d6b5f25794] Comment 655
running python squares.py 2
Bisecting: 15 revisions left to test after this (roughly 4 steps)
[b05cba3a8026b1722166076fea8f611972327f63] Comment 639
running python squares.py 2
Bisecting: 7 revisions left to test after this (roughly 3 steps)
[1e1724981bd413470808c09a778f7fe84f1c08d1] Comment 631
running python squares.py 2
Bisecting: 3 revisions left to test after this (roughly 2 steps)
[1f2d9f7b959f696935dc04d810ea4726031be4df] Comment 627
running python squares.py 2
Bisecting: 0 revisions left to test after this (roughly 1 step)
[f4a0613b7dcf4ffaf287bd9ab3a4d69aa6a7aaf8] Comment 626
running python squares.py 2
Bisecting: 0 revisions left to test after this (roughly 0 steps)
[ea87972e349ed9cd053284e9a5bb5917268739bc] Breaking argument type
running python squares.py 2
ea87972e349ed9cd053284e9a5bb5917268739bc is the first bad commit
commit ea87972e349ed9cd053284e9a5bb5917268739bc
Author: Shawn Siefkas <shawn.siefkas@meredith.com>
Date:
       Thu Nov 14 09:23:55 2013 -0600
    Breaking argument type
:100644 100644 8ee81ad44bd7734b91b72e30272d9261b3a3690e 0260586800c62910bb888f745ca7c7f86f
bisect run success
Previous HEAD position was b5755a6... Comment 500
Switched to branch 'buggy'
Traceback (most recent call last):
  File "squares.py", line 9, in <module>
   print(integer**2)
TypeError: unsupported operand type(s) for ** or pow(): 'str' and 'int'
Traceback (most recent call last):
  File "squares.py", line 9, in <module>
    print(integer**2)
TypeError: unsupported operand type(s) for ** or pow(): 'str' and 'int'
Traceback (most recent call last):
  File "squares.py", line 9, in <module>
    print(integer**2)
TypeError: unsupported operand type(s) for ** or pow(): 'str' and 'int'
Traceback (most recent call last):
  File "squares.py", line 9, in <module>
```

```
print(integer**2)
TypeError: unsupported operand type(s) for ** or pow(): 'str' and 'int'
Traceback (most recent call last):
 File "squares.py", line 9, in <module>
   print(integer**2)
TypeError: unsupported operand type(s) for ** or pow(): 'str' and 'int'
Traceback (most recent call last):
 File "squares.py", line 9, in <module>
    print(integer**2)
TypeError: unsupported operand type(s) for ** or pow(): 'str' and 'int'
Traceback (most recent call last):
 File "squares.py", line 9, in <module>
   print(integer**2)
TypeError: unsupported operand type(s) for ** or pow(): 'str' and 'int'
Traceback (most recent call last):
 File "squares.py", line 9, in <module>
   print(integer**2)
TypeError: unsupported operand type(s) for ** or pow(): 'str' and 'int'
```

Boom!

Chapter 3

Testing

3.1 Introduction

3.1.1 A few reasons not to do testing

Sensibility	Sense
It's boring	Maybe
Code is just a one off throwaway	As with most research codes
No time for it	A bit more code, a lot less debugging
Tests can be buggy too	See above
Not a professional programmer	See above
Will do it later	See above

3.1.2 A few reasons to do testing

- lazyness testing saves time
- peace of mind tests (should) ensure code is correct
- runnable specification best way to let others know what a function should do and not do
- reproducible debugging debugging that happened and is saved for later reuse
- code structure / **modularity** *since the code is designed for at least two situations*
- easier to modify since results can be tested

3.1.3 Not a panacea

Trying to improve the quality of software by doing more testing is like trying to lose weight by weighting yourself more often. - Steve McConnell

- Testing won't corrrect a buggy code
- Testing will tell you were the bugs are...
- ... if the test cases *cover* the bugs

3.1.4 Tests at different scales

Level of test	Area covered by test
Unit testing	smallest logical block of work (often < 10 lines of code)
Component testing	several logical blocks of work together
Integration testing	all components together / whole program

Always start at the smallest scale!

If a unit test is too complicated, go smaller.

3.1.5 Legacy code hardening

- Very difficult to create unit-tests for existing code
- Instead we make a regression test
- Run program as a black box:

```
setup input
run program
read output
check output against expected result
```

- Does not test correctness of code
- Checks code is a similarly wrong on day N as day 0

3.1.6 Testing vocabulary

- fixture: input data
- action: function that is being tested
- expected result: the output that should be obtained
- actual result: the output that is obtained
- **coverage**: proportion of all possible paths in the code that the tests take

3.1.7 Branch coverage:

```
if energy > 0:
    ! Do this
else:
    ! Do that

Is there a test for both energy > 0 and energy <= 0?</pre>
```

3.2 How to Test

3.2.1 Equivalence partitioning

Think hard about the different cases the code will run under: this is science, not coding!

We can't write a test for every possible input: this is an infinite amount of work.

We need to write tests to rule out different bugs. There's no need to separately test *equivalent* inputs. Let's look at an example of this question outside of coding:

- Research Project: Evolution of agricultural fields in Saskatchewan from aerial photography
- In silico translation : Compute overlap of two rectangles

```
In [1]: import matplotlib.pyplot as plt
        from matplotlib.path import Path
        import matplotlib.patches as patches
        %matplotlib inline
        ImportErrorTraceback (most recent call last)
        <ipython-input-1-e701543ea062> in <module>()
    ----> 1 import matplotlib.pyplot as plt
          2 from matplotlib.path import Path
          3 import matplotlib.patches as patches
          4 get_ipython().magic(u'matplotlib inline')
        ImportError: No module named matplotlib.pyplot
  Let's make a little fragment of matplotlib code to visualise a pair of fields.
In [2]: def show_fields(field1, field2):
            def vertices(left, bottom, right, top):
                verts = [(left, bottom),
                          (left, top),
                          (right, top),
                          (right, bottom),
                          (left, bottom)]
                return verts
            codes = [Path.MOVETO,
                     Path.LINETO,
                     Path.LINETO,
                     Path.LINETO,
                     Path.CLOSEPOLY]
            path1 = Path(vertices(*field1), codes)
            path2 = Path(vertices(*field2), codes)
            fig = plt.figure()
            ax = fig.add_subplot(111)
            patch1 = patches.PathPatch(path1, facecolor='orange', lw=2)
            patch2 = patches.PathPatch(path2, facecolor='blue', lw=2)
            ax.add_patch(patch1)
            ax.add_patch(patch2)
            ax.set_xlim(0,5)
            ax.set_ylim(0,5)
        show_fields((1.,1.,4.,4.),(2.,2.,3.,3.))
        NameErrorTraceback (most recent call last)
        <ipython-input-2-3bfe55545077> in <module>()
```

Here, we can see that the area of overlap, is the same as the smaller field, with area 1.

We could now go ahead and write a subroutine to calculate that, and also write some test cases for our answer.

But first, let's just consider that question abstractly, what other cases, not equivalent to this might there be?

For example, this case, is still just a full overlap, and is sufficiently equivalent that it's not worth another test:

But this case is no longer a full overlap, and should be tested separately:

```
In [4]: show_fields((1.,1.,4.,4.),(2.,2.,3.,4.5))
NameErrorTraceback (most recent call last)
```

On a piece of paper, sketch now the other cases you think should be treated as non-equivalent. The answers are in a separate notebook.

```
In [5]: show_fields((1.,1.,4.,4.),(2,2,4.5,4.5)) # Overlap corner
       NameErrorTraceback (most recent call last)
       <ipython-input-5-bf490d68ee7a> in <module>()
    ---> 1 show_fields((1.,1.,4.,4.),(2,2,4.5,4.5)) # Overlap corner
        <ipython-input-2-3bfe55545077> in show_fields(field1, field2)
         8
                   return verts
         9
    ---> 10 codes = [Path.MOVETO,
        11
                        Path.LINETO,
        12
                        Path.LINETO,
       NameError: global name 'Path' is not defined
In [6]: show_fields((1.,1.,4.,4.),(2.,2.,3.,4.)) # Just touching
       NameErrorTraceback (most recent call last)
       <ipython-input-6-00f0292dc5d8> in <module>()
    ----> 1 show_fields((1.,1.,4.,4.),(2.,2.,3.,4.)) # Just touching
        <ipython-input-2-3bfe55545077> in show_fields(field1, field2)
         8
                   return verts
         9
    ---> 10 codes = [Path.MOVETO,
```

```
11
                        Path.LINETO,
        12
                        Path.LINETO,
       NameError: global name 'Path' is not defined
In [7]: show_fields((1.,1.,4.,4.),(4.5,4.5,5,5)) # No overlap
       NameErrorTraceback (most recent call last)
       <ipython-input-7-bc8bec73b25e> in <module>()
    ---> 1 show_fields((1.,1.,4.,4.),(4.5,4.5,5,5)) # No overlap
        <ipython-input-2-3bfe55545077> in show_fields(field1, field2)
         8
                   return verts
         9
    ---> 10
              codes = [Path.MOVETO,
        11
                        Path.LINETO,
        12
                        Path.LINETO,
       NameError: global name 'Path' is not defined
In [8]: show_fields((1.,1.,4.,4.),(2.5,4,3.5,4.5)) # Just touching from outside
       NameErrorTraceback (most recent call last)
        <ipython-input-8-63b036f4e94c> in <module>()
    ---> 1 show_fields((1.,1.,4.,4.),(2.5,4,3.5,4.5)) # Just touching from outside
        <ipython-input-2-3bfe55545077> in show_fields(field1, field2)
         8
                   return verts
         9
    ---> 10
              codes = [Path.MOVETO,
                        Path.LINETO,
        11
        12
                        Path.LINETO,
       NameError: global name 'Path' is not defined
In [9]: show_fields((1.,1.,4.,4.),(4,4,4.5,4.5)) # Touching corner
```

NameError: global name 'Path' is not defined

3.2.2 Using our tests

OK, so how might our tests be useful?

Here's some code that **might** correctly calculate the area of overlap:

```
In [10]: def overlap(field1, field2):
    left1, bottom1, top1, right1 = field1
    left2, bottom2, top2, right2 = field2
    overlap_left=max(left1, left2)
    overlap_bottom=max(bottom1, bottom2)
    overlap_right=min(right1, right2)
    overlap_top=min(top1, top2)
    overlap_height=(overlap_top-overlap_bottom)
    overlap_width=(overlap_right-overlap_left)
    return overlap_height*overlap_width
```

So how do we check our code?

The manual approach would be to look at some cases, and, once, run it and check:

```
In [11]: overlap((1.,1.,4.,4.),(2.,2.,3.,3.))
Out[11]: 1.0
```

That looks OK.

But we can do better, we can write code which raises an error if it gets an unexpected answer:

```
In [12]: assert overlap((1.,1.,4.,4.),(2.,2.,3.,3.)) == 1.0
In [13]: assert overlap((1.,1.,4.,4.),(2.,2.,3.,4.5)) == 2.0
In [14]: assert overlap((1.,1.,4.,4.),(2.,2.,4.5,4.5)) == 4.0
In [15]: assert overlap((1.,1.,4.,4.),(4.5,4.5,5,5)) == 0.0
```

AssertionErrorTraceback (most recent call last)

```
<ipython-input-15-9b6bffd116ce> in <module>()
    ----> 1 assert overlap((1.,1.,4.,4.),(4.5,4.5,5,5)) == 0.0
        AssertionError:
In [16]: print overlap((1.,1.,4.,4.), (4.5,4.5,5,5))
0.25
In [17]: show_fields((1.,1.,4.,4.),(4.5,4.5,5,5))
        NameErrorTraceback (most recent call last)
        <ipython-input-17-4605e92c6a80> in <module>()
    ---> 1 show_fields((1.,1.,4.,4.),(4.5,4.5,5,5))
        <ipython-input-2-3bfe55545077> in show_fields(field1, field2)
          8
                    return verts
          9
    ---> 10 codes = [Path.MOVETO,
         11
                         Path.LINETO,
         12
                         Path.LINETO,
        NameError: global name 'Path' is not defined
  What? Why is this wrong?
  In our calculation, we are actually getting:
```

Both width and height are negative, resulting in a positive area. The above code didn't take into account the non-overlap correctly.

It should be:

```
In [19]: def overlap(field1, field2):
    left1, bottom1, top1, right1 = field1
    left2, bottom2, top2, right2 = field2

    overlap_left=max(left1, left2)
    overlap_bottom=max(bottom1, bottom2)
    overlap_right=min(right1, right2)
    overlap_top=min(top1, top2)
```

Note, we reran our other tests, to check our fix didn't break something else. (We call that "fallout")

3.2.3 Boundary cases

"Boundary cases" are an important area to test:

- Limit between two equivalence classes: edge and corner sharing fields
- Wherever indices appear, check values at 0, N, N+1
- Empty arrays:

```
atoms = [read_input_atom(input_atom) for input_atom in input_file]
energy = force_field(atoms)
```

- What happens if atoms is an empty list?
- What happens when a matrix/data-frame reaches one row, or one column?

3.2.4 Positive and negative tests

- Positive tests: code should give correct answer with various inputs
- Negative tests: code should crash as expected given invalid inputs, rather than lying

Bad input should be expected and should fail early and explicitly. Testing should ensure that explicit failures do indeed happen.

3.2.5 Raising exceptions

In Python, we can signal an error state by raising an error:

```
<ipython-input-23-e283d4657e88> in <module>()
----> 1 I_only_accept_positive_numbers(-5)

<ipython-input-21-6e472e931020> in I_only_accept_positive_numbers(number)
    2  # Check input
    3  if number < 0:
----> 4     raise ValueError("Input "+ str(number)+" is negative")
    5
    6  # Do something

ValueError: Input -5 is negative
```

There are standard "Exception" types, like ValueError we can raise We would like to be able to write tests like this:

But to do that, we need to learn about more sophisticated testing tools, called "test frameworks".

3.3 Classroom exercise: energy calculation

3.3.1 Diffusion model in 1D

Description: A one-dimensional diffusion model. (Could be a gas of particles, or a bunch of crowded people in a corridor, or animals in a valley habitat...)

- Agents are on a 1d axis
- Agents do not want to be where there are other agents

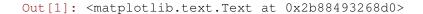
Implementation:

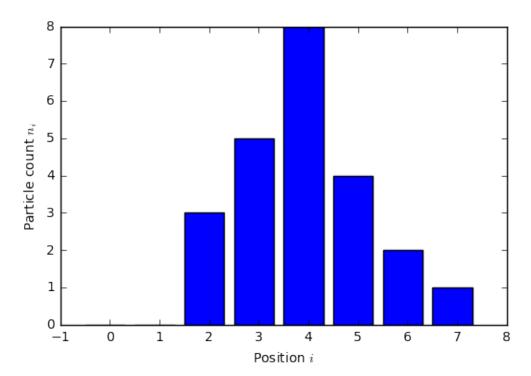
- Given a vector n of positive integers, and of arbitrary length
- Compute the energy, $E(n) = \sum_{i} n_i(n_i 1)$
- Later, we will have the likelyhood of an agent moving depend on the change in energy.

```
In [1]: import numpy as np
    from matplotlib import pyplot as plt
    %matplotlib inline

density = np.array([0, 0, 3, 5, 8, 4, 2, 1])
    fig, ax = plt.subplots()
    ax.bar(np.arange(len(density))-0.5, density)
    ax.xrange=[-0.5, len(density)-0.5]
    ax.set_ylabel("Particle count $n_i$")
    ax.set_xlabel("Position $i$")
```

/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment





Here, the total energy due to position 2 is 3(3-1)=6, and due to column 7 is 1(1-1)=0. We need to sum these to get the total energy.

3.3.2 Starting point

Create a Python module:

• Implementation file: diffusion_model.py

```
coeff: float
               Diffusion coefficient.
        11 11 11
        # implementation goes here
Writing diffusion/model.py
  • Testing file: test_diffusion_model.py
In [4]: %%writefile diffusion/test_model.py
       from .model import energy
      def test_energy():
        """ Optional description for nose reporting """
        # Test something
Writing diffusion/test_model.py
  Invoke the tests:
In [5]: %%bash
      cd diffusion
      pytest
----- test session starts ------
platform linux -- Python 3.4.3, pytest-3.0.0, py-1.4.31, pluggy-0.3.1
rootdir: /home/travis/build/UCL/rsd-engineeringcourse/ch03tests/diffusion, inifile:
collected 1 items
test_model.py .
```

Number of particles at each position i in the array

Now, write your code (in model.py), and tests (in test_model.py), testing as you do.

3.3.3 Solution

Don't look until after class!

```
# ... of the right kind (integer). Unless it is zero length,
          # in which case type does not matter.
          if density.dtype.kind != 'i' and len(density) > 0:
            raise TypeError("Density should be a array of *integers*.")
          # and the right values (positive or null)
          if any (density < 0):
            raise ValueError("Density should be an array of *positive* integers.")
          if density.ndim != 1:
            raise ValueError("Density should be an a *1-dimensional*"+
                             "array of positive integers.")
          return sum(density * (density - 1))
Overwriting diffusion/model.py
In [7]: %%writefile diffusion/test_model.py
        """ Unit tests for a diffusion model """
        from pytest import raises, approx
        from .model import energy
        def test_energy_fails_on_non_integer_density():
            with raises(TypeError) as exception:
               energy([1.0, 2, 3])
        def test_energy_fails_on_negative_density():
            with raises(ValueError) as exception: energy(
                    [-1, 2, 3])
        def test_energy_fails_ndimensional_density():
            with raises(ValueError) as exception: energy(
                    [[1, 2, 3], [3, 4, 5]])
        def test_zero_energy_cases():
          # Zero energy at zero density
          densities = [ [], [0], [0, 0, 0] ]
          for density in densities:
            assert energy(density) == approx(0)
        def test_derivative():
          from numpy.random import randint
          # Loop over vectors of different sizes (but not empty)
          for vector_size in randint(1, 1000, size=30):
            # Create random density of size N
            density = randint(50, size=vector_size)
            # will do derivative at this index
            element index = randint(vector size)
            # modified densities
            density_plus_one = density.copy()
```

```
density_plus_one[element_index] += 1
          # Compute and check result
           \# d(n^2-1)/dn = 2n
          expected = (2.0*density[element_index]
                     if density[element index] > 0
                     else 0)
          actual = energy(density_plus_one) - energy(density)
          assert expected == approx(actual)
       def test_derivative_no_self_energy():
         """ If particle is alone, then its participation to energy is zero """
         from numpy import array
         density = array([1, 0, 1, 10, 15, 0])
         density_plus_one = density.copy()
         density[1] += 1
         expected = 0
         actual = energy(density_plus_one) - energy(density)
         assert expected == approx(actual)
Overwriting diffusion/test_model.py
In [8]: %%bash
       cd diffusion
       pytest
platform linux -- Python 3.4.3, pytest-3.0.0, py-1.4.31, pluggy-0.3.1
rootdir: /home/travis/build/UCL/rsd-engineeringcourse/ch03tests/diffusion, inifile:
collected 6 items
test_model.py ...
3.3.4 Coverage
 1. Comment out from exception tests in solution
 2. in solution directory, run
In [9]: %%bash
       cd diffusion
       pytest --cov=diffusion.model -v . --cov-report=html
usage: pytest [options] [file_or_dir] [file_or_dir] [...]
pytest: error: unrecognized arguments: --cov=diffusion.model --cov-report=html
 rootdir: /home/travis/build/UCL/rsd-engineeringcourse/ch03tests/diffusion
```

Look at the coverage results

3.4 Mocking

3.4.1 Definition

Mock: verb,

- 1. to tease or laugh at in a scornful or contemptuous manner
- 2. to make a replica or imitation of something

Mocking

• *computer science*, to simulate the behaviour of real objects in controlled ways.

Stub routine

• A routine that a simulate a more computationally expensive routine, without actually performing any calculation. Strictly speaking, the term Mocking is reserved for object-oriented approaches

3.4.2 Mocking frameworks

- C: CMocka
- C++: googlemock
- Python: Mock (unittest.mock in python 3.3), doublex

3.4.3 Recording calls with mock

Mock objects record the calls made to them:

```
In [1]: from mock import Mock
        function = Mock(name="myroutine", return_value=2)
In [2]: function(1)
Out[2]: 2
In [3]: function(5, "hello", a=True)
Out[3]: 2
In [4]: function.mock_calls
Out[4]: [call(1), call(5, 'hello', a=True)]
  The arguments of each call can be recovered
In [5]: name, args, kwargs = function.mock_calls[1]
        args, kwargs
Out[5]: ((5, 'hello'), {'a': True})
  Mock objects can return different values for each call
In [6]: function = Mock(name="myroutine", side_effect=[2, "xyz"])
In [7]: function(1)
Out[7]: 2
In [8]: function(1, "hello", {'a': True})
```

```
Out[8]: 'xyz'
```

We expect an error if there are no return values left in the list:

```
In [9]: function()
                                                   Traceback (most recent call last)
        StopIteration
        <ipython-input-9-2fcbbbc1fe81> in <module>()
    ---> 1 function()
        /home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/mock/mock.py in ____
       1060
                   # in the signature
      1061
                    _mock_self._mock_check_sig(*args, **kwargs)
    -> 1062
                   return _mock_self._mock_call(*args, **kwargs)
      1063
       1064
        /home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/mock/mock.py in _mock.
       1119
       1120
                        if not callable (effect):
    -> 1121
                            result = next(effect)
       1122
                            if _is_exception(result):
       1123
                                raise result
        StopIteration:
```

3.4.4 Using mocks to model test resources

Often we want to write tests for code which interacts with remote resources. (E.g. databases, the internet, or data files.)

We don't want to have our tests *actually* interact with the remote resource, as this would mean our tests failed due to lost internet connections, for example.

Instead, we can use mocks to assert that our code does the right thing in terms of the *messages it sends*: the parameters of the function calls it makes to the remote resource.

For example, consider the following code that downloads a map from the internet:

/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a momes/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a momes

Out[12]:



We would like to test that it is building the parameters correctly. We can do this by **mocking** the requests object. We need to temporarily replace a method in the library with a mock. We can use "patch" to do this:

```
In [13]: from mock import patch
         with patch.object(requests, 'get') as mock_get:
             london_map=map_at (51.5073509, -0.1277583)
             print mock_get.mock_calls
          File "<ipython-input-13-30e527133a0b>", line 4
        print mock_get.mock_calls
    SyntaxError: Missing parentheses in call to 'print'
  Our tests then look like:
In [14]: def test_build_default_params():
             with patch.object(requests, 'get') as mock_get:
                 default_map=map_at(51.0, 0.0)
                 mock get.assert called with (
                 "http://maps.googleapis.com/maps/api/staticmap?",
                 params={
                     'sensor':'false',
                     'zoom':12,
                     'size':'400x400',
                     'center':'51.0,0.0',
                     'style':'feature:all|element:labels|visibility:off'
                 }
         test_build_default_params()
        NameError
                                                  Traceback (most recent call last)
        <ipython-input-14-0c54f762c9b1> in <module>()
        12 }
         13
    ---> 14 test_build_default_params()
        <ipython-input-14-0c54f762c9b1> in test_build_default_params()
         1 def test_build_default_params():
    ---> 2 with patch.object(requests, 'get') as mock_get:
         3
                    default_map=map_at(51.0, 0.0)
                    mock_get.assert_called_with(
                    "http://maps.googleapis.com/maps/api/staticmap?",
        NameError: name 'patch' is not defined
```

That was quiet, so it passed. When I'm writing tests, I usually modify one of the expectations, to something 'wrong', just to check it's not passing "by accident", run the tests, then change it back!

3.4.5 Testing functions that call other functions

We want to test that the above function does the right thing. It is supposed to compute the derivative of a function of a vector in a particular direction.

E.g.:

```
In [16]: partial_derivative(sum, [0,0,0], 1)
Out[16]: 1.0
```

How do we assert that it is doing the right thing? With tests like this:

```
In [17]: from mock import MagicMock

def test_derivative_2d_y_direction():
    func=MagicMock()
    partial_derivative(func, [0,0], 1)
    func.assert_any_call([0, 1.0])
    func.assert_any_call([0, 0])
test_derivative_2d_y_direction()
```

We made our mock a "Magic Mock" because otherwise, the mock results $f_x_{\text{plus_delta}}$ and f_x can't be subtracted:

3.5 Using a debugger

3.5.1 Stepping through the code

Debuggers are programs that can be used to test other programs. They allow programmers to suspend execution of the target program and inspect variables at that point.

- Mac compiled languages: Xcode
- Windows compiled languages: Visual Studio
- Linux: DDD
- all platforms: eclipse, gdb (DDD and eclipse are GUIs for gdb)
- python: spyder, pdb
- R: RStudio, debug, browser
- Python: pdb, or the ipython version ipdb

3.5.2 Using the python debugger

Unfortunately this doesn't work nicely in the notebook. But from the command line, you can run a python program with:

```
python -m pdb my_program.py
```

3.5.3 Basic navigation:

Basic command to navigate the code and the python debugger:

- help: prints the help
- help n: prints help about command n
- n(ext): executes one line of code. Executes and steps **over** functions.
- s(tep): step into current function in line of code
- 1(ist): list program around current position
- w(where): prints current stack (where we are in code)
- [enter]: repeats last command
- anypythonvariable: print the value of that variable

The python debugger is **a python shell**: it can print and compute values, and even change the values of the variables at that point in the program.

3.5.4 Breakpoints

Break points tell debugger where and when to stop We say * b somefunctionname

The debugger is, of course, most used interactively, but here I'm showing a prewritten debugger script:

```
In [3]: %%bash
        python -m pdb energy_example.py < commands</pre>
Uncaught exception. Entering post mortem debugging
Running 'cont' or 'step' will restart the program
> <string>(1) <module>()
(Pdb)
Traceback (most recent call last):
  File "/opt/python/3.4.3/lib/python3.4/pdb.py", line 1661, in main
    pdb._runscript (mainpyfile)
 File "/opt/python/3.4.3/lib/python3.4/pdb.py", line 1542, in _runscript
    self.run(statement)
  File "/opt/python/3.4.3/lib/python3.4/bdb.py", line 431, in run
    exec(cmd, globals, locals)
  File "<string>", line 1, in <module>
  File "/home/travis/build/UCL/rsd-engineeringcourse/ch03tests/energy example.py", line 2
    print energy([5, 6, 7, 8, 0, 1])
SyntaxError: invalid syntax
Traceback (most recent call last):
  File "/opt/python/3.4.3/lib/python3.4/pdb.py", line 1661, in main
   pdb._runscript(mainpyfile)
 File "/opt/python/3.4.3/lib/python3.4/pdb.py", line 1542, in _runscript
    self.run(statement)
 File "/opt/python/3.4.3/lib/python3.4/bdb.py", line 431, in run
    exec(cmd, globals, locals)
  File "<string>", line 1, in <module>
  File "/home/travis/build/UCL/rsd-engineeringcourse/ch03tests/energy_example.py", line 2
    print energy([5, 6, 7, 8, 0, 1])
SyntaxError: invalid syntax
During handling of the above exception, another exception occurred:
Traceback (most recent call last):
  File "/opt/python/3.4.3/lib/python3.4/runpy.py", line 170, in _run_module_as_main
    "__main__", mod_spec)
  File "/opt/python/3.4.3/lib/python3.4/runpy.py", line 85, in _run_code
    exec(code, run_globals)
 File "/opt/python/3.4.3/lib/python3.4/pdb.py", line 1685, in <module>
    pdb.main()
  File "/opt/python/3.4.3/lib/python3.4/pdb.py", line 1677, in main
    pdb.interaction(None, t)
  File "/opt/python/3.4.3/lib/python3.4/pdb.py", line 346, in interaction
    self._cmdloop()
  File "/opt/python/3.4.3/lib/python3.4/pdb.py", line 319, in _cmdloop
    self.cmdloop()
 File "/opt/python/3.4.3/lib/python3.4/cmd.py", line 138, in cmdloop
    stop = self.onecmd(line)
  File "/opt/python/3.4.3/lib/python3.4/pdb.py", line 412, in onecmd
    return cmd.Cmd.onecmd(self, line)
```

```
File "/opt/python/3.4.3/lib/python3.4/cmd.py", line 217, in onecmd
  return func(arg)
File "/opt/python/3.4.3/lib/python3.4/pdb.py", line 1022, in do_run
  raise Restart
pdb.Restart
```

Alternatively, break-points can be set on files: b file.py:20 will stop on line 20 of file.py.

3.5.5 Post-mortem

Debugging when something goes wrong:

- 1. Have a crash somewhere in the code
- 2. run python -m pdb file.py or run the cell with %pdb on

The program should stop where the exception was raised

- 1. use w and 1 for position in code and in call stack
- 2. use up and down to navigate up and down the call stack
- 3. inspect variables along the way to understand failure

This **does** work in the notebook.

```
%pdb on
from diffusion.model import energy
partial_derivative(energy,[5,6,7,8,0,1],5)
```

3.6 Continuous Integration

3.6.1 Test servers

Goal:

- 1. run tests nightly
- 2. run tests after each commit to github (or other)
- 3. run tests on different platforms

Various groups run servers that can be used to do this automatically. RITS run a university-wide one.

3.6.2 Memory and profiling

For compiled languages (C, C++, Fortran): * Checking for memory leaks with valgrind: valgrind --leak-check=full program * Checking cache hits and cache misses with cachegrind: valgrind --tool=cachegrind program * Profiling the code with callgrind: valgrind --tool=callgrind program

- Python: profile with runsnake
- R: Rprof

3.7 Recap example: Monte-Carlo

3.7.1 Problem: Implement and test a simple Monte-Carlo algorithm

Given an input function (energy) and starting point (density) and a temperature *T*:

- 1. Compute energy at current density.
- 2. Move randomly chosen agent randomly left or right.
- 3. Compute second energy.
- 4. Compare the two energies:
- 5. If second energy is lower, accept move.
- 6. β is a parameter which determines how likely the simulation is to move from a 'less favourable' situation to a 'more favourable' one.
- 7. Compute $P_0 = e^{-\beta(E_1 E_0)}$ and P_1 a random number between 0 and 1,
- 8. If $P_0 > P_1$, do the move anyway.
- 9. Repeat.
- the algorithm should work for (m)any energy function(s).
- there should be separate tests for separate steps! What constitutes a step?
- tests for the Monte-Carlo should not depend on other parts of code.
- Use matplotlib to plot density at each iteration, and make an animation

3.7.2 Solution

We need to break our problem down into pieces:

- 1. A function to generate a random change: random_agent(), random_direction()
- 2. A function to compute the energy before the change and after it: energy ()
- 3. A function to determine the probability of a change given the energy difference (1 if decreases, otherwise based on exponential): change_density()
- 4. A function to determine whether to execute a change or not by drawing a random numberaccept_change()
- 5. A method to iterate the above procedure: step()

Next Step: Think about the possible unit tests

- 1. Input insanity: e.g. density should non-negative integer; testing by giving negative values etc.
- 2. change_density(): density is change by a particle hopping left or right? Do all positions have an equal chance of moving?
- 3. accept_change() will move be accepted when second energy is lower?
- 4. Make a small test case for the main algorithm. (Hint: by using mocking, we can pre-set who to move where.)

```
""" A simple Monte Carlo implementation """
def __init__(self, energy, density, temperature=1, itermax=1000):
    from numpy import any, array
    density = array(density)
    self.itermax = itermax
    if temperature == 0: raise NotImplementedError(
            "Zero temperature not implemented")
    if temperature < 0e0: raise ValueError(</pre>
            "Negative temperature makes no sense")
    if len(density) < 2:
        raise ValueError("Density is too short")
    # of the right kind (integer). Unless it is zero length,
    # in which case type does not matter.
    if density.dtype.kind != 'i' and len(density) > 0:
        raise TypeError("Density should be an array of *integers*.")
    # and the right values (positive or null)
    if any (density < 0):
        raise ValueError("Density should be an array of"+
                          "*positive* integers.")
    if density.ndim != 1:
        raise ValueError("Density should be an a *1-dimensional*"+
                          "array of positive integers.")
    if sum(density) == 0:
        raise ValueError("Density is empty.")
    self.current_energy = energy(density)
    self.temperature = temperature
    self.density = density
def random_direction(self): return choice([-1, 1])
def random_agent(self, density):
    #Particle index
    particle = randint(sum(density))
    current = 0
    for location, n in enumerate (density):
        current += n
        if current > particle: break
    return location
def change_density(self, density):
    """ Move one particle left or right. """
    location = self.random_agent(density)
    # Move direction
    if (density[location]-1<0): return array(density)</pre>
    if location == 0: direction = 1
    elif location == len(density) - 1: direction = -1
    else: direction = self.random direction()
```

```
# Now make change
        result = array(density)
        result[location] -= 1
        result[location + direction] += 1
        return result
    def accept_change(self, prior, successor):
        """ Returns true if should accept change. """
        from numpy import exp
        from numpy.random import uniform
        if successor <= prior: return True
        else:
            return exp(-(successor - prior) / self.temperature) > uniform()
    def step(self):
        iteration = 0
        while iteration < self.itermax:
            new_density = self.change_density(self.density)
            new_energy = energy(new_density)
            accept = self.accept_change(self.current_energy, new_energy)
            if accept:
                self.density, self.current energy = new density, new energy
            iteration+=1
        return self.current_energy, self.density
def energy(density, coefficient=1):
  """ Energy associated with the diffusion model
      :Parameters:
      density: array of positive integers
      Number of particles at each position i in the array/geometry
  from numpy import array, any, sum
  # Make sure input is an array
  density = array(density)
  # of the right kind (integer). Unless it is zero length, in which case type does
  if density.dtype.kind != 'i' and len(density) > 0:
    raise TypeError("Density should be an array of *integers*.")
  # and the right values (positive or null)
  if any (density < 0):
    raise ValueError("Density should be an array"+
                     "of *positive* integers.")
  if density.ndim != 1:
    raise ValueError("Density should be an a *1-dimensional*"+
                     "array of positive integers.")
  return coefficient * 0.5 * sum(density * (density - 1))
```

In [3]: %matplotlib inline

```
import sys
        sys.path.append('DiffusionExample')
        from MonteCarlo import MonteCarlo, energy
        import numpy as np
        import numpy.random as random
        from matplotlib import animation
        from matplotlib import pyplot as plt
        from JSAnimation import IPython_display
        Temperature = 0.1
        density=[np.sin(i) for i in np.linspace(0.1, 3, 100)]
        density=np.array(density)*100
        density = density.astype(int)
        fig = plt.figure()
        ax = plt.axes(xlim=(-1, len(density)), ylim=(0, np.max(density)+1))
        image = ax.scatter(range(len(density)), density)
        txt_energy = plt.text(0, 100, 'Energy = 0')
        plt.xlabel('Temperature = 0.1')
        plt.ylabel('Energy Density')
        mc=MonteCarlo(energy, density, temperature = Temperature)
        def simulate(step):
            energy, density = mc.step()
            image.set_offsets(np.vstack((range(len(density)), density)).T)
            txt_energy.set_text('Energy = %f'% energy)
            return image, txt_energy
        animation.FuncAnimation(fig, simulate, frames=200, interval=50, blit=True)
/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py
  warnings.warn('Matplotlib is building the font cache using fc-list. This may take a momen
/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py
  warnings.warn('Matplotlib is building the font cache using fc-list. This may take a momen
Out[3]: <matplotlib.animation.FuncAnimation at 0x2aded26662e8>
In [4]: %%writefile DiffusionExample/test_model.py
        from MonteCarlo import MonteCarlo
        from pytest import raises, approx
        from mock import MagicMock
```

""" Check incorrect input do fail """

def test_input_sanity():

```
energy = MagicMock()
    with raises (NotImplementedError) as exception:
        MonteCarlo(sum, [1, 1, 1], 0e0)
    with raises (ValueError) as exception:
       MonteCarlo (energy, [1, 1, 1], temperature=-1e0)
    with raises(TypeError) as exception:
        MonteCarlo(energy, [1.0, 2, 3])
    with raises (ValueError) as exception:
        MonteCarlo(energy, [-1, 2, 3])
    with raises (ValueError) as exception:
        MonteCarlo(energy, [[1, 2, 3], [3, 4, 5]])
    with raises (ValueError) as exception:
        MonteCarlo(energy, [3])
    with raises (ValueError) as exception:
        MonteCarlo(energy, [0, 0])
def test_move_particle_one_over():
    """ Check density is change by a particle hopping left or right. """
    from numpy import nonzero, multiply
    from numpy.random import randint
    energy = MagicMock()
    for i in range(100):
        # Do this n times, to avoid
        # issues with random numbers
        # Create density
        density = randint(50, size=randint(2, 6))
        mc = MonteCarlo(energy, density)
        # Change it
        new_density = mc.change_density(density)
        # Make sure any movement is by one
        indices = nonzero(density - new_density)[0]
        # densities differ in two places
        assert len(indices) == 2
        \# densities differ by + and - 1
        assert multiply.reduce((density - new_density)[indices]) == -1
def test_equal_probability():
    """ Check particles have equal probability of movement. """
    from numpy import array, sqrt, count_nonzero
    energy = MagicMock()
    density = array([1, 0, 99])
    mc = MonteCarlo(energy, density)
    changes at zero = [
```

```
(density - mc.change_density(density))[0] != 0 for i in range(10000)]
            assert count_nonzero(changes_at_zero) == approx(
                0.01 * len(changes at zero),
                abs = 0.5 * sqrt(len(changes_at_zero))
        def test accept change():
            """ Check that move is accepted if second energy is lower """
            from numpy import sqrt, count_nonzero, exp
            energy = MagicMock
            mc = MonteCarlo(energy, [1, 1, 1], temperature=100.0)
            # Should always be true.
            # But do more than one draw,
            # in case randomness incorrectly crept into
            # implementation
            for i in range(10):
                assert mc.accept change (0.5, 0.4)
                assert mc.accept_change(0.5, 0.5)
            # This should be accepted only part of the time,
            # depending on exponential distribution
            prior, successor = 0.4, 0.5
            accepted = [mc.accept_change(prior, successor) for i in range(10000)]
            assert count_nonzero(accepted) / float(len(accepted)) == approx(
                exp(-(successor - prior) / mc.temperature),
                abs = 3e0 / sqrt(len(accepted))
        def test_main_algorithm():
            import numpy as np
            from numpy import testing
            from mock import Mock
            density = [1, 1, 1, 1, 1]
            energy = MagicMock()
            mc = MonteCarlo(energy, density, itermax = 5)
            acceptance = [True, True, True, True, True]
            mc.accept_change = Mock(side_effect = acceptance)
            mc.random_agent = Mock(side_effect = [0, 1, 2, 3, 4])
            mc.random\_direction = Mock(side\_effect = [1, 1, 1, 1, -1])
            np.testing.assert\_equal(mc.step()[1], [0,1,1,2,1])
Writing DiffusionExample/test_model.py
In [5]: %%bash
```

cd DiffusionExample

pytest

```
platform linux -- Python 3.4.3, pytest-3.0.0, py-1.4.31, pluggy-0.3.1
rootdir: /home/travis/build/UCL/rsd-engineeringcourse/ch03tests/DiffusionExample, inifile:
collected 5 items
test_model.py ...
```

Chapter 4

Packaging your code

4.1 Installing Libraries

We've seen that there are lots of python libraries. But how do we install them?

The main problem is this: *libraries need other libraries*

So you can't just install a library by copying code to the computer: you'll find yourself wandering down a tree of "dependencies"; libraries needed by libraries needed by the library you want.

This is actually a good thing; it means that people are making use of each others' code. There's a real problem in scientific programming, of people who think they're really clever writing their own twenty-fifth version of the same thing.

So using other people's libraries is good.

Why don't we do it more? Because it can often be quite difficult to **install** other peoples' libraries! Python has developed a good tool for avoiding this: **pip**.

4.1.1 Installing Geopy using Pip

On a computer you control, on which you have installed python via Anaconda, you will need to open a **terminal** to invoke the library-installer program, pip.

- On windows, go to start->all programs->Anaconda->Anaconda Command Prompt
- On mac, start terminal.
- On linux, open a bash shell.

Into this shell, type:

```
pip install geopy
```

The computer will install the package automatically from PyPI.

Now, close IPython notebook if you have it open, and reopen it. Check your new library is installed with:

That was actually pretty easy, I hope. This is how you'll install new libraries when you need them. Troubleshooting:

On mac or linux, you *might* get a complaint that you need "superuser", "root", or "administrator" access. If so type:

• sudo pip install geopy

and enter your password.

If you get a complaint like: 'pip is not recognized as an internal or external command', try the following:

- conda install pip (Windows)
- sudo easy_install pip (Mac, Linux)

Ask me over email if you run into trouble.

4.1.2 Installing binary dependencies with Conda

pip is the usual Python tool for installing libraries. But there's one area of library installation that is still awkward: some python libraries depend not on other **python** libraries, but on libraries in C++ or Fortran.

This can cause you to run into difficulties installing some libraries. Fortunately, for lots of these, Continuum, the makers of Anaconda, provide a carefully managed set of scripts for installing these awkward non-python libraries too. You can do this with the conda command line tool, if you're using Anaconda. Simply type

• conda install <whatever>

instead of pip install. This will fetch the python package not from PyPI, but from Anaconda's distribution for your platform, and manage any non-python dependencies too.

Typically, if you're using Anaconda, whenever you come across a python package you want, you should check if Anaconda package it first using this list: http://docs.continuum.io/anaconda/pkg-docs.html. (Or just by trying conda install and hoping!) If you can conda install it, you'll likely have less problems. But Continuum don't package everything, so you'll need to pip install from time to time.

4.1.3 Where do these libraries go?

```
In [3]: geopy.__path__
Out[3]: ['/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/geopy']
```

Your computer will be configured to keep installed Python packages in a particular place.

Python knows where to look for possible library installations in a list of places, called the "PythonPath". It will try each of these places in turn, until it finds a matching library name.

4.1.4 Libraries not in PyPI

Sometimes, such as for the Animation library in the Boids example, you'll need to download the source code directly. This won't automatically follow the dependency tree, but for simple standalone libraries, is sometimes necessary.

To install these on windows, download and unzip the library into a folder of your choice, e.g. my_python_libs.

On windows, a reasonable choice is the folder you end up in when you open the Anaconda terminal. You can get a graphical view on this folder by typing: explorer .

Make a new folder for your download and unzip the library there.

Now, you need to move so you're inside your download in the terminal:

- cd my_python_libs
- cd cd <library name> (e.g. cd JSAnimation-master)

Now, manually install the library in your PythonPath:

• python setup.py install

[You might need to do

• sudo python setup.py install

if you get prompted for 'root' or 'admin' access.]

This is all pretty awkward, but it is worth practicing this stuff, as most of the power of using programming for research resides in all the libraries that are out there.

4.2 Libraries

4.2.1 Libraries are awesome

The strength of a language lies as much in the set of libraries available, as it does in the language itself. A great set of libraries allows for a very powerful programming style:

- Write minimal code yourself
- Choose the right libraries
- · Plug them together
- Create impressive results

Not only is this efficient with your programming time, it's also more efficient with computer time. The chances are any algorithm you might want to use has already been programmed better by someone else.

4.2.2 Drawbacks of libraries.

- Sometimes, libraries are not looked after by their creator: code that is not maintained *rots*:
 - It no longer works with later versions of *upstream* libraries.
 - It doesn't work on newer platforms or systems.
 - Features that are needed now, because the field has moved on, are not added
- Sometimes, libraries are hard to get working:
 - For libraries in pure python, this is almost never a problem
 - But many libraries involve *compiled components*: these can be hard to install.

4.2.3 Contribute, don't duplicate

- You have a duty to the ecosystem of scholarly software:
 - If there's a tool or algorithm you need, find a project which provides it.
 - If there are features missing, or problems with it, fix them, don't create your own library.

4.2.4 How to choose a library

- When was the last commit?
- How often are there commits?
- Can you find the lead contributor on the internet?
- Do they respond when approached:
 - emails to developer list
 - personal emails
 - tweets
 - irc
 - issues raised on GitHub?
- Are there contributors other than the lead contributor?
- Is there discussion of the library on Stack Exchange?
- Is the code on an open version control tool like GitHub?
- Is it on standard package repositories. (PyPI, apt/yum/brew)
- Are there any tests?
- Download it. Can you build it? Do the tests pass?
- Is there an open test dashboard? (Travis/Jenkins/CDash)
- What dependencies does the library itself have? Do they pass this list?
- Are different versions of the library clearly labeled with version numbers?
- Is there a changelog?

4.2.5 Sensible Version Numbering

The best approach to version numbers clearly distinguishes kinds of change: Given a version number MAJOR.MINOR.PATCH, e.g. 2.11.14 increment the:

- MAJOR version when you make incompatible API changes,
- MINOR version when you add functionality in a backwards-compatible manner, and
- PATCH version when you make backwards-compatible bug fixes.

This is called Semantic Versioning

4.2.6 The Python Standard Library

Python comes with a powerful standard library.

Learning python is as much about learning this library as learning the language itself. You've already seen a few packages in this library: math, pdb, pytest, datetime.

4.2.7 The Python Package Index

Python's real power, however, comes with the Python Package Index: PyPI. This is a huge array of libraries, with all kinds of capabilities, all easily installable from the command line or through your Python distribution.

4.3 Python not in the Notebook

We will often want to save our Python classes, for use in multiple Notebooks. We can do this by writing text files with a .py extension, and then importing them.

4.3.1 Writing Python in Text Files

You can use a text editor like Atom for Mac or Notepad++ for windows to do this. If you create your own Python files ending in .py, then you can import them with import just like external libraries.

You can also maintain your library code in a Notebook, and use %%writefile to create your library. Libraries are usually structured with multiple files, one for each class.

We group our modules into packages, by putting them together into a folder. You can do this with explorer, or using a shell, or even with Python:

```
In [1]: import os
        if 'mazetool' not in os.listdir(os.getcwd()):
            os.mkdir('mazetool')
In [2]: %%writefile mazetool/maze.py
        from .room import Room
        from .person import Person
        class Maze (object):
            def __init__(self, name):
                self.name = name
                self.rooms = []
                self.occupants = []
            def add_room(self, name, capacity):
                result = Room(name, capacity)
                self.rooms.append(result)
                return result
            def add_exit(self, name, source, target, reverse= None):
                source.add_exit(name, target)
                if reverse:
                    target.add_exit(reverse, source)
            def add_occupant(self, name, room):
                self.occupants.append(Person(name, room))
                room.occupancy += 1
            def wander(self):
                "Move all the people in a random direction"
                for occupant in self.occupants:
                    occupant.wander()
            def describe (self):
                for occupant in self.occupants:
                    occupant.describe()
            def step(self):
                house.describe()
                print()
                house.wander()
                print()
            def simulate(self, steps):
```

```
for _ in range(steps):
                    self.step()
Writing mazetool/maze.py
In [3]: %%writefile mazetool/room.py
        from .exit import Exit
        class Room(object):
            def __init__(self, name, capacity):
                self.name = name
                self.capacity = capacity
                self.occupancy = 0
                self.exits = []
            def has_space(self):
                return self.occupancy < self.capacity</pre>
            def available exits(self):
                return [exit for exit in self.exits if exit.valid() ]
            def random_valid_exit(self):
                import random
                if not self.available_exits():
                    return None
                return random.choice(self.available_exits())
            def add_exit(self, name, target):
                self.exits.append(Exit(name, target))
Writing mazetool/room.py
In [4]: %%writefile mazetool/person.py
        class Person(object):
            def __init__(self, name, room = None):
                self.name=name
                self.room=room
            def use(self, exit):
                self.room.occupancy -= 1
                destination=exit.target
                destination.occupancy +=1
                self.room=destination
                print(self.name, "goes", exit.name, "to the", destination.name)
            def wander(self):
                exit = self.room.random_valid_exit()
                if exit:
                    self.use(exit)
```

In order to tell Python that our "mazetool" folder is a Python package, we have to make a special file called __init__.py. If you import things in there, they are imported as part of the package:

4.3.2 Loading Our Package

We just wrote the files, there is no "Maze" class in this notebook yet:

But now, we can import Maze, (and the other files will get imported via the chained Import statements, starting from the __init__.py file.

Note the files we have created are on the disk in the folder we made:

```
In [10]: import os
```

```
In [11]: os.listdir(os.path.join(os.getcwd(),'mazetool') )
Out[11]: ['room.py', 'exit.py', '__pycache__', 'maze.py', 'person.py', '__init__.py']
```

.pyc files are "Compiled" temporary python files that the system generates to speed things up. They'll be regenerated on the fly when your .py files change.

4.3.3 The Python Path

We want to import these from notebooks elsewhere on our computer: it would be a bad idea to keep all our Python work in one folder.

Supplementary material The best way to do this is to learn how to make our code into a proper module that we can install. We'll see more on that in a few lectures' time.

Alternatively, we can add a folder to the "Python Path", where python searches for modules:

I've thus added a folder to the list of places searched. If you want to do this permanently, you should set the PYTHONPATH Environment Variable, which you can learn about in a shell course, or can read about online for your operating system.

4.4 Argparse

This is the standard library for building programs with a command-line interface.

```
In [1]: %%writefile greeter.py
    #!/usr/bin/env python
    from argparse import ArgumentParser
    if __name__ == "__main__":
        parser = ArgumentParser(description = "Generate appropriate greetings")
        parser.add_argument('--title', '-t')
        parser.add_argument('--polite','-p', action="store_true")
        parser.add_argument('personal')
        parser.add_argument('family')
        arguments= parser.parse_args()
        greeting= "How do you do, " if arguments.polite else "Hey, "
        if arguments.title:
            greeting+=arguments.title+" "
        greeting+= arguments.personal + " " + arguments.family +"."
        print greeting
```

```
Writing greeter.py
In [2]: %%bash
        #!/usr/bin/env bash
        chmod u+x greeter.py
In [3]: %%bash
        ./greeter.py --help
  File "./greeter.py", line 14
   print greeting
SyntaxError: Missing parentheses in call to 'print'
In [4]: %%bash
        ./greeter.py James Hetherington
  File "./greeter.py", line 14
   print greeting
SyntaxError: Missing parentheses in call to 'print'
In [5]: %%bash
        ./greeter.py --polite James Hetherington
 File "./greeter.py", line 14
   print greeting
SyntaxError: Missing parentheses in call to 'print'
In [6]: %%bash
        ./greeter.py James Hetherington --title Dr
  File "./greeter.py", line 14
   print greeting
SyntaxError: Missing parentheses in call to 'print'
```

4.4.1 Exercise - Packaging Greengraph

We previously looked at some notebook code that enables us to explore how green space varies as we move from the city to the countryside:

Your task for the first exercise will be to transform this into a python package that can be pip installed directly from GitHub. Remember to include:

- an _init_.py file
- a setup.py file
- tests
- license and documentation
- command entry point script

You should, in the end, be able to pip install your code on a clean computer, and do something similar to

```
greengraph -- from London -- to Oxford -- steps 10 -- out graph.png
```

A formal assessed exercise rubric will be provided.

4.5 Packaging

4.5.1 Packaging

Once we've made a working program, we'd like to be able to share it with others.

A good cross-platform build tool is the most important thing: you can always have collaborators build from source.

4.5.2 Distribution tools

Distribution tools allow one to obtain a working copy of someone else's package.

Language-specific tools: PyPI, Ruby Gems, CPAN, CRAN Platform specific packagers e.g. brew, apt/yum

Until recently windows didn't have anything like brew install or apt-get You had to build an 'installer', but now there is https://chocolatey.org

4.5.3 Laying out a project

When planning to package a project for distribution, defining a suitable project layout is essential.

We can start by making our directory structure

4.5.4 Using setuptools

To make python code into a package, we have to write a setupfile:

```
In [3]: %%writefile greetings/setup.py
    from setuptools import setup, find_packages

setup(
        name = "Greetings",
        version = "0.1",
        packages = find_packages(exclude=['*test']),
        scripts = ['scripts/greet'],
        install_requires = ['argparse']
)
```

```
Overwriting greetings/setup.py
```

We can now install this code with

```
python setup.py install
```

And the package will be then available to use everywhere on the system.

And the scripts are now available as command line commands:

```
In [5]: %%bash
    #!/usr/bin/env bash
    greet --help
bash: line 2: greet: command not found

In [6]: %%bash
    greet James Hetherington
    greet --polite James Hetherington
    greet James Hetherington --title Dr

bash: line 1: greet: command not found
bash: line 2: greet: command not found
bash: line 3: greet: command not found
```

4.5.5 Installing from GitHub

We could now submit "greeter" to PyPI for approval, so everyone could pip install it. However, when using git, we don't even need to do that: we can install directly from any git URL:

4.5.6 Convert the script to a module

Of course, there's more to do when taking code from a quick script and turning it into a proper module:

```
In [8]: %%writefile greetings/greetings/greeter.py
        def greet(personal, family, title="", polite=False):
            """ Generate a greeting string for a person.
            Parameters
            personal: str
                A given name, such as Will or Jean-Luc
            family: str
               A family name, such as Riker or Picard
            title: str
               An optional title, such as Captain or Reverend
            polite: bool
                True for a formal greeting, False for informal.
            Returns
            _____
            string
               An appropriate greeting
            greeting= "How do you do, " if polite else "Hey, "
            if title:
                greeting+=title+" "
            greeting+= personal + " " + family +"."
            return greeting
Overwriting greetings/greetings/greeter.py
```

The documentation string explains how to use the function; don't worry about this for now, we'll consider this next time.

4.5.7 Write an executable script

Overwriting greetings/greetings/command.py

4.5.8 Write an entry point script stub

```
In [10]: %%writefile greetings/scripts/greet
    #!/usr/bin/env python
    from greetings.command import process
    process()
```

Writing greetings/scripts/greet

4.5.9 Write a readme file

e.g.:

```
In [11]: %%writefile greetings/README.md

Greetings!
========

This is a very simple example package used as part of the UCL
[Research Software Engineering with Python] (development.rc.ucl.ac.uk/training/eng.
```

Overwriting greetings/README.md

4.5.10 Write a license file

```
e.g.:
```

4.5.11 Write a citation file

e.g.:

```
In [13]: %%writefile greetings/CITATION.md

If you wish to refer to this course, please cite the URL http://development.rc.ucl.ac.uk/training/engineering

Portions of the material are taken from Software Carpentry http://swcarpentry.org

Overwriting greetings/CITATION.md
```

4.5.12 Define packages and executables

4.5.13 Write some unit tests

Separating the script from the logical module made this possible:

Overwriting greetings/greetings/test/test_greeter.py

Add a fixtures file:

Overwriting greetings/greetings/test/fixtures/samples.yaml

4.5.14 Developer Install

If you modify your source files, you would now find it appeared as if the program doesn't change.

That's because pip install **copies** the file.

(On my system to /Library/Python/2.7/site-packages/: this is operating system dependent.)

If you want to install a package, but keep working on it, you can do

sudo python setup.py develop

4.5.15 Distributing compiled code

If you're working in C++ or Fortran, there is no language specific repository. You'll need to write platform installers for as many platforms as you want to support.

Typically:

- dpkg for apt-get on Ubuntu and Debian
- rpm for yum on Redhat and Fedora
- homebrew on OSX (Possibly macports as well)
- An executable msi installer for Windows.

4.5.16 Homebrew

Homebrew: A ruby DSL, you host off your own webpage

See my installer for the cppcourse example

If you're on OSX, do:

brew tap jamespjh/homebrew-reactor
brew install reactor

4.6 Documentation

4.6.1 Documentation is hard

- Good documentation is hard, and very expensive.
- Bad documentation is detrimental.
- Good documentation quickly becomes bad if not kept up-to-date with code changes.
- Professional companies pay large teams of documentation writers.

4.6.2 Prefer readable code with tests and vignettes

If you don't have the capacity to maintain great documentation, focus on:

- Readable code
- Automated tests
- Small code samples demonstrating how to use the api

4.6.3 Comment-based Documentation tools

Documentation tools can produce extensive documentation about your code by pulling out comments near the beginning of functions, together with the signature, into a web page.

The most popular is Doxygen

Have a look at an example of some Doxygen output

Sphinx is nice for Python, and works with C++ as well. Here's some Sphinx-generated output and the corresponding source code Breathe can be used to make Sphinx and Doxygen work together.

Roxygen is good for R.

4.7 Example of using Sphinx

4.7.1 Write some docstrings

We're going to document our "greeter" example using docstrings with Sphinx.

There are various conventions for how to write docstrings, but the native sphinx one doesn't look nice when used with the built in help system.

In writing Greeter, we used the docstring conventions from NumPy. So we use the numpydoc sphinx extension to support these.

```
Generate a greeting string for a person.

Parameters
-----
personal: str
   A given name, such as Will or Jean-Luc

family: str
   A family name, such as Riker or Picard

title: str
   An optional title, such as Captain or Reverend
polite: bool
   True for a formal greeting, False for informal.

Returns
-----
string
   An appropriate greeting
```

4.7.2 Set up sphinx

Invoke the sphinx-quickstart command to build Sphinx's configuration file automatically based on questions at the command line:

sphinx-quickstart

Which responds:

```
Welcome to the Sphinx 1.2.3 quickstart utility.

Please enter avalues for the following settings (just press Enter to accept a default value, if one is given in brackets).

Enter the root path for documentation.

> Root path for the documentation [.]:
```

and then look at and adapt the generated config, a file called conf.py in the root of the project. This contains the project's Sphinx configuration, as Python variables:

```
#Add any Sphinx extension module names here, as strings. They can be
#extensions coming with Sphinx (named 'sphinx.ext.*') or your custom
# ones.
extensions = [
    'sphinx.ext.autodoc', # Support automatic documentation
    'sphinx.ext.coverage', # Automatically check if functions are documented
```

```
'sphinx.ext.mathjax', # Allow support for algebra
'sphinx.ext.viewcode', # Include the source code in documentation
'numpydoc' # Support NumPy style docstrings
]
```

To proceed with the example, we'll copy a finished conf.py into our folder, though normally you'll always use sphinx-quickstart

```
In [1]: %%writefile greetings/conf.py
        import sys
        import os
        extensions = [
            'sphinx.ext.autodoc', # Support automatic documentation
            'sphinx.ext.coverage', # Automatically check if functions are documented
            'sphinx.ext.mathjax',  # Allow support for algebra
            'sphinx.ext.viewcode', # Include the source code in documentation
                                    # Support NumPy style docstrings
            'numpydoc'
        templates_path = ['_templates']
        source suffix = '.rst'
        master doc = 'index'
        project = u'Greetings'
        copyright = u'2014, James Hetherington'
        version = '0.1'
        release = '0.1'
        exclude_patterns = ['_build']
        pygments style = 'sphinx'
        htmlhelp_basename = 'Greetingsdoc'
        latex_elements = {
        latex_documents = [
          ('index', 'Greetings.tex', u'Greetings Documentation',
           u'James Hetherington', 'manual'),
        man pages = [
            ('index', 'greetings', u'Greetings Documentation',
             [u'James Hetherington'], 1)
        texinfo_documents = [
          ('index', 'Greetings', u'Greetings Documentation',
           u'James Hetherington', 'Greetings', 'One line description of project.',
           'Miscellaneous'),
        1
```

4.7.3 Define the root documentation page

Overwriting greetings/conf.py

Sphinx uses RestructuredText another wiki markup format similar to Markdown.

You define an "index.rst" file to contain any preamble text you want. The rest is autogenerated by sphinx-quickstart

4.7.4 Run sphinx

We can run Sphinx using:

```
In [3]: %%bash
        cd greetings/
        sphinx-build . doc
Running Sphinx v1.4.9
making output directory...
loading pickled environment... not yet created
building [mo]: targets for 0 po files that are out of date
building [html]: targets for 1 source files that are out of date
updating environment: 1 added, 0 changed, 0 removed
reading sources... [100%] index
looking for now-outdated files... none found
pickling environment... done
checking consistency... done
preparing documents... done
writing output... [100%] index
generating indices... genindex
writing additional pages... search
copying static files... done
copying extra files... done
dumping search index in English (code: en) ... done
dumping object inventory... done
build succeeded, 1 warning.
/home/travis/build/UCL/rsd-engineeringcourse/ch04packaging/greetings/index.rst:6: WARNING:
Traceback (most recent call last):
  File "/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/sphinx/ext/autodoc
    __import___(self.modname)
ImportError: No module named 'greetings'
```

4.7.5 Sphinx output

Sphinx's output is html. We just created a simple single function's documentation, but Sphinx will create multiple nested pages of documentation automatically for many functions.

4.8 Software Project Management

4.8.1 Software Engineering Stages

- Requirements
- Functional Design
- Architectural Design
- Implementation
- Integration

4.8.2 Requirements Engineering

Requirements capture obviously means describing the things the software needs to be able to do.

A common approach is to write down lots of "user stories", describing how the software helps the user achieve something:

As a clinician, when I finish an analysis, I want a report to be created on the test results, so that I can send it to the patient.

As a role, when condition or circumstance applies I want a goal or desire so that benefits occur.

These are easy to map into the Gherkin behaviour driven design test language.

4.8.3 Functional and architectural design

Engineers try to separate the functional design, how the software appears to and is used by the user, from the architectural design, how the software achieves that functionality.

Changes to functional design require users to adapt, and are thus often more costly than changes to architectural design.

4.8.4 Waterfall

The *Waterfall* design philosophy argues that the elements of design should occur in order: first requirements capture, then functional design, then architectural design. This approach is based on the idea that if a mistake is made in the design, then programming effort is wasted, so significant effort is spent in trying to ensure that requirements are well understood and that the design is correct before programming starts.

4.8.5 Why Waterfall?

Without a design approach, programmers resort to designing as we go, typing in code, trying what works, and making it up as we go along. When trying to collaborate to make software with others this can result in lots of wasted time, software that only the author understands, components built by colleagues that don't work together, or code that the programmer thinks is nice but that doesn't meet the user's requirements.

4.8.6 Problems with Waterfall

Waterfall results in a contractual approach to development, building an us-and-them relationship between users, business types, designers, and programmers.

I built what the design said, so I did my job.

Waterfall results in a paperwork culture, where people spend a long time designing standard forms to document each stage of the design, with less time actually spent *making things*.

Waterfall results in excessive adherence to a plan, even when mistakes in the design are obvious to people doing the work.

4.8.7 Software is not made of bricks

The waterfall approach to software engineering comes from the engineering tradition applied to building physical objects, where Architects and Engineers design buildings, and builders build them according to the design.

Software is intrinsically different:

4.8.8 Software is not made of bricks

Software is not the same 'stuff' as that from which physical systems are constructed. Software systems differ in material respects from physical systems. Much of this has been rehearsed by Fred Brooks in his classic 'No Silver Bullet' paper. First, complexity and scale are different in the case of software systems: relatively functionally simple software systems comprise more independent parts, placed in relation to each other, than do physical systems of equivalent functional value. Second, and clearly linked to this, we do not have well developed components and composition mechanisms from which to build software systems (though clearly we are working hard on providing these) nor do we have a straightforward mathematical account that permits us to reason about the effects of composition.

4.8.9 Software is not made of bricks

Third, software systems operate in a domain determined principally by arbitrary rules about information and symbolic communication whilst the operation of physical systems is governed by the laws of physics. Finally, software is readily changeable and thus is changed, it is used in settings where our uncertainty leads us to anticipate the need to change.

- Prof. Anthony Finkelstein, UCL Dean of Engineering, and Professor of Software Systems Engineering

4.8.10 The Agile Manifesto

In 2001, authors including Martin Folwer, Ward Cunningham and Kent Beck met in a Utah ski resort, and published the following manifesto.

Manifesto for Agile Software Development

We are uncovering better ways of developing software by doing it and helping others do it. Through this work we have come to value:

- Individuals and interactions over processes and tools
- Working software over comprehensive documentation
- Customer collaboration over contract negotiation
- Responding to change over following a plan

That is, while there is value in the items on the right, we value the items on the left more.

4.8.11 Agile is not absence of process

The Agile movement is not anti-methodology, in fact, many of us want to restore credibility to the word methodology. We want to restore a balance. We embrace modeling, but not in order to file some diagram in a dusty corporate repository. We embrace documentation, but not hundreds of pages of never-maintained and rarely-used tomes. We plan, but recognize the limits of planning in a turbulent environment. Those who would brand proponents of XP or SCRUM or any of the other Agile Methodologies as "hackers" are ignorant of both the methodologies and the original definition of the term hacker

– Jim Highsmith.

4.8.12 Elements of an Agile Process

- Continuous delivery
- Self-organising teams
- Iterative development
- · Ongoing design

4.8.13 Ongoing Design

Agile development doesn't eschew design. Design documents should still be written, but treated as living documents, updated as more insight is gained into the task, as work is done, and as requirements change.

Use of a Wiki or version control repository to store design documents thus works much better than using Word documents!

Test-driven design and refactoring are essential techniques to ensure that lack of "Big Design Up Front" doesn't produce badly constructed spaghetti software which doesn't meet requirements. By continously scouring our code for smells, and stopping to refactor, we evolve towards a well-structured design with weakly interacting units. By starting with tests which describe how our code should behave, we create executable specifications, giving us confidence that the code does what it is supposed to.

4.8.14 Iterative Development

Agile development maintains a backlog of features to be completed and bugs to be fixed. In each iteration, we start with a meeting where we decide which backlog tasks will be attempted during the development cycle, estimating how long each will take, and selecting an achievable set of goals for the "sprint". At the end of each cycle, we review the goals completed and missed, and consider what went well, what went badly, and what could be improved.

We try not to add work to a cycle mid-sprint. New tasks that emerge are added to the backlog, and considered in the next planning meeting. This reduces stress and distraction.

4.8.15 Continuous Delivery

In agile development, we try to get as quickly as possible to code that can be *demonstrated* to clients. A regular demo of progress to clients at the end of each development iteration says so much more than sharing a design document. "Release early, release often" is a common slogan. Most bugs are found by people *using* code – so exposing code to users as early as possible will help find bugs quickly.

4.8.16 Self-organising teams

Code is created by people. People work best when they feel ownership and pride in their work. Division of responsibilities into designers and programmers results in a "Code Monkey" role, where the craftspersonship and sense of responsibility for code quality is lost. Agile approaches encourage programmers, designers, clients, and businesspeople to see themselves as one team, working together, with fluid roles. Programmers grab issues from the backlog according to interest, aptitude, and community spirit.

4.8.17 Agile in Research

Agile approaches, where we try to turn the instincts and practices which emerge naturally when smart programmers get together into well-formulated best practices, have emerged as antidotes to both the chaotic free-form typing in of code, and the rigid paperwork-driven approaches of Waterfall.

If these approaches have turned out to be better even in industrial contexts, where requirements for code can be well understood, they are even more appropriate in a research context, where we are working in poorly understood fields with even less well captured requirements.

4.8.18 Conclusion

- Don't ignore design
- See if there's a known design pattern that will help
- Do try to think about how your code will work before you start typing
- Do use design tools like UML to think about your design without coding straight away
- Do try to write down some user stories
- Do maintain design documents.

BUT

- Do change your design as you work, updating the documents if you have them
- Don't go dark never do more than a couple of weeks programming without showing what you've done to colleagues
- Don't get isolated from the reasons for your code's existence, stay involved in the research, don't be a Code Monkey.
- Do keep a list of all the things your code needs, estimate and prioritise tasks carefully.

4.9 Software Licensing

4.9.1 Reuse

This course is distributed under the Creative Commons By Attribution license, which means you can modify and reuse the materials, so long as you credit UCL Research IT Services.

4.9.2 Disclaimer

Here we attempt to give some basic advice on choosing a license for your software. But:

- we are NOT lawyers
- opinions differ (and flamewars are boring)
- this training does NOT constitute legal advice.

For an in-depth discussion of software licenses, read the O'Reilly book.

Your department, or UCL, may have policies about applying licenses to code you create while a UCL employee or student. This training doesn't address this issue, and does not represent UCL policy – seek advice from your supervisor or manager if concerned.

4.9.3 Choose a license

It is important to choose a license and to create a *license file* to tell people what it is.

The license lets people know whether they can reuse your code and under what terms. This course has one, for example.

Your license file should typically be called LICENSE.txt or similar. GitHub will offer to create a license file automatically when you create a new repository.

4.9.4 Open source doesn't stop you making money

A common misconception about open source software is the thought that open source means you can't make any money. This is *wrong*.

Plenty of people open source their software and profit from:

- The software under a different license e.g. Saxon
- Consulting. For example: Continuum who help maintain NumPy

- Manuals. For example: VTK
- Add-ons. For example: Puppet
- Server software, which open source client software interacts with. For example: GitHub API clients

4.9.5 Plagiarism vs promotion

Many researchers worry about people stealing their work if they open source their code. But often the biggest problem is not theft, but the fact no one is aware of your work.

Open source is a way to increase the probability that someone else on the planet will care enough about your work to cite you.

So when thinking about whether to open source your code, think about whether you're more worried about anonymity or theft.

4.9.6 Your code is good enough

New coders worry that they'll be laughed at if they put their code online. Don't worry. Everyone, including people who've been coding for decades, writes shoddy code that is full of bugs.

The only thing that will make your code better, is *other people reading it*.

For small scripts that no one but you will ever use, my recommendation is to use an open repository anyway. Find a buddy, and get them to comment on it.

4.9.7 Worry about license compatibility and proliferation

Not all open source code can be used in all projects. Some licenses are legally incompatible.

This is a huge and annoying problem. As an author, you might not care, but you can't anticipate the exciting uses people might find by mixing your code with someone else's.

Use a standard license from the small list that are well-used. Then people will understand. *Don't make up your own*.

When you're about to use a license, see if there's a more common one which is recommended, e.g.: using the opensource.org proliferation report

4.9.8 Academic license proliferation

Academics often write their own license terms for their software.

For example:

XXXX NON-COMMERCIAL EDUCATIONAL LICENSE Copyright (c) 2013 Prof. Foo. All rights reserved.

You may use and modify this software for any non-commercial purpose within your educational institution. Teaching, academic research, and personal experimentation are examples of purpose which can be non-commercial.

You may redistribute the software and modifications to the software for non-commercial purposes, but only to eligible users of the software (for example, to another university student or faculty to support joint academic research).

Please don't do this. Your desire to slightly tweak the terms is harmful to the future software ecosystem. Also, *Unless you are a lawyer, you cannot do this safely!*

4.9.9 Licenses for code, content, and data.

Licenses designed for code should not be used to license data or prose.

Don't use Creative Commons for software, or GPL for a book.

4.9.10 Licensing issues

- Permissive vs share-alike
- Non-commercial and academic Use Only
- Patents
- Use as a web service

4.9.11 Permissive vs share-alike

Some licenses require all derived software to be licensed under terms that are similarly free. Such licenses are called "Share Alike" or "Copyleft".

• Licenses in this class include the GPL.

Those that don't are called "Permissive"

• These include Apache, BSD, and MIT licenses.

If you want your code to be maximally reusable, use a permissive license If you want to force other people using your code to make derivatives open source, use a copyleft license.

If you want to use code that has a permissive license, it's safe to use it and keep your code secret. If you want to use code that has a copyleft license, you'll have to release your code under such a license.

4.9.12 Academic use only

Some researchers want to make their code free for 'academic use only'. None of the standard licenses state this, and this is a reason why academic bespoke licenses proliferate.

However, there is no need for this, in our opinion.

Use of a standard Copyleft license precludes derived software from being sold without also publishing the source So use of a Copyleft license precludes commercial use.

This is a very common way of making a business from open source code: offer the code under GPL for free but offer the code under more permissive terms, allowing for commercial use, for a fee.

4.9.13 Patents

Intellectual property law distinguishes copyright from patents. This is a complex field, which I am far from qualified to teach!

People who think carefully about intellectual property law distinguish software licenses based on how they address patents. Very roughly, if a you want to ensure that contributors to your project can't then go off and patent their contribution, some licenses, such as the Apache license, protect you from this.

4.9.14 Use as a web service

If I take copyleft code, and use it to host a web service, I have not sold the software.

Therefore, under some licenses, I do not have to release any derivative software. This "loophole" in the GPL is closed by the AGPL ("Affero GPL")

4.9.15 Library linking

If I use your code just as a library, without modifying it or including it directly in my own code, does the copyleft term of the GPL apply?

Yes

If you don't want it to, use the LGPL. ("Lesser GPL"). This has an exception for linking libraries.

4.9.16 Citing software

Almost all software licenses require people to credit you for what they used ("attribution").

In an academic context, it is useful to offer a statement as to how best to do this, citing *which paper to cite in all papers which use the software*.

This is best done with a CITATION file in your repository.

To cite ggplot2 in publications, please use:

H. Wickham. ggplot2: elegant graphics for data analysis. Springer New York, 2009.

A BibTeX entry for LaTeX users is

```
@Book{, author = {Hadley Wickham}, title = {ggplot2: elegant graphics for data analysis}, publisher = {Springer New York}, year = {2009}, isbn = {978-0-387-98140-6}, url = {http://had.co.nz/ggplot2/book}, }
```

4.9.17 Referencing the license in every file

Some licenses require that you include license information in every file. Others do not.

Typically, every file should contain something like:

```
In [1]: # (C) University College London 2010-2014
     # This software is licensed under the terms of the <foo license>
     # See <somewhere> for the license details.
```

Check your license at opensource.org for details of how to apply it to your software. For example, for the GPL

4.9.18 Choose a license

See GitHub's advice on how to choose a license

4.9.19 Open source does not equal free maintenance

One common misunderstanding of open source software is that you'll automatically get loads of contributors from around the internets. This is wrong. Most open source projects get no commits from anyone else

Open source does *not* guarantee your software will live on with people adding to it after you stop working on it.

Learn more about these issues from the website of the Software Sustainability Institute

4.10 Managing software issues

4.10.1 Issues

Code has *bugs*. It also has *features*, things it should do.

A good project has an organised way of managing these. Generally you should use an issue tracker.

4.10.2 Some Issue Trackers

There are lots of good issue trackers.

The most commonly used open source ones are Trac and Redmine.

Cloud based issue trackers include Lighthouse and GitHub.

Commercial solutions include Jira.

In this course, we'll be using the GitHub issue tracker.

4.10.3 Anatomy of an issue

- Reporter
- Description
- Owner
- Type [Bug, Feature]
- Component
- Status
- Severity

4.10.4 Reporting a Bug

The description should make the bug reproducible:

- Version
- Steps

If possible, submit a minimal reproducing code fragment.

4.10.5 Owning an issue

- Whoever the issue is assigned to works next.
- If an issue needs someone else's work, assign it to them.

4.10.6 Status

- Submitted
- Accepted
- Underway
- Blocked

4.10.7 Resolutions

- Resolved
- Will Not Fix
- Not reproducible
- Not a bug (working as intended)

4.10.8 Bug triage

Some organisations use a severity matrix based on:

- Severity [Wrong answer, crash, unusable, workaround, cosmetic...]
- Frequency [All users, most users, some users...]

4.10.9 The backlog

The list of all the bugs that need to be fixed or features that have been requested is called the "backlog".

4.10.10 Development cycles

Development goes in cycles.

Cycles range in length from a week to three months. In a given cycle:

- Decide which features should be implemented
- Decide which bugs should be fixed
- Move these issues from the Backlog into the current cycle. (Aka Sprint)

4.10.11 GitHub issues

GitHub doesn't have separate fields for status, component, severity etc. Instead, it just has labels, which you can create and delete.

See for example Jupyter

In [1]:

Chapter 5

Construction

5.1 Construction

Software *design* gets a lot of press (Object orientation, UML, design patterns) In this session we're going to look at advice on software *construction* This lecture is available as an IPython Notebook

5.1.1 Construction vs Design

For a given piece of code, there exist several different ways one could write it:

- Choice of variable names
- Choice of comments
- Choice of layout

The consideration of these questions is the area of Software Construction.

5.1.2 Low-level design decisions

We will also look at some of the lower-level software design decisions in the context of this section:

- Division of code into subroutines
- Subroutine access signatures
- Choice of data structures for readability

5.1.3 Algorithms and structures

We will not, in this session, be looking at decisions as to how design questions impact performance:

- Choice of algorithms
- Choice of data structures for performance
- Choice of memory layout

We will consider these in a future session.

5.1.4 Architectural design

We will not, in this session, be looking at the large-scale questions of how program components interact, the stategic choices that govern how software behaves at the large scale:

• Where do objects get made?

- Which objects own or access other objects?
- How can I hide complexity in one part of the code from other parts of the code?

We will consider these in a future session.

5.1.5 Construction

So, we've excluded most of the exciting topics. What's left is the bricks and mortar of software: how letters and symbols are used to build code which is readable.

5.1.6 Literate programming

In literature, books are enjoyable for different reasons:

- The beauty of stories
- The beauty of plots
- The beauty of characters
- The beauty of paragraphs
- The beauty of sentences
- The beauty of words

Software has beauty at these levels too: stories and characters correspond to architecture and object design, plots corresponds to algorithms, but the rhythm of sentences and the choice of words corresponds to software construction.

5.1.7 Programming for humans

- Remember you're programming for humans as well as computers
- A program is the best, most rigourous way to describe an algorithm
- Code should be pleasant to read, a form of scholarly communication

Read CodeComplete

5.1.8 **Setup**

This notebook is based on a number of fragments of code, with an implicit context. We've made a library to set up the context so the examples work:

```
In [1]: %%writefile context.py
    from mock import Mock
    array=[]
    agt=[]
    ws=[]
    agents=[]
    counter=0
    x=Mock()
    y=None
    agent=Mock()
    value=0
    bird_types=["Starling", "Hawk"]
    import numpy as np
    from mock import Mock
```

```
average=np.mean
        hawk=Mock()
        starling=Mock()
        Mock.__sub__=Mock()
        sInput="2.0"
        input ="2.0"
        iOffset=1
        offset = 1
        anothervariable=1
        flag1=True
        variable=1
        flag2=False
        def do_something(): pass
        from mock import Mock
        Mock.__sub__=Mock()
        Mock.__abs__=Mock()
        chromosome=None
        start codon=None
        subsequence=Mock()
        transcribe=Mock()
        ribe=Mock()
        find=Mock()
        hawk=Mock()
        starling=Mock()
        can_see=Mock()
        my_name=""
        your_name=""
        flag1=False
        flag2=False
        start=0.0
        end=1.0
        step=0.1
        birds=[Mock()] *2
        resolution=100
        pi=3.141
        result= [0]*resolution
        import numpy as np
        import math
        data= [math.sin(y) for y in np.arange(0,pi,pi/resolution)]
        import yaml
        import os
Writing context.py
```

5.2 Coding Conventions

5.2.1 One code, many layouts:

Consider the following fragment of python:

```
In [1]: from context import *
```

```
ImportErrorTraceback (most recent call last)
        <ipython-input-1-5c72e5712007> in <module>()
    ---> 1 from context import *
        /home/travis/build/UCL/rsd-engineeringcourse/ch05construction/context.py in <module
    ----> 1 from mock import Mock
          2 array=[]
          3 agt=[]
          4 ws=[]
          5 agents=[]
        ImportError: No module named mock
In [2]: import species
        def AddToReaction(name, reaction):
            reaction.append(species.Species(name))
  this could also have been written:
In [3]: from species import Species
        def add_to_reaction(a_name,
                             a_reaction):
          l_species = Species(a_name)
          a_reaction.append( l_species )
5.2.2 So many choices
  • Layout
  • Naming

    Syntax choices

5.2.3 Layout
In [4]: reaction= {
            "reactants": ["H", "H", "O"],
            "products": ["H2O"]
In [5]: reaction2=(
          "reactants":
            "H",
            "Н",
            "O"
          ],
          "products":
```

"H20"

```
}
```

5.2.4 Layout choices

- Brace style
- Line length
- Indentation
- Whitespace/Tabs

5.2.5 Naming Conventions

5.2.6 Hungarian Notation

Prefix denotes *type*:

5.2.7 Newlines

- Newlines make code easier to read
- Newlines make less code fit on a screen

Use newlines to describe your code's rhythm

5.2.8 Syntax Choices

```
In [9]: anothervariable+=1
    if ((variable==anothervariable) and flag1 or flag2): do_something()
```

```
NameErrorTraceback (most recent call last)
        <ipython-input-9-3a5cade5ae03> in <module>()
    ----> 1 anothervariable+=1
          2 if ((variable==anothervariable) and flag1 or flag2): do_something()
        NameError: name 'anothervariable' is not defined
In [10]: anothervariable = anothervariable + 1
         variable_equality = (variable == anothervariable);
         if ((variable_equality and flag1) or flag2):
            do something()
        NameErrorTraceback (most recent call last)
        <ipython-input-10-effa6eeab38c> in <module>()
    ----> 1 anothervariable = anothervariable + 1
         2 variable_equality = (variable == anothervariable);
          3 if ((variable_equality and flag1) or flag2):
               do_something()
        NameError: name 'anothervariable' is not defined
```

5.2.9 Syntax choices

- Explicit operator precedence
- Compound expressions
- Package import choices

5.2.10 Coding Conventions

You should try to have an agreed policy for your team for these matters.

If your language sponsor has a standard policy, use that.

```
E.g. Python PEP8
E.g. Google's guide for R
E.g. Google's style guide for C++
```

5.2.11 Lint

There are automated tools which enforce coding conventions and check for common mistakes.

```
These are called linters
E.g. pip install pep8
```

```
bash: line 1: pep8: command not found
```

It is a good idea to run a linter before every commit, or include it in your CI tests.

5.3 Comments

5.3.1 Why comment?

- You're writing code for people, as well as computers.
- Comments can help you build code, by representing your design
- Comments explain subtleties in the code which are not obvious from the syntax
- Comments explain why you wrote the code the way you did

5.3.2 Bad Comments

"I write good code, you can tell by the number of comments." This is wrong.

5.3.3 Comments which are obvious

```
In [1]: from context import *
        ImportErrorTraceback (most recent call last)
        <ipython-input-1-5c72e5712007> in <module>()
    ---> 1 from context import *
        /home/travis/build/UCL/rsd-engineeringcourse/ch05construction/context.py in <module
    ----> 1 from mock import Mock
          2 array=[]
          3 agt=[]
          4 ws=[]
          5 agents=[]
        ImportError: No module named mock
In [2]: counter=counter+1 # Increment the counter
        for element in array: # Loop over elements
            pass
        NameErrorTraceback (most recent call last)
        <ipython-input-2-ff3c29d8ec10> in <module>()
    ---> 1 counter=counter+1 # Increment the counter
```

```
NameError: name 'counter' is not defined
5.3.4 Comments which could be replaced by better style
In [3]: for i in range(len(agt)): #for each agent
          agt[i].theta+=ws[i]
                                  # Increment the angle of each agent
                                  #by its angular velocity
          agt[i].x+=r*sin(agt[i].theta) #Move the agent by the step-size
          agt[i].y+=r*cos(agt[i].theta) #r in the direction indicated
        NameErrorTraceback (most recent call last)
        <ipython-input-3-ae976b13e6e4> in <module>()
    ----> 1 for i in range(len(agt)): #for each agent
          2 agt[i].theta+=ws[i]
                                      # Increment the angle of each agent
                                      #by its angular velocity
            agt[i].x+=r*sin(agt[i].theta) #Move the agent by the step-size
            agt[i].y+=r*cos(agt[i].theta) #r in the direction indicated
        NameError: name 'agt' is not defined
  Is good. But:
In [4]: for agent in agents:
          agent.turn()
          agent.move()
        class Agent (object):
           def turn(self):
                self.direction+=self.angular_velocity;
           def move(self):
               self.x+=Agent.step_length*sin(self.direction)
               self.y+=Agent.step_length*cos(self.direction)
        NameErrorTraceback (most recent call last)
        <ipython-input-4-88f1b92aa3da> in <module>()
    ----> 1 for agent in agents:
            agent.turn()
          3
             agent.move()
          5 class Agent (object):
```

2 for element in array: # Loop over elements

pass

```
NameError: name 'agents' is not defined
```

is probably better.

is OK.

5.3.5 Comments vs expressive code

The proper use of comments is to compensate for our failure to express yourself in code. Note that I used the word failure. I meant it. Comments are always failures.

- Robert Martin, Clean Code.

I wouldn't disagree, but still, writing "self-documenting" code is very hard, so do comment if you're unsure!

5.3.6 Comments which belong in an issue tracker

```
In [5]: x.clear() # Code crashes here sometimes
        class Agent (object):
            pass
            # TODO: Implement pretty-printer method
        NameErrorTraceback (most recent call last)
        <ipython-input-5-9535676f4e95> in <module>()
    ----> 1 x.clear() # Code crashes here sometimes
          2 class Agent (object):
          3
                pass
                # TODO: Implement pretty-printer method
        NameError: name 'x' is not defined
  BUT comments that reference issues in the tracker can be good.
In [6]: if x.safe_to_clear(): # Guard added as temporary workaround for #32
           x.clear()
        NameErrorTraceback (most recent call last)
        <ipython-input-6-4e78b63ee55f> in <module>()
    ----> 1 if x.safe_to_clear(): # Guard added as temporary workaround for #32
         2 x.clear()
        NameError: name 'x' is not defined
```

5.3.7 Comments which only make sense to the author today

5.3.8 Comments which are unpublishable

5.3.9 Good commenting: pedagogical comments

Code that is good style, but you're not familiar with, or that colleagues might not be familiar with

```
In [9]: # This is how you define a decorator in python
    def double(decorated_function):
        # Here, the result function forms a closure over
        # the decorated function
        def result_function(input):
            return decorated_function(decorated_function(input))
        # The returned result is a function
        return result_function

@double
def try_me_twice():
        pass
```

5.3.10 Good commenting: reasons and definitions

Comments which explain coding definitions or reasons for programming choices.

5.4 Refactoring

5.4.1 Refactoring

To refactor is to:

- Make a change to the design of some software
- Which improves the structure or readability
- But which leaves the actual behaviour of the program completely unchanged.

5.4.2 A word from the Master

Refactoring is a controlled technique for improving the design of an existing code base. Its essence is applying a series of small behavior-preserving transformations, each of which "too small to be worth doing". However the cumulative effect of each of these transformations is quite significant. By doing them in small steps you reduce the risk of introducing errors. You also avoid having the system broken while you are carrying out the restructuring - which allows you to gradually refactor a system over an extended period of time.

Martin Fowler

5.4.3 List of known refactorings

The next few sections will present some known refactorings

We'll show before and after code, present any new coding techniques needed to do the refactoring, and describe *code smells*: how you know you need to refactor.

5.4.4 Replace magic numbers with constants

Smell: Raw numbers appear in your code Before:

for i in range (100):

for j in range(i+1, 100):

result[j] += data[i] * data[i-j] / 100

```
NameErrorTraceback (most recent call last)
        <ipython-input-2-6072360c557d> in <module>()
    ---> 1 data= [math.sin(x) for x in np.arange(0,3.141,3.141/100)]
          2 result= [0] *100
          3 for i in range (100):
                for j in range(i+1, 100):
                    result[j] += data[i] * data[i-j] / 100
        NameError: name 'np' is not defined
  after:
In [3]: resolution=100
        pi=3.141
        data= [math.sin(x) for x in np.arange(0,pi,pi/resolution)]
        result= [0] * resolution
        for i in range(resolution):
            for j in range(i + 1, resolution):
                result[j] += data[i] * data[i-j] / resolution
        NameErrorTraceback (most recent call last)
        <ipython-input-3-60a4b84d3b9b> in <module>()
          1 resolution=100
          2 pi=3.141
    ---> 3 data= [math.sin(x) for x in np.arange(0,pi,pi/resolution)]
          4 result= [0]*resolution
          5 for i in range (resolution):
        NameError: name 'np' is not defined
5.4.5 Replace repeated code with a function
Smell: Fragments of repeated code appear
  Before:
In [4]: if abs(hawk.facing-starling.facing) < hawk.viewport:</pre>
            hawk.hunting()
        if abs(starling.facing-hawk.facing)<starling.viewport:</pre>
            starling.flee()
```

```
NameErrorTraceback (most recent call last)
        <ipython-input-4-20296c1d98b5> in <module>()
    ----> 1 if abs(hawk.facing-starling.facing)<hawk.viewport:
                hawk.hunting()
          4 if abs(starling.facing-hawk.facing)<starling.viewport:
                starling.flee()
        NameError: name 'hawk' is not defined
  After:
In [5]: def can_see(source, target):
            return (source.facing-target.facing) < source.viewport</pre>
        if can_see(hawk, starling):
            hawk.hunting()
        if can_see(starling, hawk):
            starling.flee()
        NameErrorTraceback (most recent call last)
        <ipython-input-5-916d574fa707> in <module>()
                return (source.facing-target.facing) < source.viewport
          3
    ----> 4 if can_see(hawk, starling):
          5
               hawk.hunting()
          6
        NameError: name 'hawk' is not defined
```

5.4.6 Change of variable name

Smell: Code needs a comment to explain what it is for Before:

```
In [6]: z=find(x,y)
    if z:
        ribe(x)

NameErrorTraceback (most recent call last)
```

```
<ipython-input-6-1c1f4e45be04> in <module>()
    ---> 1 z=find(x,y)
          2 if z:
          3
                ribe(x)
        NameError: name 'find' is not defined
  After:
In [7]: gene = subsequence(chromosome, start_codon)
        if gene:
            transcribe(gene)
        NameErrorTraceback (most recent call last)
        <ipython-input-7-51cf56d26aee> in <module>()
    ----> 1 gene = subsequence(chromosome, start_codon)
          2 if gene:
          3
               transcribe(gene)
        NameError: name 'subsequence' is not defined
5.4.7 Separate a complex expression into a local variable
```

Smell: An expression becomes long

```
NameErrorTraceback (most recent call last)

<ipython-input-9-d5cc1290bffa> in <module>()
----> 1 same_names= (my_name==your_name)
        2 flags_OK=flag1 or flag2
        3 if same_names and flags_OK: do_something()

NameError: name 'my_name' is not defined
```

5.4.8 Replace loop with iterator

Smell: Loop variable is an integer from 1 to something Before:

```
In [10]: sum=0
         for i in range(resolution):
             sum+=data[i]
        NameErrorTraceback (most recent call last)
        <ipython-input-10-a9a14e677ac8> in <module>()
          1 \text{ sum}=0
          2 for i in range (resolution):
              sum+=data[i]
    ---> 3
        NameError: name 'data' is not defined
  After:
In [11]: sum=0
         for value in data:
             sum+=value
        NameErrorTraceback (most recent call last)
        <ipython-input-11-b267c3b4dd44> in <module>()
         1 sum=0
    ---> 2 for value in data:
          3
               sum+=value
        NameError: name 'data' is not defined
```

5.4.9 Replace hand-written code with library code

Smell: It feels like surely someone else must have done this at some point Before:

5.4.10 Replace set of arrays with array of structures

Smell: A function needs to work corresponding indices of several arrays: Before:

Warning: this refactoring greatly improves readability but can make code slower, depending on memory layout. Be careful.

5.4.11 Replace constants with a configuration file

Smell: You need to change your code file to explore different research scenarios Before:

```
In [16]: flight_speed=2.0 # mph
         bounds=[0,0,100,100]
         turning_circle=3.0 # m
         bird_counts= {"hawk": 5, "starling": 500}
  After:
In [17]: %%writefile config.yaml
         bounds: [0,0,100,100]
         counts:
             hawk: 5
             starling: 500
         speed: 2.0
         turning_circle: 3.0
Writing config.yaml
In [18]: config=yaml.load(open("config.yaml"))
        NameErrorTraceback (most recent call last)
        <ipython-input-18-3954c9087a04> in <module>()
    ---> 1 config=yaml.load(open("config.yaml"))
        NameError: name 'yaml' is not defined
```

See YAML and PyYaml and Python OS

5.4.12 Replace global variables with function arguments

Smell: A global variable is assigned and then used inside a called function:

```
In [19]: viewport=pi/4
    if hawk.can_see(starling):
        hawk.hunt(starling)

class Hawk(object):
    def can_see(self,target):
        return (self.facing-target.facing) < viewport

NameErrorTraceback (most recent call last)</pre>
```

```
<ipython-input-19-95713c91a097> in <module>()
          1 viewport=pi/4
    ----> 2 if hawk.can_see(starling):
               hawk.hunt(starling)
          3
          5 class Hawk (object):
        NameError: name 'hawk' is not defined
  Becomes:
In [20]: viewport=pi/4
         if hawk.can_see(starling, viewport):
             hawk.hunt(starling)
         class Hawk (object):
             def can_see(self, target, viewport):
                 return (self.facing-target.facing) < viewport</pre>
        NameErrorTraceback (most recent call last)
        <ipython-input-20-2c352b33e3b6> in <module>()
          1 viewport=pi/4
    ----> 2 if hawk.can_see(starling, viewport):
          3
               hawk.hunt(starling)
          5 class Hawk (object):
        NameError: name 'hawk' is not defined
```

5.4.13 Merge neighbouring loops

Smell: Two neighbouring loops have the same for statement

```
3
4 for bird in birds:
5    bird.lay_eggs()

NameError: name 'birds' is not defined

Becomes:

In [22]: for bird in birds:
    bird.build_nest()
    bird.lay_eggs()

NameErrorTraceback (most recent call last)

<ipython-input-22-663360464b37> in <module>()
----> 1 for bird in birds:
    2    bird.build_nest()
    3    bird.lay_eggs()

NameError: name 'birds' is not defined
```

5.4.14 Break a large function into smaller units

Smell: A function or subroutine no longer fits on a page in your editor Smell: A line of code is indented more than three levels Smell: A piece of code interacts with the surrounding code through just a few variables Before:

```
In [23]: def do_calculation():
             for predator in predators:
                 for prey in preys:
                      if predator.can_see(prey):
                         predator.hunt(prey)
                      if predator.can_reach(prey):
                          predator.eat (prey)
  After:
In [24]: def do_calculation():
             for predator in predators:
                 for prey in preys:
                     predate(predator, prey)
         def predate(predator, prey):
             if predator.can_see(prey):
                 predator.hunt(prey)
             if predator.can_reach(prey):
                 predator.eat (prey)
```

5.4.15 Separate code concepts into files or modules

Smell: You find it hard to locate a piece of code Smell: You get a lot of version control conflicts

5.4.16 Refactoring is a safe way to improve code

You may think you can see how to rewrite a whole codebase to be better

However, you may well get lost halfway through the exercise.

By making the changes as small, reversible, incremental steps, you can reach your target design more reliably.

5.4.17 Tests and Refactoring

Badly structured code cannot be unit tested. There are no "units".

Before refactoring, ensure you have a robust regression test.

This will allow you to Refactor with confidence

As you refactor, if you create any new units (functions, modules, classes), add new tests for them.

5.4.18 Refactoring Summary

- Replace magic numbers with constants
- Replace repeated code with a function
- Change of variable/function/class name
- Replace loop with iterator
- Replace hand-written code with library code
- Replace set of arrays with array of structures
- Replace constants with a configuration file
- Replace global variables with function arguments
- Break a large function into smaller units
- Separate code concepts into files or modules

And many more

Read The Refactoring Book

Chapter 6

Design

6.1 Object-Oriented Design

In this session, we will finally discuss the thing most people think of when they refer to "Software Engineering": the deliberate *design* of software. We will discuss processes and methodologies for planned development of large-scale software projects: *Software Architecture*.

The software engineering community has, in large part, focused on an object-oriented approach to the design and development of large scale software systems. The basic concepts of object orientation are necessary to follow much of the software engineering conversation.

6.1.1 Design processes

In addition to object-oriented architecture, software engineers have focused on the development of processes for robust, reliable software development. These codified ways of working hope to enable organisations to repeatably and reliably complete complex software projects in a way that minimises both development and maintainance costs, and meets user requirements.

6.1.2 Design and research

Software engineering theory has largely been developed in the context of commercial software companies. The extent to which the practices and processes developed for commercial software are applicable in a research context is itself an active area of research.

6.2 Recap of Object-Orientation

6.2.1 Classes: User defined types

```
In [1]: class Person(object):
    def __init__(self,name,age):
        self.name=name
        self.age=age
    def grow_up(self):
        self.age+=1

    james=Person("James",37)
    james.home="London"
```

6.2.2 Declaring a class

Class: A user-defined type

```
In [2]: class MyClass(object):
     pass
```

6.2.3 Object instances

Instance: A particular object instantiated from a class.

```
In [3]: my_object = MyClass()
```

6.2.4 Method

Method: A function which is "built in" to a class

```
In [4]: from context import *
        ImportErrorTraceback (most recent call last)
        <ipython-input-4-5c72e5712007> in <module>()
    ----> 1 from context import *
        /home/travis/build/UCL/rsd-engineeringcourse/ch05construction/context.py in <module
    ----> 1 from mock import Mock
          2 array=[]
          3 agt=[]
          4 ws=[]
          5 agents=[]
        ImportError: No module named mock
In [5]: class MyClass(object):
            def someMethod(self, argument):
                pass
        my_object=MyClass()
        my_object.someMethod(value)
        NameErrorTraceback (most recent call last)
        <ipython-input-5-e72d837778ff> in <module>()
          5 my_object=MyClass()
```

---> 6 my_object.someMethod(value)

```
NameError: name 'value' is not defined
```

6.2.5 Constructor

Constructor: A special method called when instantiating a new object

6.2.6 Member Variable

Member variable: a value stored inside an instance of a class.

6.3 Object refactorings

6.3.1 Replace add-hoc structure with user defined classes

Smell: A data structure made of nested arrays and dictionaries becomes unwieldy Before:

```
NameErrorTraceback (most recent call last)
        <ipython-input-8-e200ad58da32> in <module>()
          2 birds = [{"position": random(),
                      "velocity": random(),
    ---> 4
                      "type": kind} for kind in bird_types]
          6 average_position = average([bird["position"] for bird in birds])
        NameError: name 'bird_types' is not defined
  After:
In [9]: class Bird(object):
            def init (self, type):
                from random import random
                self.type = type
                self.position = random()
                self.velocity = random()
        birds = [Bird(type) for type in bird_types]
        average_position = average([bird.position for bird in birds])
        NameErrorTraceback (most recent call last)
        <ipython-input-9-598a6cc8751f> in <module>()
                   self.velocity = random()
    ----> 8 birds = [Bird(type) for type in bird_types]
          9 average_position = average([bird.position for bird in birds])
        NameError: name 'bird_types' is not defined
```

6.3.2 Replace function with a method

Smell: A function is always called with the same kind of thing Before:

```
NameErrorTraceback (most recent call last)
        <ipython-input-10-2b1bfb37897c> in <module>()
                return (source.facing-target.facing) < source.viewport
          3
    ----> 4 if can_see(hawk, starling):
               hawk.hunt()
        NameError: name 'hawk' is not defined
  After:
In [11]: class Bird(object):
             def can_see(self, target):
                 return (self.facing-target.facing) < self.viewport</pre>
         if hawk.can_see(starling):
             hawk.hunt()
        NameErrorTraceback (most recent call last)
        <ipython-input-11-a10ba1572ef2> in <module>()
          3
                    return (self.facing-target.facing) < self.viewport
    ----> 5 if hawk.can_see(starling):
                hawk.hunt()
        NameError: name 'hawk' is not defined
```

6.3.3 Replace method arguments with class members

Smell: A variable is nearly always used in arguments to a class.

6.3.4 Replace global variable with class and member

Smell: A global variable is referenced by a few functions

```
In [14]: name="James"
         birthday=[19,10,76]
         today=[29,10]
         if today==birthday[0:2]:
             print "Happy Birthday, ", name
         else:
             print "No birthday for you today."
No birthday for you today.
In [15]: class Person(object):
             def __init__(self, birthday, name):
                 self.birth_day=birthday[0]
                 self.birth_month=birthday[1]
                 self.birth_year=birthday[2]
                 self.name=name
             def check_birthday(self, today_day, today_month):
                 if not self.birth_day == today_day:
                     return False
                 if not self.birth_month == today_month:
                     return False
                 return True
             def greet_appropriately(self, today):
                 if self.check_birthday(*today):
                     print "Happy Birthday", self.name
                 else:
                     print "No birthday for you."
         james=Person([19, 10, 76], "James")
         james.greet_appropriately([29,10])
No birthday for you.
```

6.3.5 Object Oriented Refactoring Summary

- Replace ad-hoc structure with a class
- Replace function with a method
- Replace method argument with class member
- Replace global variable with class data

6.4 Class design

The concepts we have introduced are common between different object oriented languages. Thus, when we design our program using these concepts, we can think at an architectural level, independent of language syntax.

```
In [1]: class Particle(object):
    def __init__(self, position, velocity):
        self.position=position
```

6.4.1 UML

UML is a conventional diagrammatic notation used to describe "class structures" and other higher level aspects of software design.

Computer scientists get worked up about formal correctness of UML diagrams and learning the conventions precisely. Working programmers can still benefit from using UML to describe their designs.

6.4.2 YUML

We can see a YUML model for a Particle class with position and velocity data and a move () method using the YUML online UML drawing tool.

http://yuml.me/diagram/boring/class/[Particle|position;velocity|move%28%29

Here's how we can use Python code to get an image back from YUML:

```
In [2]: import requests
    import IPython

def yuml(model):
        result=requests.get("http://yuml.me/diagram/boring/class/"+model)
        return IPython.core.display.Image(result.content)

ImportErrorTraceback (most recent call last)

<ipython-input-2-7898472b6edf> in <module>()
----> 1 import requests
        2 import IPython
        3
        4 def yuml(model):
        5 result=requests.get("http://yuml.me/diagram/boring/class/"+model)

ImportError: No module named requests
```

```
In [3]: yuml("[Particle|position;velocity|move()]")

        NameErrorTraceback (most recent call last)

        <ipython-input-3-e7a403e069ec> in <module>()
----> 1 yuml("[Particle|position;velocity|move()]")

        NameError: name 'yuml' is not defined
```

6.4.3 Information Hiding

Sometimes, our design for a program would be broken if users start messing around with variables we don't want them to change.

Robust class design requires consideration of which subroutines are intended for users to use, and which are internal. Languages provide features to implement this: access control.

In python, we use leading underscores to control whether member variables and methods can be accessed from outside the class.

```
In [4]: class MyClass(object):
            def __init__(self):
                self.__private_data=0
                self._private_data=0
                self.public_data=0
            def __private_method(self): pass
            def _private_method(self): pass
            def public_method(self): pass
            def called_inside(self):
                self.__private_method()
                self._private_method()
                self.__private_data=1
                self._private_data=1
        MyClass().called_inside()
        MyClass()._private_method() # Works, but forbidden by convention
        MyClass().public_method() # OK
        print MyClass()._private_data
        print MyClass().public_data
0
0
In [5]: MyClass().__private_method() # Generates error
```

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```
AttributeErrorTraceback (most recent call last)

<ipython-input-5-f273bcb10b88> in <module>()
----> 1 MyClass().__private_method() # Generates error

AttributeError: 'MyClass' object has no attribute '__private_method'

In [6]: print MyClass().__private_data # Generates error

AttributeErrorTraceback (most recent call last)

<ipython-input-6-9da94df448bc> in <module>()
----> 1 print MyClass().__private_data # Generates error

AttributeError: 'MyClass' object has no attribute '__private_data'
```

6.4.4 Property accessors

Python provides a mechanism to make functions appear to be variables. This can be used if you want to change the way a class is implemented without changing the interface:

Note that the code behaves the same way to the outside user. The implementation detail is hidden by private variables. In languages without this feature, such as C++, it is best to always make data private, and always access data through functions:

```
In [9]: class Person(object):
    def __init__(self):
        self._name = "James Hetherington"
    def name(self):
        return self._name
```

```
assert (Person().name() == "James Hetherington")
```

But in Python this is unnecessary.

6.4.5 Class Members

Class, or static members, belong to the class as a whole, and are shared between instances.

6.5 Inheritance and Polymorphism

6.5.1 Object-based vs Object-Oriented

So far we have seen only object-based programming, not object-oriented programming. Using Objects doesn't mean your code is object-oriented.

To understand object-oriented programming, we need to introduce **polymorphism** and **inheritance**.

6.5.2 Inheritance

- Inheritance allows related classes to share code
- Inheritance allows a program to reflect the *ontology* of kinds of thing in a program.

6.5.3 Ontology and inheritance

- A bird is a kind of animal
- An eagle is a kind of bird
- A starling is also a kind of bird
- All animals can be born and die
- Only birds can fly (Ish.)
- Only eagles hunt
- Only starlings flock

6.5.4 Inheritance in python

6.5.5 Inheritance terminology

- A derived class derives from a base class
- A subclass inherits from a superclass

(These are different terms for the same thing.)

- Eagle is a subclass of the Animal superclass.
- Animal is the base class of the Eagle derived class

6.5.6 Inheritance and constructors

6.5.7 Inheritance UML diagrams

UML shows inheritance with an open triangular arrow pointing from subclass to superclass.

6.5.8 Aggregation vs Inheritance

If one object *has* or *owns* one or more objects, this is *not* inheritance.

For example, in my solution to the Boids task from last week, the overal Model owned several Boids, and each Boid owned two 2-vectors, one for position and one for velocity.

6.5.9 Aggregation in UML

The Boids situation can be represented thus:

The open diamond indicates **Aggregation**, the closed diamond **composition**. (A given boid might belong to multiple models, a given position vector is forever part of the corresponding Boid.)

The asterisk represents cardinality, a model may contain multiple Boids.

6.5.10 Refactoring to inheritance

Smell: Repeated code between two classes which are both ontologically subtypes of something Before:

```
In [15]: class Person(object):
             def __init__(self, age, job):
                 self.age = age
                 self.job = job
             def birthday(self):
                 self.age += 1
         class Pet (object):
             def __init__(self, age, owner):
                 self.age = age
                 self.owner = owner
             def birthday(self):
                 self.age += 1
  After:
In [16]: class Animal(object):
             def __init__(self, age):
                 self.age = age
             def birthday(self):
                 self.age += 1
         class Person(Animal):
```

```
def __init__(self, age, job):
    self.job = job
    super(Person, self).__init__(age)
```

6.5.11 Polymorphism

```
In [17]: class Dog(object):
             def noise(self):
                 return "Bark"
         class Cat (object):
             def noise(self):
                 return "Miaow"
         class Pig(object):
             def noise(self): return "Oink"
         class Cow(object):
             def noise(self): return "Moo"
         animals=[Dog(), Dog(), Cat(), Pig(), Cow(), Cat()]
         for animal in animals:
             print animal.noise()
Bark
Bark
Miaow
Oink
Moo
Miaow
```

This will print "Bark Bark Miaow Oink Moo Miaow"

If two classes support the same method, but it does different things for the two classes, then if an object is of an unknown class, calling the method will invoke the version for whatever class the instance is an instance of.

6.5.12 Polymorphism and Inheritance

Often, polymorphism uses multiple derived classes with a common base class. However, duck typing in Python means that all that is required is that the types support a common **Concept** (Such as iterable, or container, or, in this case, the Noisy concept.)

A common base class is used where there is a likely **default** that you want several of the derived classes to have.

pass

6.5.13 Undefined Functions and Polymorphism

In the above example, we put in a dummy noise for Animals that don't know what type they are.

Instead, we can explicitly deliberately leave this undefined, and we get a crash if we access an undefined method.

6.5.14 Refactoring to Polymorphism

Smell: a function uses a big set of if statements or a case statement to decide what to do: Before:

```
In [21]: class Animal(object):
    def __init__(self,type):
        self.type=type

def noise(self):
    if self.type=="Dog":
        return "Bark"
    elif self.type=="Cat":
        return "Miaow"
    elif self.type=="Cow":
        return "Moo"
```

which is better replaced by the code above.

6.5.15 Interfaces and concepts

In C++, it is common to define classes which declare dummy methods, called "virtual" methods, which specify the methods which derived classes must implement. Classes which define these methods, which cannot be instantiated into actual objects, are called "abstract base" classes or "interfaces".

Python's Duck Typing approach means explicitly declaring these is unnesssary: any class concept which implements appropriately named methods will do. These as user-defined **concepts**, just as "iterable" or "container" are built-in Python concepts. A class is said to "implement and interface" or "satisfy a concept".

6.5.16 Interfaces in UML

Interfaces implementation in UML is indicated thus:

6.5.17 Further UML

UML is a much larger diagram language than the aspects we've shown here.

- Message sequence charts show signals passing back and forth between objects (Web Sequence Diagrams)
- Entity Relationship Diagrams can be used to show more general relationships between things in a system

6.6 Patterns

6.6.1 Class Complexity

We've seen that using object orientation can produce quite complex class structures, with classes owning each other, instantiating each other, and inheriting from each other.

There are lots of different ways to design things, and decisions to make.

Should I inherit from this class, or own it as a member variable? ("is a" vs "has a")

6.6.2 Design Patterns

Programmers have noticed that there are certain ways of arranging classes that work better than others. These are called "design patterns".

They were first collected on one of the world's first Wikis, as the Portland Pattern Repository

6.6.3 Reading a pattern

A description of a pattern in a book such as the Gang Of Four book usually includes:

- Intent
- Motivation
- Applicability
- Structure
- Participants
- Collaborations
- Consequences
- Implementation
- Sample Code

6.6.4 Introducing Some Patterns

There are lots and lots of design patterns, and it's a great literature to get into to read about design questions in programming and learn from other people's experience.

We'll just show a few in this session:

- Factory Method
- Builder
- Handle-Body
- Strategy

6.7 Factory Pattern

6.7.1 Factory Pattern

Here's what the Gang of Four Book says about Factory Method:

Intent: Define an interface for creating an object, but let subclasses decide which class to instantiate. Factory Method lets a class defer instantiation to subclasses.

Applicability: Use the Factory method pattern when:

- A class can't anticipate the class of objects it must create
- A class wants its subclasses to specify the objects it creates

This is pretty hard to understand, so let's look at an example.

6.7.2 Factory UML

```
In [1]: import requests
    import IPython

def yuml(model):
        result=requests.get("http://yuml.me/diagram/boring/class/"+model)
        return IPython.core.display.Image(result.content)

ImportErrorTraceback (most recent call last)
        <ipython-input-1-7898472b6edf> in <module>()
```

```
---> 1 import requests
          2 import IPython
          4 def yuml(model):
                result=requests.get("http://yuml.me/diagram/boring/class/"+model)
        ImportError: No module named requests
In [2]: yuml("[Product]^-[ConcreteProduct], "+
             "[Creator| (v) FactoryMethod()]^-[ConcreteCreator| FactoryMethod()], "+
             "[ConcreteCreator] - . -> [ConcreteProduct]")
        NameErrorTraceback (most recent call last)
        <ipython-input-2-615977b6c146> in <module>()
    ----> 1 yuml("[Product]^-[ConcreteProduct], "+
          2
                 "[Creator| (v) FactoryMethod()]^-[ConcreteCreator| FactoryMethod()], "+
          3
                 "[ConcreteCreator] - . -> [ConcreteProduct] ")
        NameError: name 'yuml' is not defined
```

6.7.3 Factory Example

An "agent based model" is one like the Boids model from last week: agents act and interact under certain rules. Complex phenomena can be described by simple agent behaviours.

6.7.4 Agent model constructor

This logic is common to many kinds of Agent based model, so we can imagine a common class for agent based models: the constructor could parse a configuration specifying how many agents of each type to create, their initial conditions and so on.

However, this common constructor doesn't know what kind of agent to create; as a common base, it could be a model of boids, or the agents could be remote agents on foreign servers, or they could even be physical hardware robots connected to the driving model over Wifi!

We need to defer the construction of the agents. We can do this with polymorphism: each derived class of the ABM can have an appropriate method to create its agents:

```
In [4]: class AgentModel(object):
    def __init__(self, config):
        self.agents=[]
    for agent_config in config:
        self.agents.append(self.create(**agent_config))
```

This is the *factory method* pattern: a common design solution to the need to defer the construction of daughter objects to a derived class.

6.7.5 Agent derived classes

The type that is created is different in the different derived classes:

Agents are the base product, boids or robots are a ConcreteProduct.

```
In [6]: class WebAgentFactory(AgentModel):
    def __init__(self, url):
        self.url=url
        self.connection=AmazonCompute.connect(url)
        AgentModel.__init__(self)
    def create(self, agent_config):
        return OnlineAgent(agent_config, self.connection)
```

There is no need to define an explicit base interface for the "Agent" concept in Python: anything that responds to "simulate" and "interact" methods will do: this is our Agent concept.

6.7.6 Refactoring to Patterns

I personally have got into a terrible tangle trying to make base classes which somehow "promote" themselves into a derived class based on some code in the base class.

This is an example of an "Antipattern": like a Smell, this is a recognised Wrong Way of doing things. What I should have written was a Creator with a FactoryMethod. Consider the following code:

```
In [7]: class AgentModel(object):
          def simulate(self):
            for agent in agents:
              for target in agents:
                agent.interact(target)
              agent.simulate()
        class BirdModel(AgentModel):
          def init (self, config):
            self.boids=[]
            for boid_config in config:
                self.boids.append(Boid(**boid_config))
        class WebAgentFactory(AgentModel):
          def __init__(self, url, config):
            self.url=url
            connection=AmazonCompute.connect(url)
            AgentModel.__init__(self)
            self.web_agents=[]
            for agent config in config:
              self.web_agents.append(OnlineAgent(agent_config, connection))
```

The agent creation loop is almost identical in the two classes; so we can be sure we need to refactor it away; but the **type** that is created is different in the two cases, so this is the smell that we need a factory pattern.

6.8 Builder

6.8.1 Builder Pattern

Intent: Separate the steps for constructing a complex object from its final representation.

6.8.2 Builder example

Let's continue our Agent Based modelling example.

There's a lot more to defining a model than just adding agents of different kinds: we need to define boundary conditions, specify wind speed or light conditions.

We could define all of this for an imagined advanced Model with a very very long constructor, with lots of optional arguments:

6.8.3 Builder preferred to complex constructor

However, long constructors easily become very complicated. Instead, it can be cleaner to define a Builder for models. A builder is like a deferred factory: each step of the construction process is implemented as an individual method call, and the completed object is returned when the model is ready.

```
In [11]: Model=Mock() # Create a temporary mock so the example works!
        NameErrorTraceback (most recent call last)
        <ipython-input-11-93f12523ddf9> in <module>()
    ---> 1 Model=Mock() # Create a temporary mock so the example works!
        NameError: name 'Mock' is not defined
In [12]: class ModelBuilder(object):
             def start_model(self):
                 self.model=Model()
                 self.model.xlim = None
                 self.model.ylim = None
             def set_bounds(self, xlim, ylim):
                 self.model.xlim=xlim
                 self.model.ylim=ylim
             def add_agent(self, xpos, ypos):
                 pass # Implementation here
             def finish(self):
                 self.validate()
                 return self.model
             def validate(self):
                 assert(self.model.xlim is not None)
                 # Check that the all the
                 # parameters that need to be set
                 # have indeed been set.
```

Inheritance of an Abstract Builder for multiple concrete builders could be used where there might be multiple ways to build models with the same set of calls to the builder: for example a version of the model builder yielding models which can be executed in parallel on a remote cluster.

6.8.4 Using a builder

```
model=builder.finish()
    model.simulate()
   TypeErrorTraceback (most recent call last)
    <ipython-input-13-d948c830f77a> in <module>()
     1 builder=ModelBuilder()
----> 2 builder.start_model()
     4 builder.set_bounds(500, 500)
     5 builder.add_agent(40, 40)
    <ipython-input-12-88795908ff65> in start_model(self)
     1 class ModelBuilder(object):
     2 def start_model(self):
---> 3
              self.model=Model()
              self.model.xlim = None
     4
              self.model.ylim = None
   TypeError: __init__() takes exactly 7 arguments (1 given)
```

6.8.5 Avoid staged construction without a builder.

We could, of course, just add all the building methods to the model itself, rather than having the model be yielded from a separate builder.

This is an antipattern that is often seen: a class whose __init__ constructor alone is insufficient for it to be ready to use. A series of methods must be called, in the right order, in order for it to be ready to use.

This results in very fragile code: its hard to keep track of whether an object instance is "ready" or not. Use the builder pattern to keep deferred construction in control.

We might ask why we couldn't just use a validator in all of the methods that must follow the deferred constructors; to check they have been called. But we'd need to put these in *every* method of the class, whereas with a builder, we can validate only in the finish method.

```
In [14]: %matplotlib inline
```

```
2159
   2160
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
   2077
                        kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
   2078
                    with self.builtin trap:
-> 2079
                        result = fn(*args,**kwargs)
   2080
                    return result
   2081
    <decorator-gen-104> in matplotlib(self, line)
    /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
            # but it's overkill for just that one bit of state.
   186
   187
            def magic deco(arg):
--> 188
                call = lambda f, \stara, \star \stark: f(\stara, \star \stark)
    189
   190
                if callable (arg):
    /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/pylab.pyc in ma-
                    print("Available matplotlib backends: %s" % backends_list)
    98
    99
                else:
--> 100
                    gui, backend = self.shell.enable_matplotlib(args.gui)
    101
                    self._show_matplotlib_backend(args.gui, backend)
   102
    /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
   2933
  2934
                from IPython.core import pylabtools as pt
-> 2935
                qui, backend = pt.find_qui_and_backend(qui, self.pylab_qui_select)
  2936
   2937
                if qui != 'inline':
    /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/pylabtools.pyc in find
   257
   258
--> 259
            import matplotlib
    260
            if qui and qui != 'auto':
    261
```

ImportError: No module named matplotlib

6.9 Strategy Pattern

Define a family of algorithms, encapsulate each one, and make them interchangeable. Strategy lets the algorithm vary independently from clients that use it.

6.9.1 Strategy pattern example: sunspots

```
In [15]: from numpy import linspace, exp, log, sqrt, array
         import math
         from scipy.interpolate import UnivariateSpline
         from scipy.signal import lombscargle
         from scipy.integrate import cumtrapz
         from numpy.fft import rfft,fft,fftfreq
         import csv
         from StringIO import StringIO
         from datetime import datetime
         import requests
         import matplotlib.pyplot as plt
         %matplotlib inline
        ImportErrorTraceback (most recent call last)
        <ipython-input-15-0cfc82b090e7> in <module>()
    ----> 1 from numpy import linspace, exp, log, sqrt, array
          2 import math
          3 from scipy.interpolate import UnivariateSpline
          4 from scipy.signal import lombscargle
          5 from scipy.integrate import cumtrapz
        ImportError: No module named numpy
  Consider the sequence of sunspot observations:
In [16]: def load_sunspots():
              url_base="http://www.quandl.com/api/v1/datasets/SIDC/SUNSPOTS_A.csv"
              x=requests.get(url_base,params={'trim_start':'1700-12-31',
                                                  'trim_end':'2014-01-01',
                                                  'sort_order':'asc'})
              data=csv.reader(StringIO(x.text)) #Convert requests result to look
                                                 #like a file buffer before
                                                 # reading with CSV
              data.next() # Skip header row
              return [float(row[1]) for row in data]
In [17]: spots=load_sunspots()
         plt.plot(spots)
```

6.9.2 Sunspot cycle has periodicity

```
In [18]: spectrum=rfft(spots)
    plt.figure()
    plt.plot(abs(spectrum))
    plt.savefig('fixed.png')

    NameErrorTraceback (most recent call last)

    <ipython-input-18-34013178b9ac> in <module>()
----> 1 spectrum=rfft(spots)
    2
    3 plt.figure()
    4 plt.plot(abs(spectrum))
    5 plt.savefig('fixed.png')

NameError: name 'rfft' is not defined
```

6.9.3 Years are not constant length

There's a potential problem with this analysis however:

- Years are not constant length
- Leap years exist
- But, the Fast Fourier Transform assumes evenly spaced intervals

6.9.4 Strategy Pattern for Algorithms

6.9.5 Uneven time series

The Fast Fourier Transform cannot be applied to uneven time series.

We could:

- Ignore this problem, and assume the effect is small
- Interpolate and resample to even times
- Use a method which is robust to unevenly sampled series, such as LSSA

We also want to find the period of the strongest periodic signal in the data, there are various different methods we could use for this also, such as integrating the fourier series by quadrature to find the mean frequency, or choosing the largest single value.

6.9.6 Too many classes!

We could implement a base class for our common code between the different approaches, and define derived classes for each different algorithmic approach. However, this has drawbacks:

- The constructors for each derived class will need arguments for all the numerical method's control parameters, such as the degree of spline for the interpolation method, the order of quadrature for integrators, and so on.
- Where we have multiple algorithmic choices to make (interpolator, periodogram, peak finder...) the number of derived classes would explode: class SunspotAnalyzerSplineFFTTrapeziumNearMode is a bit unweildy.
- The algorithmic choices are not then available for other projects
- This design doesn't fit with a clean Ontology of "kinds of things": there's no Abstract Base for spectrogram generators...

6.9.7 Apply the strategy pattern:

- We implement each algorithm for generating a spectrum as its own Strategy class.
- They all implement a common interface
- · Arguments to strategy constructor specify parameters of algorithms, such as spline degree
- One strategy instance for each algorithm is passed to the constructor for the overall analysis

First, we'll define a helper class for our time series.

```
In [19]: class Series(object):
    """Enhance NumPy N-d array with some helper functions for clarity"""
    def __init__(self, data):
        self.data=array(data)
        self.count=self.data.shape[0]
        self.start=self.data[0,0]
        self.end=self.data[-1,0]
        self.range=self.end-self.start
        self.step=self.range/self.count
        self.times=self.data[:,0]
        self.values=self.data[:,1]
        self.plot_data=[self.times, self.values]
        self.inverse_plot_data=[1.0/self.times[20:], self.values[20:]]
```

Then, our class which contains the analysis code, *except* the numerical methods

```
start_date_str='1700-12-31'
                 end date str='2014-01-01'
                 self.start_date=self.format_date(start_date_str)
                 end_date=self.format_date(end_date_str)
                 url base=("http://www.quandl.com/api/v1/datasets/"+
                            "SIDC/SUNSPOTS A.csv")
                 x=requests.get(url_base,params={'trim_start':start_date_str,
                                                   'trim_end':end_date_str,
                                                   'sort_order':'asc'})
                 secs_per_year=(datetime(2014,1,1)-datetime(2013,1,1)
                         ).total_seconds()
                 data=csv.reader(StringIO(x.text)) #Convert requests
                                                     #result to look
                                                     #like a file buffer before
                                                     #reading with CSV
                 data.next() # Skip header row
                 self.series=Series([[
                          (self.format_date(row[0])-self.start_date
                              ).total seconds()/secs per year
                           , float(row[1])] for row in data])
             def __init__(self, frequency_strategy):
                 self.load_data()
                 self.frequency_strategy=frequency_strategy
             def frequency_data(self):
                 return self.frequency_strategy.transform(self.series)
  Our existing simple fourier strategy
In [21]: class FourierNearestFrequencyStrategy(object):
             def transform(self, series):
                 transformed=fft(series.values)[0:series.count/2]
                 frequencies=fftfreq(series.count, series.step)[0:series.count/2]
                 return Series(zip(frequencies, abs(transformed)/series.count))
  A strategy based on interpolation to a spline
In [22]: class FourierSplineFrequencyStrategy(object):
             def next power of two(self, value):
                 "Return the next power of 2 above value"
                 return 2**(1+int(log(value)/log(2)))
             def transform(self, series):
                 spline=UnivariateSpline(series.times, series.values)
                 # Linspace will give us *evenly* spaced points in the series
                 fft_count= self.next_power_of_two(series.count)
                 points=linspace(series.start,series.end,fft_count)
                 regular_xs=[spline(point) for point in points]
                 transformed=fft (regular_xs) [0:fft_count/2]
                 frequencies=fftfreq(fft_count,
                          series.range/fft_count) [0:fft_count/2]
                 return Series(zip(frequencies, abs(transformed)/fft_count))
  A strategy using the Lomb-Scargle Periodogram
```

304

def load data(self):

```
In [23]: class LombFrequencyStrategy(object):
             def transform(self, series):
                 frequencies=array(linspace(1.0/series.range,
                     0.5/series.step, series.count))
                 result= lombscargle(series.times,
                         series.values, 2.0 * math.pi * frequencies)
                 return Series(zip(frequencies, sqrt(result/series.count)))
  Define our concrete solutions with particular strategies
In [24]: fourier_model=AnalyseSunspotData(FourierSplineFrequencyStrategy())
         lomb_model=AnalyseSunspotData(LombFrequencyStrategy())
         nearest_model=AnalyseSunspotData(FourierNearestFrequencyStrategy())
        NameErrorTraceback (most recent call last)
        <ipython-input-24-82e75651bb61> in <module>()
    ----> 1 fourier_model=AnalyseSunspotData(FourierSplineFrequencyStrategy())
          2 lomb_model=AnalyseSunspotData(LombFrequencyStrategy())
          3 nearest_model=AnalyseSunspotData(FourierNearestFrequencyStrategy())
        <ipython-input-20-2850e087581a> in __init__(self, frequency_strategy)
         27
         28
                def __init__(self, frequency_strategy):
    ---> 29
                    self.load_data()
         30
                    self.frequency strategy=frequency strategy
         31
        <ipython-input-20-2850e087581a> in load_data(self)
          7
                  start_date_str='1700-12-31'
          8
                   end date str='2014-01-01'
    ---> 9
                   self.start_date=self.format_date(start_date_str)
         10
                    end_date=self.format_date(end_date_str)
                    url_base=("http://www.quandl.com/api/v1/datasets/"+
         11
        <ipython-input-20-2850e087581a> in format date(self, date)
          2
               def format date(self, date):
                    date format="%Y-%m-%d"
          3
                   return datetime.strptime(date, date_format)
    ---> 4
          5
              def load data(self):
        NameError: global name 'datetime' is not defined
  Use these new tools to compare solutions
```

comparison+=lomb_model.frequency_data().inverse_plot_data+['g']

In [25]: comparison=fourier_model.frequency_data().inverse_plot_data+['r']

```
comparison+=nearest_model.frequency_data().inverse_plot_data+['b']
         deviation=365*(fourier_model.series.times-linspace(
             fourier_model.series.start,
             fourier_model.series.end,
             fourier model.series.count))
        NameErrorTraceback (most recent call last)
        <ipython-input-25-0c678a42afa0> in <module>()
    ----> 1 comparison=fourier_model.frequency_data().inverse_plot_data+['r']
          2 comparison+=lomb_model.frequency_data().inverse_plot_data+['g']
          3 comparison+=nearest_model.frequency_data().inverse_plot_data+['b']
          5 deviation=365*(fourier_model.series.times-linspace(
        NameError: name 'fourier_model' is not defined
In [26]: plt.plot(*comparison)
        plt.xlim(0,16)
        NameErrorTraceback (most recent call last)
        <ipython-input-26-53b99d3c9394> in <module>()
    ----> 1 plt.plot(*comparison)
          2 plt.xlim(0,16)
        NameError: name 'plt' is not defined
6.9.8 Results: Deviation of year length from average
In [27]: plt.plot(deviation)
        NameErrorTraceback (most recent call last)
        <ipython-input-27-fc1f64d48ca3> in <module>()
    ----> 1 plt.plot(deviation)
        NameError: name 'plt' is not defined
```

6.10 Model-View-Controller

6.10.1 Separate graphics from science!

Whenever we are coding a simulation or model we want to:

- Implement the maths of the model
- Visualise, plot, or print out what is going on.

We often see scientific programs where the code which is used to display what is happening is mixed up with the mathematics of the analysis. This is hard to understand.

We can do better by separating the Model from the View, and using a "Controller" to manage them.

6.10.2 Model

```
In [28]: import numpy as np
         class Model(object):
             def __init__(self):
                 self.positions=np.random.rand(100,2)
                 self.speeds = (np.random.rand(100,2) +
                             np.array([-0.5, -0.5])[np.newaxis,:])
                 self.deltat=0.01
             def simulation step(self):
                 self.positions += self.speeds * self.deltat
             def agent_locations(self):
                 return self.positions
        ImportErrorTraceback (most recent call last)
        <ipython-input-28-7d3193731885> in <module>()
    ---> 1 import numpy as np
          3 class Model (object):
          4 def __init__(self):
                    self.positions=np.random.rand(100,2)
        ImportError: No module named numpy
6.10.3 View
```

```
In [29]: class View(object):
             def __init__(self, model):
                 from matplotlib import pyplot as plt
                 self.figure=plt.figure()
                 axes=plt.axes()
                 self.model=model
                 self.scatter=axes.scatter(
```

```
model.agent_locations()[:,0],
                         model.agent_locations()[:,1])
             def update(self):
                 self.scatter.set_offsets(
                     self.model.agent_locations())
6.10.4 Controller
In [30]: class Controller(object):
             def __init__(self):
                 self.model=Model() # Or use Builder
                 self.view=View(self.model)
                 def animate(frame_number):
                     self.model.simulation_step()
                     self.view.update()
                 self.animator=animate
             def go(self):
                 from JSAnimation import IPython_display
                 from matplotlib import animation
                 anim = animation.FuncAnimation(self.view.figure,
                                                 self.animator,
                                                 frames=200,
                                                 interval=50)
                 return anim
In [31]: contl=Controller()
        TypeErrorTraceback (most recent call last)
        <ipython-input-31-88447969c51b> in <module>()
    ----> 1 contl=Controller()
        <ipython-input-30-deba2a30eee1> in __init__(self)
          1 class Controller(object):
         2
               def __init__(self):
    ---> 3
                    self.model=Model() # Or use Builder
                    self.view=View(self.model)
          4
          5
                    def animate(frame_number):
        TypeError: __init__() takes exactly 7 arguments (1 given)
In [32]: from matplotlib import pyplot as plt
         %matplotlib inline
         contl.go()
```

6.11 Exercise: Refactoring The Bad Boids

6.11.1 Bad_Boids

I have written some *very bad* code implementing our Boids flocking example.

Here's the Github link.

Please fork it on GitHub, and clone your fork.

```
git clone git@github.com:yourname/bad-boids.git
# OR git clone https://github.com/yourname/bad-boids.git
```

For the Exercise, you should start from the GitHub repository, but here's my terrible code:

```
In [1]: """
        A deliberately bad implementation of
        [Boids] (http://dl.acm.org/citation.cfm?doid=37401.37406)
        for use as an exercise on refactoring.
        m m m
        from matplotlib import pyplot as plt
        from matplotlib import animation
        import random
        # Deliberately terrible code for teaching purposes
        boids_x = [random.uniform(-450,50.0) for x in range(50)]
        boids_y=[random.uniform(300.0,600.0) for x in range(50)]
        boid_x_velocities=[random.uniform(0,10.0) for x in range(50)]
        boid_y_velocities=[random.uniform(-20.0,20.0) for x in range(50)]
        boids=(boids_x,boids_y,boid_x_velocities,boid_y_velocities)
        def update boids(boids):
            xs, ys, xvs, yvs=boids
            # Fly towards the middle
            for i in range(len(xs)):
                for j in range(len(xs)):
                    xvs[i] = xvs[i] + (xs[j] - xs[i]) *0.01/len(xs)
            for i in range(len(xs)):
                for j in range(len(xs)):
                     yvs[i] = yvs[i] + (ys[j] - ys[i]) *0.01/len(xs)
```

```
# Fly away from nearby boids
        for i in range(len(xs)):
            for j in range(len(xs)):
                if (xs[j]-xs[i])**2 + (ys[j]-ys[i])**2 < 100:
                    xvs[i] = xvs[i] + (xs[i] - xs[j])
                    yvs[i] = yvs[i] + (ys[i] - ys[j])
        # Try to match speed with nearby boids
        for i in range(len(xs)):
            for j in range(len(xs)):
                if (xs[j]-xs[i])**2 + (ys[j]-ys[i])**2 < 10000:
                    xvs[i]=xvs[i]+(xvs[j]-xvs[i])*0.125/len(xs)
                    yvs[i] = yvs[i] + (yvs[j] - yvs[i]) *0.125/len(xs)
        # Move according to velocities
        for i in range(len(xs)):
            xs[i]=xs[i]+xvs[i]
            ys[i]=ys[i]+yvs[i]
    figure=plt.figure()
    axes=plt.axes(xlim=(-500, 1500), ylim=(-500, 1500))
   scatter=axes.scatter(boids[0],boids[1])
   def animate(frame):
       update boids (boids)
       scatter.set_offsets(zip(boids[0],boids[1]))
   anim = animation.FuncAnimation(figure, animate,
                                    frames=200, interval=50)
    ImportErrorTraceback (most recent call last)
    <ipython-input-1-39c9b8ed0fee> in <module>()
     5 """
---> 7 from matplotlib import pyplot as plt
      8 from matplotlib import animation
    ImportError: No module named matplotlib
```

If you go into your folder and run the code:

```
cd bad_boids
python bad_boids.py
```

You should be able to see some birds flying around, and then disappearing as they leave the window.

6.11.2 Your Task

Transform bad_boids **gradually** into better code, while making sure it still works, using a Refactoring approach.

6.11.3 A regression test

First, have a look at the regression test I made.

To create it, I saved out the before and after state for one iteration of some boids, using ipython:

```
import yaml
import boids
from copy import deepcopy
before=deepcopy(boids.boids)
boids.update_boids(boids.boids)
after=boids.boids
fixture={"before":before, "after":after}
fixture_file=open("fixture.yml", 'w')
fixture_file.write(yaml.dump(fixture))
fixture_file.close()
```

6.11.4 Invoking the test

Then, I used the fixture file to define the test:

6.11.5 Make the regression test fail

Check the tests pass:

nosetests

Edit the file to make the test fail, see the fail, then reset it:

```
git checkout boids.py
```

6.11.6 Start Refactoring

Look at the code, consider the list of refactorings, and make changes

Each time, do a git commit on your fork, and write a commit message explaining the refactoring you did.

Try to keep the changes as small as possible.

If your refactoring creates any units, (functions, modules, or classes) write a unit test for the unit: it is a good idea to get away from regression testing as soon as you can.

Chapter 7

Advanced Python Programming

... or, how to avoid repeating yourself.

7.1 Avoid Boiler-Plate

Code can often be annoyingly full of "boiler-plate" code: characters you don't really want to have to type. Not only is this tedious, it's also time-consuming and dangerous: unnecessary code is an unnecessary potential place for mistakes.

There are two important phrases in software design that we've spoken of before in this context:

Once And Only Once

Don't Repeat Yourself (DRY)

All concepts, ideas, or instructions should be in the program in just one place. Every line in the program should say something useful and important.

We refer to code that respects this principle as DRY code.

In this chapter, we'll look at some techniques that can enable us to refactor away repetitive code.

Since in many of these places, the techniques will involve working with functions as if they were variables, we'll learn some **functional** programming. We'll also learn more about the innards of how Python implements classes.

We'll also think about how to write programs that *generate* the more verbose, repetitive program we could otherwise write. We call this **metaprogramming**.

7.2 Functional programming

7.2.1 Functional Programming

Understanding to think in a *functional programming* style is almost as important as object orientation for building DRY, clear scientific software, and is just as conceptually difficult.

Programs are composed of functions: they take data in (which we call *parameters* or *arguments*) and send data out (through return statements.)

A conceptual trick which is often used by computer scientists to teach the core idea of functional programming is this: to write a program, in theory, you only ever need functions with **one** argument, even when you think you need two or more. Why?

Let's define a program to add two numbers:

```
Out[1]: 11
```

How could we do this, in a fictional version of Python which only defined functions of one argument? In order to understand this, we'll have to understand several of the concepts of functional programming. Let's start with a program which just adds five to something:

OK, we could define lots of these, one for each number we want to add. But that would be infinitely repetitive. So, let's try to metaprogram that: we want a function which returns these add_N() functions. Let's start with the easy case: a function which returns a function which adds 5 to something:

OK, so what happened there? Well, we defined a function **inside** the other function. We can always do that:

When we do this, the functions enclosed inside the outer function are **local** functions, and can't be seen outside:

There's not really much of a difference between functions and other variables in python. A function is just a variable which can have () put after it to call the code!

And we know that one of the things we can do with a variable is return it. So we can return a function, and then call it outside:

So now, to finish this, we just need to return a function to add an arbitrary amount:

We can make this even prettier: let's make another variable pointing to our define_adder() function:

```
In [14]: add = define_adder
```

And now we can do the real magic:

```
In [15]: add(8)(5)
Out[15]: 13
```

7.2.2 Closures

You may have noticed something a bit weird:

In the definition of define_adder, increment is a local variable. It should have gone out of scope and died at the end of the definition. How can the amount the returned adder function is adding still be kept?

This is called a **closure**. In Python, whenever a function definition references a variable in the surrounding scope, it is preserved within the function definition.

You can close over global module variables as well:

And note that the closure stores a reference to the variable in the surrounding scope: ("Late Binding")

7.2.3 Map and Reduce

We often want to apply a function to each variable in an array, to return a new array. We can do this with a list comprehension:

But this is sufficiently common that there's a quick built-in:

```
In [19]: map(add_five, numbers)
Out[19]: [5, 6, 7, 8, 9, 10, 11, 12, 13, 14]
```

This **map** operation is really important conceptually when understanding efficient parallel programming: different computers can apply the *mapped* function to their input at the same time. We call this Single Program, Multiple Data. (SPMD) **map** is half of the **map-reduce** functional programming paradigm which is key to the efficient operation of much of today's "data science" explosion.

Let's continue our functional programming mind-stretch by looking at reduce operations.

We very often want to loop with some kind of accumulator, such as when finding a mean, or finding a maximum:

```
In [20]: def summer(data):
             sum = 0.0
             for x in data:
                 sum+=x
             return sum
In [21]: summer(range(10))
Out[21]: 45.0
In [22]: import sys
         def my_max(data):
             # Start with the smallest possible number
             highest = sys.float_info.min
             for x in data:
                 if x>highest:
                     highest=x
             return highest
In [23]: my_max([2,5,10,-11,-5])
Out[23]: 10
```

These operations, where we have some variable which is building up a result, and the result is updated with some operation, can be gathered together as a functional program, taking in the operation to be used to combine results as an argument:

```
In [24]: def accumulate(initial, operation, data):
             accumulator=initial
             for x in data:
                 accumulator=operation(accumulator, x)
             return accumulator
         def my_sum(data):
             def_{add}(a,b):
                 return a+b
             return accumulate(0, _add, data)
In [25]: my_sum(range(5))
Out [25]: 10
In [26]: def bigger(a,b):
             if b>a:
                 return b
             return a
         def my_max(data):
             return accumulate(sys.float_info.min, bigger, data)
         my_max([2,5,10,-11,-5])
```

```
Out [26]: 10
```

Now, because these operations, *bigger*, *and* add, are such that e.g. (a+b)+c = a+(b+c), i.e. they are **associative**, we could apply our accumulation to the left half and the right half of the array, each on a different computer, and then combine the two halves:

```
1+2+3+4=(1+2)+(3+4)
```

Indeed, with a bigger array, we can divide-and-conquer more times:

```
1+2+3+4+5+6+7+8=((1+2)+(3+4))+((5+6)+(7+8))
```

So with enough parallel computers, we could do this operation on eight numbers in three steps: first, we use four computers to do one each of the pairwise adds.

Then, we use two computers to add the four totals.

Then, we use one of the computers to do the final add of the two last numbers.

You might be able to do the maths to see that with an N element list, the number of such steps is proportional to the logarithm of N.

We say that with enough computers, reduction operations are O(ln N)

This course isn't an introduction to algorithms, but we'll talk more about this O() notation when we think about programming for performance.

Anyway, this accumulate-under-an-operation process, is so fundamental to computing that it's usually in standard libraries for languages which allow functional programming:

```
In [27]: from functools import reduce

def my_max(data):
    return reduce(bigger, data, sys.float_info.min)

my_max([2,5,10,-11,-5])

Out[27]: 10
```

7.2.4 Lambda Functions

When doing functional programming, we often want to be able to define a function on the fly:

The syntax here is that these two definitions are identical:

7.2.5 Using functional programming for numerical methods

2080

2081

Probably the most common use in research computing for functional programming is the application of a numerical method to a function. For example:

```
In [32]: % matplotlib inline
        ImportErrorTraceback (most recent call last)
        <ipython-input-32-2b1da000a957> in <module>()
    ----> 1 get ipython().magic(u'matplotlib inline')
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2156
                    magic_name, _, magic_arg_s = arg_s.partition(' ')
       2157
                    magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
    -> 2158
                    return self.run_line_magic(magic_name, magic_arg_s)
       2159
       2160
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
                            kwarqs['local_ns'] = sys._qetframe(stack_depth).f_locals
       2077
       2078
                        with self.builtin_trap:
    -> 2079
                            result = fn(*args, **kwargs)
```

return result

```
/opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
                # but it's overkill for just that one bit of state.
        187
                def magic deco(arg):
    --> 188
                    call = lambda f, *a, **k: f(*a, **k)
        189
        190
                    if callable (arg):
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/pylab.pyc in ma-
                        print("Available matplotlib backends: %s" % backends_list)
         99
                    else:
    --> 100
                        gui, backend = self.shell.enable_matplotlib(args.gui)
        101
                        self._show_matplotlib_backend(args.gui, backend)
        102
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2933
       2934
                    from IPython.core import pylabtools as pt
                    gui, backend = pt.find_gui_and_backend(gui, self.pylab_gui_select)
    -> 2935
       2936
       2937
                    if gui != 'inline':
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/pylabtools.pyc in find
        257
        258
    --> 259
                import matplotlib
        260
        261
                if qui and qui != 'auto':
        ImportError: No module named matplotlib
In [33]: from scipy.optimize import newton
         from numpy import linspace, zeros
         from matplotlib import pyplot as plt
         solve_me=lambda x: x * *2-x
         print newton(solve_me, 2), newton(solve_me, 0.2)
         xs=linspace(-1,2,50)
         solved=[xs,map(solve_me,xs),xs,zeros(50)]
         plt.plot(*solved)
        ImportErrorTraceback (most recent call last)
```

<decorator-gen-104> in matplotlib(self, line)

```
---> 1 from scipy.optimize import newton
          2 from numpy import linspace, zeros
          3 from matplotlib import pyplot as plt
          5 solve me=lambda x: x**2-x
        ImportError: No module named scipy.optimize
  Sometimes such tools return another function:
In [34]: def derivative(func, eps):
             def _func_derived(x):
                 return (func(x+eps)-func(x))/eps
             return _func_derived
         straight = derivative(solve_me, 0.01)
        NameErrorTraceback (most recent call last)
        <ipython-input-34-b327c74a4af1> in <module>()
          6 return _func_derived
    ----> 8 straight = derivative(solve_me, 0.01)
        NameError: name 'solve_me' is not defined
In [35]: straight(3)
        NameErrorTraceback (most recent call last)
        <ipython-input-35-89be818b7b08> in <module>()
    ----> 1 straight(3)
        NameError: name 'straight' is not defined
In [36]: derived=(xs,map(solve_me,xs),xs,map(derivative(solve_me,0.01),xs))
         plt.plot(*derived)
         print newton(derivative(solve_me, 0.01), 0)
```

<ipython-input-33-f06b0e6b48cd> in <module>()

```
<ipython-input-36-bcb1ff4c793b> in <module>()
    ---> 1 derived=(xs,map(solve_me,xs),xs,map(derivative(solve_me,0.01),xs))
          2 plt.plot(*derived)
          3 print newton(derivative(solve me, 0.01), 0)
        NameError: name 'xs' is not defined
  Of course, coding your own numerical methods is bad:
In [37]: import scipy.misc
         def derivative(func):
             def _func_derived(x):
                 return scipy.misc.derivative(solve_me,x)
             return _func_derived
         newton(derivative(solve_me),0)
        ImportErrorTraceback (most recent call last)
        <ipython-input-37-72dbc210b0da> in <module>()
    ---> 1 import scipy.misc
          2.
          3 def derivative(func):
          4 def _func_derived(x):
                    return scipy.misc.derivative(solve_me,x)
        ImportError: No module named scipy.misc
```

NameErrorTraceback (most recent call last)

If you've done a moderate amount of calculus, then you'll find similarities between functional programming in computer science and Functionals in the calculus of variations.

7.3 Iterators and Generators

We've seen that in Python, anything which can be iterated over is called an iterable:

```
In [1]: bowl = {
          "apple" : 5,
          "banana" : 3,
          "orange" : 7
      }

for fruit in bowl:
          print fruit.upper()
```

ORANGE APPLE BANANA

Surprisingly often, we want to iterate over something that takes a moderately large amount of storage to store. For example, our map images in the green-graph example.

Our green-graph example involved making an array of all the maps between London and Birmingham. This kept them all in memory at the same time: first we downloaded all the maps, then we counted the green pixels in each of them.

This would NOT work if we used more points. We need to use a generator

7.3.1 Iterators

Consider the basic python range function:

While this was executing, the range() statement allocated a million integers. This is very inefficient. We don't actually need a million integers **at once**, just each integer **in turn** up to a million. xrange is like range, but yields an iterable which is not an array.

An generator object, like xrange(3), when we iterate over it, works by defining a next () method which moves the iterator forward:

```
In [6]: a=iter(xrange(3))
In [7]: a.next()
Out[7]: 0
In [8]: a.next()
Out[8]: 1
```

```
In [9]: a.next()
Out[9]: 2
  At the end, StopIteration is raised as an exception:
In [10]: a.next()
        StopIterationTraceback (most recent call last)
        <ipython-input-10-aa817a57a973> in <module>()
    ----> 1 a.next()
        StopIteration:
  We can turn an iterator back into a list with the list constructor function:
In [11]: list(xrange(5))
Out[11]: [0, 1, 2, 3, 4]
In [12]: total=0
         for x in xrange(int(1e6)): total+= x
         print total
499999500000
  Similarly:
In [13]: basket.items()
        NameErrorTraceback (most recent call last)
        <ipython-input-13-e578031bb616> in <math><module>()
    ----> 1 basket.items()
        NameError: name 'basket' is not defined
In [14]: basket.iteritems()
        NameErrorTraceback (most recent call last)
```

7.3.2 Defining Our Own Iterable

We can make our own iterators by defining *classes* that implement next() and **iter**() methods: this is the iterator protocol.

For each of the *concepts*, in Python, like sequence, container, iterable, python defines a **protocol**, a set of methods a class must implement, in order to be treated as a member of that concept.

The iterator protocol is the protocol that defines things that support for x in y:.

To define an iterator, the methods that must be supported are <code>next()</code> and <code>__iter__()</code>.

next () must update the iterator.

We'll see why we need to define __iter__ in a moment.

```
In [15]: class fib_iterator(object):
             def __init__(self, limit, seed1=1, seed2=1):
                 self.limit = limit
                 self.previous = seed1
                 self.current = seed2
             def __iter__(self):
                 return self
             def next(self):
                  (self.previous, self.current) = (
                          self.current, self.previous+self.current)
                 self.limit -=1
                 if self.limit<0: raise StopIteration()</pre>
                 return self.current
In [16]: x=fib_iterator(5)
In [17]: x.next()
Out[17]: 2
In [18]: x.next()
Out[18]: 3
In [19]: x.next()
Out[19]: 5
In [20]: x.next()
Out[20]: 8
In [21]: for x in fib_iterator(5):
             print x
```

```
5 8 13 In [22]: sum(fib_iterator(1000))
Out[22]: 297924218508143360336882819981631900915673130543819759032778173440536722190488904
```

7.3.3 A shortcut to iterables: the __iter__ method.

2

In fact, if, to be iterated over, a class just wants to behave as if it were some other iterable, you can just implement __iter__ and return iter(some_other_iterable), without implementing next. For example, an image class might want to implement some metadata, but behave just as if it were just a 1-d pixel array when being iterated:

```
In [23]: from numpy import array
         from matplotlib import pyplot as plt
         class MyImage(object):
             def __init__(self, pixels):
                 self.pixels=array(pixels,dtype='uint8')
                 self.channels=self.pixels.shape[2]
             def __iter__(self):
                 # return an iterator over the pixels
                 # See future NumPy lecture for using reshape
                 return iter(self.pixels.reshape(-1, self.channels))
             def show(self):
                 plt.imshow(self.pixels, interpolation="None")
         x = [[[255, 255, 0], [0, 255, 0]], [[0, 0, 255], [255, 255, 255]]]
         image=MyImage(x)
        ImportErrorTraceback (most recent call last)
        <ipython-input-23-b5f4ef22da0f> in <module>()
    ---> 1 from numpy import array
          2 from matplotlib import pyplot as plt
          4 class MyImage(object):
                def __init__(self, pixels):
        ImportError: No module named numpy
In [24]: %matplotlib inline
         image.show()
```

```
ImportErrorTraceback (most recent call last)
    <ipython-input-24-ba3d96948f60> in <module>()
---> 1 get ipython().magic(u'matplotlib inline')
     2 image.show()
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
               magic_name, _, magic_arg_s = arg_s.partition(' ')
  2156
  2157
               magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
-> 2158
               return self.run_line_magic(magic_name, magic_arg_s)
  2159
  2160
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc in
  2077
                       kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
  2078
                    with self.builtin_trap:
-> 2079
                       result = fn(*args, **kwargs)
  2080
                    return result
  2081
    <decorator-gen-104> in matplotlib(self, line)
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
   186
            # but it's overkill for just that one bit of state.
   187
           def magic_deco(arg):
--> 188
               call = lambda f, *a, **k: f(*a, **k)
   189
   190
               if callable(arg):
    /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/pylab.pyc in ma-
    98
                    print("Available matplotlib backends: %s" % backends_list)
    99
               else:
--> 100
                    qui, backend = self.shell.enable matplotlib(args.qui)
   101
                    self._show_matplotlib_backend(args.gui, backend)
   102
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc in
  2933
  2934
               from IPython.core import pylabtools as pt
-> 2935
               gui, backend = pt.find_gui_and_backend(gui, self.pylab_gui_select)
  2936
  2937
               if gui != 'inline':
```

/opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/pylabtools.pyc in find

```
11 11 11
        257
        258
    --> 259
               import matplotlib
        260
        261
                if gui and gui != 'auto':
        ImportError: No module named matplotlib
In [25]: image.channels
        NameErrorTraceback (most recent call last)
        <ipython-input-25-1f8baeb53897> in <module>()
    ---> 1 image.channels
        NameError: name 'image' is not defined
In [26]: from webcolors import rgb_to_name
         for pixel in image:
             print rgb_to_name(pixel)
        ImportErrorTraceback (most recent call last)
        <ipython-input-26-755abc5ac407> in <module>()
    ---> 1 from webcolors import rgb_to_name
          2 for pixel in image:
                print rgb_to_name(pixel)
        ImportError: No module named webcolors
```

The **iterator** protocol is to implement both <u>__iter__</u> and next, while the **iterable** protocol is to implement <u>__iter__</u> and return an something iterable.

7.3.4 Generators

There's a fair amount of "boiler-plate" in the above class-based definition of an iterable. Python provides another way to specify something which meets the iterator protocol: **generators**.

A function which has yield statements instead of a return statement returns temporarily: it automagically becomes something which implements next.

Each call of next() returns control to the function where it left off.

Control passes back-and-forth between the generator and the caller. Our fibonacci example therefore becomes a function rather than a class.

7.3.5 Context managers

We saw that instead of separately opening and closeing a file, we can have the file be automatically closed using a context manager:

How could we define our own one of these, if we too have clean-up code we always want to run after a calling function has done its work, or set-up code we want to do first?

We can define a class that meets an appropriate protocol:

However, this is pretty verbose! Again, a generator with yield makes for an easier syntax:

Again, we use yield to temporarily return from a function.

7.3.6 Decorators

When doing functional programming, we may often want to define mutator functions which take in one function and return a new function, such as our derivative example earlier.

It turns out that, quite often, we want to apply one of these to a function as we're defining a class. For example, we may want to specify that after certain methods are called, data should always be stored:

```
return _with_data_save
         class SomeClass(object):
             def __init__(self):
                 self.data=[]
                 self.stored data=[]
             def _step1(self, ins):
                 self.data=[x*2 for x in ins]
             step1=reset_required(_step1)
In [41]: x=SomeClass()
In [42]: x.step1("Hello")
         x.data
Out[42]: ['HH', 'ee', 'll', 'll', 'oo']
In [43]: x.step1("World")
         x.data
Out[43]: ['WW', 'oo', 'rr', 'll', 'dd']
In [44]: x.stored data
Out[44]: [['HH', 'ee', 'll', 'll', 'oo'], ['WW', 'oo', 'rr', 'll', 'dd']]
  Python provides some "syntactic sugar" to make this kind of coding prettier:
In [45]: def reset_required(func):
             def _with_data_save(self, *args):
                 func(self, *args)
                 self.stored_data.append(self.data)
             return _with_data_save
         class SomeClass(object):
             def __init__(self):
                 self.data=[]
                 self.stored_data=[]
             @reset required
             def step1(self, ins):
                 self.data=[x*2 for x in ins]
In [46]: x=SomeClass()
         x.step1("Hello")
         x.step1("World")
         print x.stored data
[['HH', 'ee', 'll', 'll', 'oo'], ['WW', 'oo', 'rr', 'll', 'dd']]
```

Any function which accepts a function as its first argument and returns a function can be used as a **decorator** like this.

Much of Python's standard functionality is implemented as decorators: we've seen @contextmanager, @classmethod and @attribute. The @contextmanager metafunction, for example, takes in an iterator, and yields a class conforming to the context manager protocol.

7.3.7 Test generators

A few weeks ago we saw a test which loaded its test cases from a YAML file and asserted each input with each output. This was nice and concise, but had one flaw: we had just one test, covering all the fixtures, so we got just one . in the test output when we ran the tests, and if any test failed, the rest were not run. We can do a nicer job with a test **generator**:

Each time a function beginning with test_does a yield it results in another test.

7.3.8 Negative test contexts managers

We have seen this:

```
In [48]: from nose.tools import assert_raises

with assert_raises(AttributeError):
    x=2
    x.foo()

ImportErrorTraceback (most recent call last)

<ipython-input-48-56da23bf94db> in <module>()
----> 1 from nose.tools import assert_raises
    2
    3 with assert_raises(AttributeError):
    4    x=2
    5    x.foo()

ImportError: No module named nose.tools
```

We can now see how nose might have implemented this:

7.3.9 Negative test decorators

Nose also implements a very nice negative test decorator:

```
In [51]: from nose.tools import raises
         @raises(TypeError, ValueError)
         def test raises type error():
             raise TypeError("This test passes")
        ImportErrorTraceback (most recent call last)
        <ipython-input-51-d45731226a53> in <module>()
    ----> 1 from nose.tools import raises
          3 @raises(TypeError, ValueError)
          4 def test_raises_type_error():
            raise TypeError("This test passes")
        ImportError: No module named nose.tools
In [52]: test_raises_type_error()
        NameErrorTraceback (most recent call last)
        <ipython-input-52-56bcddeb3998> in <module>()
    ----> 1 test_raises_type_error()
        NameError: name 'test_raises_type_error' is not defined
In [53]: @raises(Exception)
         def test_that_fails_by_passing():
            pass
```

```
NameErrorTraceback (most recent call last)
        <ipython-input-53-d2839aa37f2c> in <module>()
    ---> 1 @raises(Exception)
          2 def test_that_fails_by_passing():
               pass
        NameError: name 'raises' is not defined
In [54]: test_that_fails_by_passing()
        NameErrorTraceback (most recent call last)
        <ipython-input-54-fbd84a070d60> in <module>()
    ----> 1 test_that_fails_by_passing()
        NameError: name 'test_that_fails_by_passing' is not defined
  We could reimplement this ourselves now too:
In [55]: def homemade_raises_decorator(exception):
             def wrap_function(func): #Closure over exception
                 # Define a function which runs another function under the assert_raises of
                 def _output(*args): #Closure over func and exception
                     with assert_raises(exception):
                         func(*args)
                 # Return it
                 return _output
             return wrap_function
In [56]: @homemade_raises_decorator(TypeError)
         def test_raises_type_error():
             raise TypeError("This test passes")
In [57]: test_raises_type_error()
        NameErrorTraceback (most recent call last)
        <ipython-input-57-56bcddeb3998> in <module>()
    ----> 1 test_raises_type_error()
        <ipython-input-55-ea4ce6ae73a4> in _output(*args)
                    # Define a function which runs another function under the assert_raise
```

7.4 Exceptions

7.4.1 Exceptions

When we learned about testing, we saw that Python complains when things go wrong by raising an "Exception" naming a type of error:

Exceptions are objects, forming a class hierarchy. We just raised an instance of the ZeroDivisionError class, making the program crash.

So we can see that a zero division error is a particular kind of Arithmetic Error.

```
1 x=1
2
----> 3 for y in x: print y

TypeError: 'int' object is not iterable

In [4]: inspect.getmro(TypeError)

Out[4]: (TypeError, StandardError, Exception, BaseException, object)
```

In [5]: class MyCustomErrorType(ArithmeticError):

When we were looking at testing, we saw that it is important for code to crash with a meaningful exception type when something is wrong. We raise an Exception with raise. Often, we can look for an appropriate exception from the standard set to raise.

However, we may want to define our own exceptions. Doing this is as simple as inheriting from Exception:

```
pass
        raise(MyCustomErrorType("Problem"))
        MyCustomErrorTypeTraceback (most recent call last)
        <ipython-input-5-59beeb91fa6a> in <module>()
               pass
    ---> 4 raise(MyCustomErrorType("Problem"))
        MyCustomErrorType: Problem
  You can add custom data to your exception:
In [6]: class MyCustomErrorType(Exception):
            def __init__(self, category=None):
                self.category=category
            def __str__(self):
                return "Error, cateory " + str(self. category)
        raise (MyCustomErrorType (404))
        MyCustomErrorTypeTraceback (most recent call last)
        <ipython-input-6-7f8db3bcfb4d> in <module>()
                    return "Error, cateory " + str(self. category)
          7
```

```
----> 8 raise(MyCustomErrorType(404))

MyCustomErrorType: Error, cateory 404
```

The real power of exceptions comes, however, not in letting them crash the program, but in letting your program handle them. We say that an exception has been "thrown" and then "caught".

```
In [7]: import yaml
        try:
            config=yaml.load(open("datasource.yaml"))
            user=config["userid"]
            password=config["password"]
        except IOError:
            user="anonymous"
            password=None
        except Exception:
            print "Also handled the base exception type"
        print user
        ImportErrorTraceback (most recent call last)
        <ipython-input-7-f88718395532> in <module>()
    ----> 1 import yaml
          2
          3 try:
              config=yaml.load(open("datasource.yaml"))
                user=config["userid"]
        ImportError: No module named yaml
```

Note that we specify only the error we expect to happen and want to handle. Sometimes you see code that catches everything:

337

There was a mistyped function name there ('lod'), but we did not notice the error, as the generic except caught it. Therefore, we should catch only the error we want.

```
In [9]: with open('datasource2.yaml','w') as outfile:
            outfile.write('userid: jamespjh\n')
            outfile.write('password: secret\n')
        with open('datasource3.yaml','w') as outfile:
            outfile.write('user: jamespjh\n')
            outfile.write('password: secret\n')
In [10]: def read credentials(source):
             try:
                datasource=open(source)
                config=yaml.load(datasource)
                user=config["userid"]
                password=config["password"]
                datasource.close()
             except IOError:
                user="anonymous"
                password=None
             return user, password
In [11]: print read_credentials('datasource2.yaml')
        NameErrorTraceback (most recent call last)
        <ipython-input-11-34f90ae010c6> in <module>()
    ---> 1 print read_credentials('datasource2.yaml')
        <ipython-input-10-e8681b65ffe8> in read_credentials(source)
          2 try:
          3
                 datasource=open(source)
               datasource=open(source)
config=yaml.load(datasource)
    ---> 4
                 user=config["userid"]
          5
                 password=config["password"]
        NameError: global name 'yaml' is not defined
In [12]: print read_credentials('datasource.yaml')
('anonymous', None)
In [13]: print read_credentials('datasource3.yaml')
        NameErrorTraceback (most recent call last)
```

This last code has a flaw: the file was successfully opened, the missing key was noticed, but not explicitly closed. It's normally OK, as python will close the file as soon as it notices there are no longer any references to datasource in memory, after the function exits. But this is not good practice, you should keep a file handle for as short a time as possible.

The finally clause is executed whether or not an exception occurs.

The last optional clause of a try statement, an else clause is called only if an exception is NOT raised. It can be a better place than the try clause to put code other than that which you expect to raise the error, and which you do not want to be executed if the error is raised. It is executed in the same circumstances as code put in the end of the try block, the only difference is that errors raised during the else clause are not caught. Don't worry if this seems useless to you; most languages implementations of try/except don't support such a clause.

Exceptions do not have to be caught close to the part of the program calling them. They can be caught anywhere "above" the calling point in the call stack: control can jump arbitrarily far in the program: up to the except clause of the "highest" containing try statement.

```
In [16]: def f4(x):
             if x==0:
                 return
             if x==1:
                 raise ArithmeticError()
             if x==2:
                 raise SyntaxError()
             if x==3:
                 raise TypeError()
In [17]: def f3(x):
             try:
                 print "F3Before"
                 f4(x)
                 print "F3After"
             except ArithmeticError:
                 print "F3Except"
In [18]: def f2(x):
             try:
                 print "F2Before"
                 f3(x)
                 print "F2After"
             except SyntaxError:
                 print "F2Except"
In [19]: def f1(x):
             try:
                 print "F1Before"
                 f2(x)
                 print "F1After"
             except TypeError:
                 print "F1Except"
In [20]: f1(0)
F1Before
F2Before
F3Before
F3After
F2After
F1After
In [21]: f1(1)
F1Before
F2Before
F3Before
F3Except
F2After
F1After
```

```
In [22]: f1(2)
F1Before
F2Before
F3Before
F2Except
F1After

In [23]: f1(3)
F1Before
F2Before
F3Before
F1Except
```

7.4.2 Design with Exceptions

Now we know how exceptions work, we need to think about the design implications... How best to use them.

Traditional software design theory will tell you that they should only be used to describe and recover from **exceptional** conditions: things going wrong. Normal program flow shouldn't use them.

Python's designers take a different view: use of exceptions in normal flow is considered OK. For example, all iterators raise a StopIteration exception to indicate the iteration is complete.

A commonly recommended python design pattern is to use exceptions to determine whether an object implments a protocol (concept/interface), rather than testing on type.

For example, we might want a function which can be supplied *either* a data series *or* a path to a location on disk where data can be found. We can examine the type of the supplied content:

```
In [24]: import yaml
         def analysis(source):
             if type(source) == dict:
                 name=source['modelname']
                 content=open(source)
                 source=yaml.load(content)
                 name=source['modelname']
             print name
        ImportErrorTraceback (most recent call last)
        <ipython-input-24-c48710300e4c> in <module>()
    ---> 1 import yaml
          2 def analysis(source):
              if type(source) == dict:
                    name=source['modelname']
          4
                else:
        ImportError: No module named yaml
```

```
In [25]: analysis({'modelname':'Super'})
        NameErrorTraceback (most recent call last)
        <ipython-input-25-46f865e131c0> in <module>()
    ----> 1 analysis({'modelname':'Super'})
        NameError: name 'analysis' is not defined
In [26]: with open('example.yaml','w') as outfile:
             outfile.write('modelname: brilliant\n')
In [27]: analysis('example.yaml')
        NameErrorTraceback (most recent call last)
        <ipython-input-27-56d44188df75> in <module>()
    ----> 1 analysis('example.yaml')
        NameError: name 'analysis' is not defined
  However, we can also use the try-it-and-handle-exceptions approach to this.
In [28]: def analysis(source):
             try:
               name=source['modelname']
             except TypeError:
               content=open(source)
               source=yaml.load(content)
               name=source['modelname']
             print name
         analysis('example.yaml')
        NameErrorTraceback (most recent call last)
        <ipython-input-28-25400e5e9f76> in <module>()
          8
                print name
    ---> 10 analysis('example.yaml')
        <ipython-input-28-25400e5e9f76> in analysis(source)
```

```
4 except TypeError:
5 content=open(source)
----> 6 source=yaml.load(content)
7 name=source['modelname']
8 print name

NameError: global name 'yaml' is not defined
```

This approach is more extensible, and behaves properly if we give it some other data-source which responds like a dictionary or string.

```
In [29]: def analysis(source):
              name=source['modelname']
            except TypeError:
               # Source was not a dictionary-like object
               # Maybe it is a file path
              try:
                content=open(source)
                source=yaml.load(content)
                name=source['modelname']
               except IOError:
                 # Maybe it was already raw YAML content
                source=yaml.load(source)
                name=source['modelname']
            print name
         analysis("modelname: Amazing")
       NameErrorTraceback (most recent call last)
        <ipython-input-29-6d833521c7c4> in <module>()
        15
            print name
        16
    ---> 17 analysis("modelname: Amazing")
        <ipython-input-29-6d833521c7c4> in analysis(source)
        11 except IOError:
        12
                  # Maybe it was already raw YAML content
    ---> 13
                  source=yaml.load(source)
        14
                   name=source['modelname']
        15
              print name
       NameError: global name 'yaml' is not defined
```

Sometimes we want to catch an error, partially handle it, perhaps add some extra data to the exception, and then re-raise to be caught again further up the call stack.

The keyword "raise" with no argument in an except: clause will cause the caught error to be rethrown. Doing this is the only circumstance where it is safe to do except: without catching a specific type of error.

It can be useful to catch and re-throw an error as you go up the chain, doing any clean-up needed for each layer of a program.

The error will finally be caught and not re-thrown only at a higher program layer that knows how to recover. This is known as the "throw low catch high" principle.

7.5 Operator overloading

Warning: Advanced Topic!

7.5.1 Operator overloading

We need to use a metaprogramming trick to make this teaching notebook work. I want to be able to put explanatory text in between parts of a class definition, so I'll define a decorator to help me build up a class definition gradually.

Imagine we wanted to make a library to describe some kind of symbolic algebra system:

```
third=Term([],[],2)
result=Expression([first, second, third])
```

This is pretty cumbersome.

What we'd really like is to have 2x+y give an appropriate expression.

First, we'll define things so that we can construct our terms and expressions in different ways.

```
In [5]: class Term(object):
            def __init__(self, *args):
                lead=args[0]
                if type(lead) ==type(self):
                     # Copy constructor
                    self.data = dict(lead.data)
                     self.coefficient = lead.coefficient
                elif type(lead) == int:
                     self.from constant(lead)
                elif type(lead) == str:
                     self.from_symbol(*args)
                elif type(lead) == dict:
                     self.from_dictionary(*args)
                else:
                     self.from_lists(*args)
            def from_constant(self, constant):
                self.coefficient = constant
                self.data={}
            def from_symbol(self, symbol, coefficient=1, power=1):
                self.coefficient = coefficient
                self.data={symbol:power}
            def from_dictionary(self, data, coefficient=1):
                self.data = data
                self.coefficient = coefficient
            def from_lists(self, symbols=[], powers=[], coefficient=1):
                self.coefficient=coefficient
                self.data={symbol: exponent for symbol, exponent
                        in zip(symbols, powers)}
In [6]: class Expression(object):
            def __init__(self, terms=[]):
                self.terms = list(terms)
  We could define add() and multiply() operations on expressions and terms:
In [7]: @extend(Term)
        class Term(object):
            def add(self, *others):
                return Expression((self,)+others)
In [8]: @extend(Term)
        class Term(object):
```

```
def multiply(self, *others):
                 result_data=dict(self.data)
                 result coeff = self.coefficient
                 # Convert arguments to Terms first if they are
                 # constants or integers
                 others=map(Term, others)
                 for another in others:
                     for symbol, exponent in another.data.iteritems():
                         if symbol in result_data:
                             result_data[symbol] += another.data[symbol]
                         else:
                              result_data[symbol] = another.data[symbol]
                     result_coeff *= another.coefficient
                 return Term(result_data, result_coeff)
In [9]: @extend(Expression)
        class Expression(object):
            def add(self, *others):
                 result = Expression(self.terms)
                 for another in others:
                     if type(another) == Term:
                         result.terms.append(another)
                     else:
                         result.terms+=another.terms
                 return result
  We can now construct the above expression as:
In [10]: x=Term('x')
         y=Term('y')
         first=Term(5).multiply(Term('x'), Term('x'), Term('y'))
         second=Term(7).multiply(Term('x'))
         third=Term(2)
         expr=first.add(second,third)
  This is better, but we still can't write the expression in a 'natural' way.
  However, we can define what * and + do when applied to Terms!:
In [11]: @extend(Term)
         class Term(object):
             def __add__(self, other):
                  return self.add(other)
             def __mul__(self, other):
                  return self.multiply(other)
In [12]: @extend(Expression)
         class Expression(object):
             def multiply(self, another):
```

```
# Distributive law left as exercise
pass

def __add__(self, other):
    return self.add(other)

In [13]: x_plus_y=Term('x')+'y'
    x_plus_y.terms[0].data

Out[13]: {'x': 1}

In [14]: five_x_ysq=Term('x')*5*'y'*'y'
    print five_x_ysq.data, five_x_ysq.coefficient
{'y': 2, 'x': 1} 5
```

This is called operator overloading. We can define what add and multiply mean when applied to our class.

Note that this only works so far if we multiply on the right-hand-side! However, we can define a multiplication that works backwards, which is used as a fallback if the left multiply raises an error:

It's not easy at the moment to see if these things are working!

We can add another operator method __str__, which defines what happens if we try to print our class:

```
else:
                          return symbol+'^'+str(power)
                  symbol_strings=[symbol_string(symbol, power)
                          for symbol, power in self.data.iteritems()]
                  prod='*'.join(symbol_strings)
                  if not prod:
                      return str(self.coefficient)
                  if self.coefficient==1:
                      return prod
                  else:
                      return str(self.coefficient) + ' * ' + prod
In [20]: @extend(Expression)
         class Expression(object):
             def __str__(self):
                  return '+'.join(map(str, self.terms))
In [21]: first=Term(5) \star'x'\star'x'\star'y'
         second=Term(7) * 'x'
         third=Term(2)
         expr=first+second+third
In [22]: print expr
5*y*x^2+7*x+2
```

We can add lots more operators to classes. __eq_ to determine if objects are equal. __getitem_ to apply [1] to your object. Probably the most exciting one is __call__, which overrides the () operator; allows us to define classes that *behave like functions*! We call these callables.

```
In [23]: class Greeter(object):
    def __init__(self, greeting):
        self.greeting = greeting

def __call__(self, name):
        print self.greeting, name

    greeter_instance = Greeter("Hello")

    greeter_instance("James")
Hello James
```

We've now come full circle in the blurring of the distinction between functions and objects! The full power of functional programming is really remarkable.

If you want to know more about the topics in this lecture, using a different language syntax, I recommend you watch the Abelson and Sussman "Structure and Interpretation of Computer Programs" lectures. These are the Computer Science equivalent of the Feynman Lectures!

7.6 Metaprogramming

Warning: Advanced topic!

7.6.1 Metaprogramming globals

Consider a bunch of variables, each of which need initialising and incrementing:

The right hand side of these assignments doesn't respect the DRY principle. We could of course define a variable for our initial value:

However, this is still not as DRY as it could be: what if we wanted to replace the assignment with, say, a class constructor and a buy operation:

We had to make the change in three places. Whenever you see a situation where a refactoring or change of design might require you to change the code in multiple places, you have an opportunity to make the code DRYer.

In this case, metaprogramming for incrementing these variables would involve just a loop over all the variables we want to initialise:

However, this trick **doesn't** work for initialising a new variable:

```
In [5]: from nose.tools import assert_raises
    with assert_raises(NameError):
        baskets=[bananas, apples, oranges, kiwis]

ImportErrorTraceback (most recent call last)
        <ipython-input-5-8e0f88fd6e9c> in <module>()
----> 1 from nose.tools import assert_raises
```

```
2 with assert_raises(NameError):
3    baskets=[bananas, apples, oranges, kiwis]
ImportError: No module named nose.tools
```

So can we declare a new variable programmatically? Given a list of the **names** of fruit baskets we want, initialise a variable with that name?

Wow, we can! Every module or class in Python, is, under the hood, a special dictionary, storing the values in its **namespace**. So we can create new variables by assigning to this dictionary. globals() gives a reference to the attribute dictionary for the current module

This is **metaprogramming**.

I would NOT recommend using it for an example as trivial as the one above. A better, more Pythonic choice here would be to use a data structure to manage your set of fruit baskets:

Or even, using a dictionary comprehension:

Which is the nicest way to do this, I think. Code which feels like metaprogramming is needed to make it less repetitive can often instead be DRYed up using a refactored data structure, in a way which is cleaner and more easy to understand. Nevertheless, metaprogramming is worth knowing.

7.6.2 Metaprogramming class attributes

We can metaprogram the attributes of a **module** using the globals() function.

We will also want to be able to metaprogram a class, by accessing its attribute dictionary.

This will allow us, for example, to programmatically add members to a class.

```
In [10]: class Boring(object):
    pass
```

If we are adding our own attributes, we can just do so directly:

And these turn up, as expected, in an attribute dictionary for the class:

```
In [13]: x.__dict__
Out[13]: {'name': 'James'}
```

We can use getattr to access this special dictionary:

```
In [14]: getattr(x, 'name')
Out[14]: 'James'
```

If we want to add an attribute given it's name as a string, we can use setattr:

And we could do this in a loop to programmatically add many attributes.

The real power of accessing the attribute dictionary comes when we realise that there is *very little difference* between member data and member functions.

Now that we know, from our functional programming, that **a function is just a variable that can be** *called* **with** (), we can set an attribute to a function, and it becomes a member function!

```
In [16]: setattr(Boring, 'describe', lambda self: self.name+ " is "+str(self.age))
In [17]: x.describe()
Out[17]: 'James is 38'
In [18]: x.describe
Out[18]: <bound method Boring.<lambda> of <__main__.Boring object at 0x2abff574c610>>
In [19]: Boring.describe
Out[19]: <unbound method Boring.<lambda>>
```

Note that we set this method as an attribute of the class, not the instance, so it is available to other instances of Boring:

We can define a standalone function, and then **bind** it to the class. It's first argument automagically becomes self.

```
In [22]: def broken_birth_year(b_instance):
    import datetime
        current=datetime.datetime.now().year
    return current-b_instance.age

In [23]: Boring.birth_year=broken_birth_year

In [24]: x.birth_year()

Out[24]: 1978

In [25]: x.birth_year

Out[25]: <bound method Boring.broken_birth_year of <__main__.Boring object at 0x2abff574c6

In [26]: x.birth_year.__name__

Out[26]: 'broken_birth_year'</pre>
```

7.6.3 Metaprogramming function locals

We can access the attribute dictionary for the local namespace inside a function with locals () but this cannot be written to.

Lack of safe programmatic creation of function-local variables is a flaw in Python.

7.6.4 Metaprogramming warning!

Use this stuff **sparingly**!

The above example worked, but it produced Python code which is not particularly understandable. Remember, your objective when programming is to produce code which is **descriptive of what it does**.

The above code is **definitely** less readable, less maintainable and more error prone than:

```
In [30]: class Person(object):
    def __init__(self, name, age, job, children_count):
        self.name=name
        self.age=age
        self.job=job
        self.children_count=children_count
```

Sometimes, metaprogramming will be **really** helpful in making non-repetitive code, and you should have it in your toolbox, which is why I'm teaching you it. But doing it all the time overcomplicated matters. We've talked a lot about the DRY principle, but there is another equally important principle:

KISS: Keep it simple, Stupid!

Whenever you write code and you think, "Gosh, I'm really clever", you're probably *doing it wrong*. Code should be about clarity, not showing off.

Chapter 8

Performance programming

We've spent most of this course looking at how to make code readable and reliable. For research work, it is often also important that code is efficient: that it does what it needs to do *quickly*.

It is very hard to work out beforehand whether code will be efficient or not: it is essential to *Profile* code, to measure its performance, to determine what aspects of it are slow.

When we looked at Functional programming, we claimed that code which is conceptualised in terms of actions on whole data-sets rather than individual elements is more efficient. Let's measure the performance of some different ways of implementing some code and see how they perform.

8.1 Two Mandelbrots

You're probably familiar with a famous fractal called the Mandelbrot Set.

For a complex number c, c is in the Mandelbrot set if the series $z_{i+1} = z_i^2 + c$ (With $z_0 = c$) stays close to 0. Traditionally, we plot a color showing how many steps are needed for $|z_i| > 2$, whereupon we are sure the series will diverge.

Here's a trivial python implementation:

```
In [1]: def mandel1(position, limit=50):
            value=position
            while abs(value) < 2:</pre>
                 limit-=1
                 value=value**2+position
                 if limit<0:</pre>
                     return 0
            return limit
In [2]: xmin=-1.5
        ymin=-1.0
        xmax=0.5
        vmax=1.0
        resolution=300
        xstep=(xmax-xmin)/resolution
        ystep=(ymax-ymin)/resolution
        xs=[(xmin+(xmax-xmin)*i/resolution) for i in range(resolution)]
        ys=[(ymin+(ymax-ymin)*i/resolution) for i in range(resolution)]
```

```
In [3]: %%timeit
        data=[[mandel1(complex(x,y)) for x in xs] for y in ys]
1 loop, best of 3: 497 ms per loop
In [4]: data1=[[mandel1(complex(x,y)) for x in xs] for y in ys]
In [5]: %matplotlib inline
        import matplotlib.pyplot as plt
        plt.imshow(data1, interpolation='none')
        ImportErrorTraceback (most recent call last)
        <ipython-input-5-ac497b0414b2> in <module>()
    ---> 1 get_ipython().magic(u'matplotlib inline')
          2 import matplotlib.pyplot as plt
          3 plt.imshow(data1,interpolation='none')
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2156
                   magic_name, _, magic_arg_s = arg_s.partition(' ')
       2157
                    magic name = magic name.lstrip(prefilter.ESC MAGIC)
    -> 2158
                   return self.run_line_magic(magic_name, magic_arg_s)
       2159
       2160
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc in
       2077
                           kwarqs['local_ns'] = sys._qetframe(stack_depth).f_locals
                        with self.builtin_trap:
       2078
    -> 2079
                            result = fn(*args, **kwargs)
       2080
                        return result
       2081
        <decorator-gen-104> in matplotlib(self, line)
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
                # but it's overkill for just that one bit of state.
        186
        187
                def magic_deco(arg):
    --> 188
                   call = lambda f, *a, **k: f(*a, **k)
        189
        190
                    if callable (arg):
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/pylab.pyc in ma-
         98
                        print("Available matplotlib backends: %s" % backends_list)
         99
                    else:
    --> 100
                        gui, backend = self.shell.enable_matplotlib(args.gui)
        101
                        self._show_matplotlib_backend(args.gui, backend)
```

```
2934
                    from IPython.core import pylabtools as pt
    -> 2935
                    gui, backend = pt.find_gui_and_backend(gui, self.pylab_gui_select)
       2936
       2937
                    if gui != 'inline':
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/pylabtools.pyc in find
        258
    --> 259
                import matplotlib
        260
        261
                if qui and qui != 'auto':
        ImportError: No module named matplotlib
  We will learn this lesson how to make a version of this code which works Ten Times faster:
In [6]: import numpy as np
        def mandel_numpy(position,limit=50):
            value=position
            diverged_at_count=np.zeros(position.shape)
            while limit>0:
                limit-=1
                value=value**2+position
                diverging=value*np.conj(value)>4
                first_diverged_this_time=np.logical_and(diverging, diverged_at_count==0)
                diverged_at_count[first_diverged_this_time] = limit
                value[diverging] = 2
            return diverged_at_count
        ImportErrorTraceback (most recent call last)
        <ipython-input-6-e40c7ebb2599> in <module>()
    ---> 1 import numpy as np
          2 def mandel_numpy(position,limit=50):
                value=position
          4
                diverged_at_count=np.zeros(position.shape)
          5
                while limit>0:
        ImportError: No module named numpy
```

/opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is

In [7]: ymatrix, xmatrix=np.mgrid[ymin:ymax:ystep,xmin:xmax:xstep]

```
NameErrorTraceback (most recent call last)
        <ipython-input-7-e716a80bbaa4> in <module>()
    ---> 1 ymatrix,xmatrix=np.mgrid[ymin:ymax:ystep,xmin:xmax:xstep]
        NameError: name 'np' is not defined
In [8]: values=xmatrix + 1j*ymatrix
        NameErrorTraceback (most recent call last)
        <ipython-input-8-e6be35132a99> in <module>()
    ----> 1 values=xmatrix + 1j*ymatrix
        NameError: name 'xmatrix' is not defined
In [9]: data_numpy=mandel_numpy(values)
        NameErrorTraceback (most recent call last)
        <ipython-input-9-aa34e074c59e> in <module>()
    ---> 1 data_numpy=mandel_numpy(values)
        NameError: name 'mandel_numpy' is not defined
In [10]: %matplotlib inline
         import matplotlib.pyplot as plt
         plt.imshow(data_numpy,interpolation='none')
        ImportErrorTraceback (most recent call last)
        <ipython-input-10-ea4b9624d0f7> in <module>()
    ---> 1 get_ipython().magic(u'matplotlib inline')
          2 import matplotlib.pyplot as plt
          3 plt.imshow(data_numpy,interpolation='none')
```

```
/opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
                magic_name, _, magic_arg_s = arg_s.partition(' ')
   2156
  2157
                magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
-> 2158
                return self.run_line_magic(magic_name, magic_arg_s)
   2159
   2160
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
                        kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
   2077
   2078
                    with self.builtin_trap:
-> 2079
                        result = fn(*args, **kwargs)
   2080
                    return result
   2081
    <decorator-gen-104> in matplotlib(self, line)
    /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
            # but it's overkill for just that one bit of state.
   187
            def magic deco(arg):
                call = lambda f, \stara, \star \stark: f(\stara, \star \stark)
--> 188
    189
   190
                if callable (arg):
    /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/pylab.pyc in ma-
                    print("Available matplotlib backends: %s" % backends_list)
    99
                else:
--> 100
                    qui, backend = self.shell.enable_matplotlib(args.qui)
    101
                    self._show_matplotlib_backend(args.gui, backend)
   102
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
   2933
   2934
                from IPython.core import pylabtools as pt
-> 2935
                gui, backend = pt.find_gui_and_backend(gui, self.pylab_gui_select)
   2936
   2937
                if qui != 'inline':
    /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/pylabtools.pyc in find
    257
    258
--> 259
            import matplotlib
    260
    261
            if gui and gui != 'auto':
```

ImportError: No module named matplotlib

```
In [11]: %%timeit
         data_numpy=mandel_numpy(values)
        NameErrorTraceback (most recent call last)
        <ipython-input-11-2fe069eac38d> in <module>()
    ----> 1 get_ipython().run_cell_magic(u'timeit', u'', u'data_numpy=mandel_numpy(values)
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2113
                        magic_arg_s = self.var_expand(line, stack_depth)
       2114
                       with self.builtin_trap:
    -> 2115
                            result = fn(magic_arg_s, cell)
       2116
                        return result
       2117
        <decorator-gen-58> in timeit(self, line, cell)
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
             # but it's overkill for just that one bit of state.
                def magic_deco(arg):
        187
                   call = lambda f, *a, **k: f(*a, **k)
    --> 188
        189
        190
                   if callable(arg):
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
       1042
                        number = 1
      1043
                        for \_ in range(1, 10):
    -> 1044
                            time_number = timer.timeit(number)
       1045
                            worst_tuning = max(worst_tuning, time_number / number)
       1046
                            if time_number >= 0.2:
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
       137
                    gc.disable()
        138
                    try:
    --> 139
                        timing = self.inner(it, self.timer)
        140
                    finally:
        141
                        if gcold:
        <magic-timeit> in inner(_it, _timer)
        NameError: global name 'mandel_numpy' is not defined
  Note we get the same answer:
```

In [12]: sum(sum(abs(data_numpy-data1)))

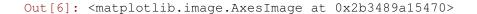
```
NameErrorTraceback (most recent call last)
        <ipython-input-12-92cc7bdebea0> in <module>()
    ---> 1 sum(sum(abs(data_numpy-data1)))
        NameError: name 'data_numpy' is not defined
In [1]: xmin=-1.5
        ymin=-1.0
        xmax=0.5
        ymax=1.0
        resolution=300
        xstep=(xmax-xmin)/resolution
        ystep= (ymax-ymin) / resolution
        xs=[(xmin+(xmax-xmin)*i/resolution) for i in range(resolution)]
        ys=[(ymin+(ymax-ymin)*i/resolution) for i in range(resolution)]
In [2]: def mandel1(position, limit=50):
            value=position
            while abs(value)<2:</pre>
                limit-=1
                value=value**2+position
                if limit<0:</pre>
                    return 0
            return limit
In [3]: data1=[[mandel1(complex(x,y)) for x in xs] for y in ys]
```

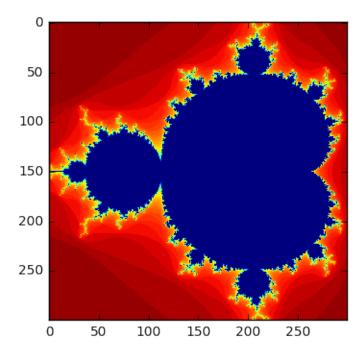
8.2 Many Mandelbrots

Let's compare our naive python implementation which used a list comprehension, taking 662ms, with the following:

Interestingly, not much difference. I would have expected this to be slower, due to the normally high cost of **appending** to data.

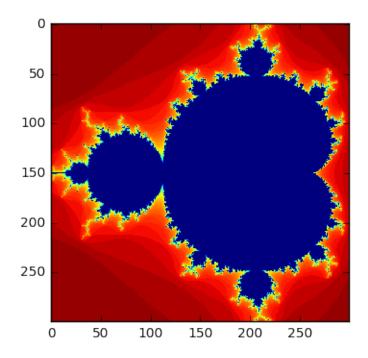
/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment





We ought to be checking if these results are the same by comparing the values in a test, rather than re-plotting. This is cumbersome in pure Python, but easy with NumPy, so we'll do this later. Let's try a pre-allocated data structure:

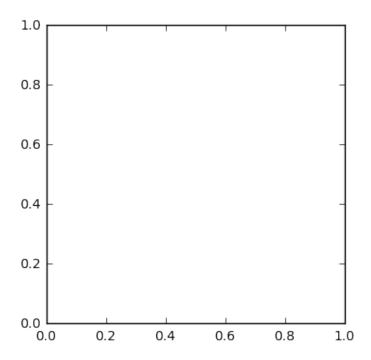
```
In [10]: plt.imshow(data3,interpolation='none')
Out[10]: <matplotlib.image.AxesImage at 0x2b3489a7f160>
```



Nope, no gain there. Let's try using functional programming approaches:

```
/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/pyplot.
  3027
                                filternorm=filternorm, filterrad=filterrad,
  3028
                                imlim=imlim, resample=resample, url=url, data=data,
-> 3029
                                **kwargs)
  3030
            finally:
  3031
                ax.hold(washold)
   /home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/__init_
  1817
                            warnings.warn(msg % (label_namer, func.__name__),
  1818
                                          RuntimeWarning, stacklevel=2)
-> 1819
                    return func(ax, *args, **kwargs)
  1820
                pre_doc = inner.__doc___
  1821
                if pre_doc is None:
   /home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/axes/_a:
  4920
                                      resample=resample, **kwargs)
  4921
-> 4922
                im.set_data(X)
  4923
                im.set_alpha(alpha)
  4924
                if im.get_clip_path() is None:
   /home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/image.pg
   447
                if (self._A.dtype != np.uint8 and
   448
                        not np.can_cast(self._A.dtype, np.float)):
--> 449
                    raise TypeError("Image data can not convert to float")
   450
    451
                if (self._A.ndim not in (2, 3) or
```

TypeError: Image data can not convert to float



That was a tiny bit slower.

So, what do we learn from this? Our mental image of what code should be faster or slower is often wrong, or doesn't make much difference. The only way to really improve code performance is empirically, through measurements.

8.3 NumPy for Performance

8.3.1 NumPy constructors

We saw previously that NumPy's core type is the ndarray, or N-Dimensional Array:

```
In [1]: import numpy as np
        np.zeros([3,4,2])
Out[1]: array([[[ 0.,
                  [ 0.,
                         0.],
                  [ 0.,
                         0.],
                  [ 0.,
                          0.]],
                 [[ 0.,
                          0.],
                  [ 0.,
                          0.],
                  [ 0.,
                          0.],
                  [ 0.,
                          0.]],
                 [[ 0.,
                          0.],
                  [ 0.,
                          0.],
                  [ 0.,
                         0.],
                  [ 0.,
                         0.]])
```

The real magic of numpy arrays is that most python operations are applied, quickly, on an elementwise basis:

```
In [2]: x = np.arange(0, 256, 4).reshape(8, 8)
                           8,
                               12,
                                    16, 20, 24,
Out [2]: array([[ 0,
                      4,
               [ 32,
                     36,
                          40,
                               44,
                                    48, 52, 56,
                    68,
                         72, 76, 80,
                                        84, 88,
               [ 64,
               [ 96, 100, 104, 108, 112, 116, 120, 124],
               [128, 132, 136, 140, 144, 148, 152, 156],
               [160, 164, 168, 172, 176, 180, 184, 188],
               [192, 196, 200, 204, 208, 212, 216, 220],
               [224, 228, 232, 236, 240, 244, 248, 252]])
```

Numpy's mathematical functions also happen this way, and are said to be "vectorized" functions.

```
In [3]: np.sqrt(x)
Out[3]: array([[ 0.
                             2.
                                          2.82842712,
                                                      3.46410162,
                            4.47213595,
                                         4.89897949, 5.29150262],
                4.
                            6. ,
              [ 5.65685425,
                                         6.32455532,
                                                      6.63324958,
                6.92820323, 7.21110255,
                                          7.48331477,
                                                      7.745966691,
                     , 8.24621125,
                                        8.48528137,
                                                      8.71779789,
              [ 8.
                8.94427191,
                            9.16515139,
                                         9.38083152,
                                                      9.59166305],
              [ 9.79795897, 10.
                                  , 10.19803903, 10.39230485,
               10.58300524, 10.77032961, 10.95445115, 11.13552873],
              [ 11.3137085 , 11.48912529, 11.66190379, 11.83215957,
                    , 12.16552506, 12.32882801, 12.489996 ],
              [ 12.64911064, 12.80624847, 12.9614814 ,
                                                      13.11487705,
               13.26649916, 13.41640786,
                                         13.56465997,
                                                      13.7113092 ],
              [ 13.85640646, 14.
                                  , 14.14213562, 14.28285686,
               14.4222051 , 14.56021978, 14.69693846,
                                                      14.83239697],
              [ 14.96662955,
                            15.09966887,
                                         15.23154621,
                                                      15.3622915 ,
               15.49193338,
                                         15.74801575,
                                                      15.87450787]])
                           15.62049935,
```

Numpy contains many useful functions for creating matrices. In our earlier lectures we've seen linspace and arange for evenly spaced numbers.

```
In [4]: np.linspace (0, 10, 21)
Out[4]: array([ 0. , 0.5, 1. , 1.5, 2. , 2.5,
                                                   3.,
                                                         3.5,
                                                               4.,
                         5.5,
                   5.,
                                6., 6.5,
                                           7.,
                                                         8.,
              4.5,
                                                   7.5,
              9.,
                   9.5, 10. 1)
In [5]: np.arange(0, 10, 0.5)
Out[5]: array([ 0. , 0.5, 1. , 1.5, 2. , 2.5, 3. , 3.5, 4. , 4.5, 5. ,
                  6., 6.5, 7., 7.5, 8., 8.5, 9.,
```

Here's one for creating matrices like coordinates in a grid:

```
In [6]: xmin=-1.5
    ymin=-1.0
    xmax=0.5
    ymax=1.0
    resolution=300
    xstep=(xmax-xmin)/resolution
    ystep=(ymax-ymin)/resolution

ymatrix, xmatrix=np.mgrid[ymin:ymax:ystep,xmin:xmax:xstep]
```

We can add these together to make a grid containing the complex numbers we want to test for membership in the Mandelbrot set.

8.3.2 Arraywise Algorithms

We can use this to apply the mandelbrot algorithm to whole ARRAYS

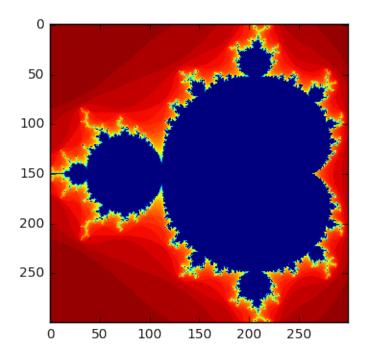
So can we just apply our mandel1 function to the whole matrix?

ValueError: The truth value of an array with more than one element is ambiguous. Us

No. The *logic* of our current routine would require stopping for some elements and not for others. We can ask numpy to **vectorise** our method for us:

/home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment home/travis/virtualenv/python3.4.3/lib/python3.4/site-packages/matplotlib/font_manager.py warnings.warn('Matplotlib is building the font cache using fc-list. This may take a moment

Out[16]: <matplotlib.image.AxesImage at 0x2b896b0a52b0>



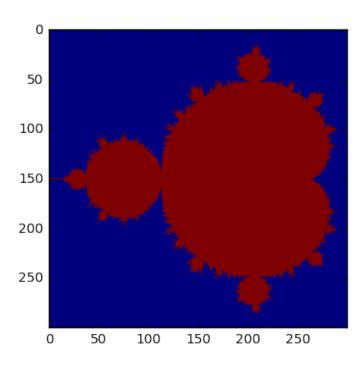
Is that any faster?

This is not significantly faster. When we use *vectorize* it's just hiding an plain old python for loop under the hood. We want to make the loop over matrix elements take place in the "C Layer".

What if we just apply the Mandelbrot algorithm without checking for divergence until the end:

OK, we need to prevent it from running off to ∞

```
In [20]: def mandel_numpy(position,limit=50):
             value=position
             while limit>0:
                 limit-=1
                 value=value**2+position
                 diverging=abs(value)>2
                 # Avoid overflow
                 value[diverging] = 2
             return abs(value)<2</pre>
In [21]: data6=mandel_numpy(values)
In [22]: %%timeit
         data6=mandel_numpy(values)
10 loops, best of 3: 79.2 ms per loop
In [23]: from matplotlib import pyplot as plt
         %matplotlib inline
         plt.imshow(data6,interpolation='none')
Out[23]: <matplotlib.image.AxesImage at 0x2b896b14d4e0>
```



Wow, that was TEN TIMES faster. There's quite a few NumPy tricks there, let's remind ourselves of how they work:

```
In [24]: diverging=abs(z3)>2
    z3[diverging]=2
```

When we apply a logical condition to a NumPy array, we get a logical array.

In [25]: x=np.arange(10) *1.0

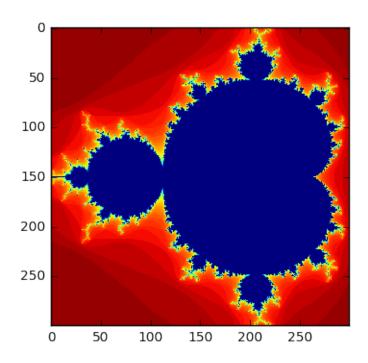
```
y=np.ones([10])*5
        z=x>\lambda
        print z
         File "<ipython-input-25-6ba89fb0264c>", line 4
       print z
   SyntaxError: Missing parentheses in call to 'print'
  Logical arrays can be used to index into arrays:
In [26]: x[x>80]
Out[26]: array([ 84, 88, 92, 96, 100, 104, 108, 112, 116, 120, 124, 128, 132,
               136, 140, 144, 148, 152, 156, 160, 164, 168, 172, 176, 180, 184,
               188, 192, 196, 200, 204, 208, 212, 216, 220, 224, 228, 232, 236,
               240, 244, 248, 2521)
In [27]: x[np.logical_not(z)]
             ______
       NameError
                                                Traceback (most recent call last)
       <ipython-input-27-f3fc2721f547> in <module>()
   ----> 1 x[np.logical_not(z)]
       NameError: name 'z' is not defined
  And you can use such an index as the target of an assignment:
In [28]: x[z]=5
        print x
         File "<ipython-input-28-751bbe5e9db6>", line 2
       print x
```

Note that we didn't compare two arrays to get our logical array, but an array to a scalar integer – this was broadcasting again.

SyntaxError: Missing parentheses in call to 'print'

8.3.3 More Mandelbrot

Of course, we didn't calculate the number-of-iterations-to-diverge, just whether the point was in the set. Let's correct our code to do that:



Note that here, all the looping over mandelbrot steps was in Python, but everything below the loop-over-positions happened in C. The code was amazingly quick compared to pure Python.

Can we do better by avoiding a square root?

Probably not worth the time I spent thinking about it!

8.3.4 NumPy Testing

Now, let's look at calculating those residuals, the differences between the different datasets.

For our non-numpy datasets, numpy knows to turn them into arrays:

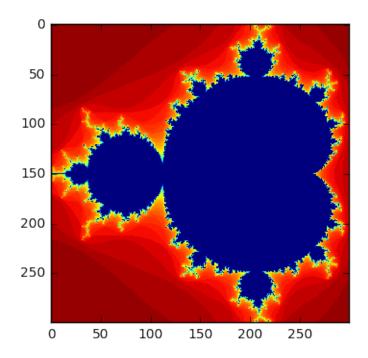
But this doesn't work for pure non-numpy arrays

```
In [38]: data2=[]
         for y in ys:
             row=[]
             for x in xs:
                 row.append(mandel1(complex(x,y)))
             data2.append(row)
        NameError
                                                    Traceback (most recent call last)
        <ipython-input-38-12f1bb5ea1a8> in <module>()
          1 data2=[]
    ----> 2 for y in ys:
          3
                row=[]
               for x in xs:
          4
                    row.append(mandel1(complex(x,y)))
        NameError: name 'ys' is not defined
In [39]: data2-data1
        NameError
                                                    Traceback (most recent call last)
        <ipython-input-39-f2646eae3452> in <module>()
    ----> 1 data2-data1
        NameError: name 'datal' is not defined
  So we have to convert to NumPy arrays explicitly:
In [40]: sum(sum((np.array(data2)-np.array(data1))**2))
        NameError
                                                    Traceback (most recent call last)
        <ipython-input-40-cbdf843fcaea> in <module>()
    ----> 1 sum(sum((np.array(data2)-np.array(data1))**2))
        NameError: name 'data1' is not defined
  NumPy provides some convenient assertions to help us write unit tests with NumPy arrays:
In [41]: x = [1e-5, 1e-3, 1e-1]
         y = np.arccos(np.cos(x))
         np.testing.assert_allclose(x, y, rtol=1e-6, atol=1e-20)
```

8.3.5 Arraywise operations are fast

Note that we might worry that we carry on calculating the mandelbrot values for points that have already diverged.

```
In [43]: def mandel6(position, limit=50):
             value=np.zeros(position.shape)+position
             calculating=np.ones(position.shape,dtype='bool')
             diverged at count=np.zeros(position.shape)
             while limit>0:
                 limit-=1
                 value[calculating] = value[calculating] * *2 + position[calculating]
                 diverging_now=np.zeros(position.shape,dtype='bool')
                 diverging_now[calculating]=value[calculating]
                                                   ]*np.conj(value[calculating])>4
                 calculating=np.logical_and(calculating,
                                             np.logical_not(diverging_now))
                 diverged_at_count[diverging_now]=limit
             return diverged_at_count
In [44]: data8=mandel6(values)
In [45]: %%timeit
         data8=mandel6(values)
10 loops, best of 3: 61.1 ms per loop
In [46]: plt.imshow(data8,interpolation='none')
Out[46]: <matplotlib.image.AxesImage at 0x2b896b242748>
```



This was not faster even though it was doing less work

This often happens: on modern computers, **branches** (if statements, function calls) and **memory access** is usually the rate-determining step, not maths.

Complicating your logic to avoid calculations sometimes therefore slows you down. The only way to know is to **measure**

8.3.6 Indexing with arrays

We've been using Boolean arrays a lot to get access to some elements of an array. We can also do this with integers:

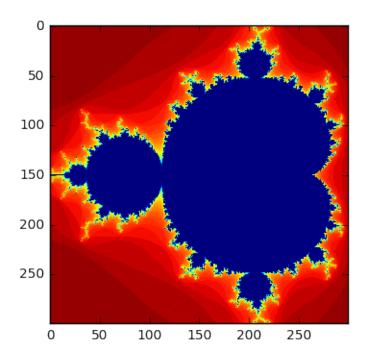
```
In [47]: x=np.arange(64)
         y=x.reshape([8,8])
                                         6,
Out[47]: array([[ 0,
                     1, 2, 3, 4, 5,
                     9, 10, 11, 12, 13, 14, 15],
                [ 8,
                [16, 17, 18, 19, 20, 21, 22, 23],
                [24, 25, 26, 27, 28, 29, 30, 31],
                [32, 33, 34, 35, 36, 37, 38, 39],
                [40, 41, 42, 43, 44, 45, 46, 47],
                [48, 49, 50, 51, 52, 53, 54, 55],
                [56, 57, 58, 59, 60, 61, 62, 63]])
In [48]: y[[0,5,2]]
Out[48]: array([[ 0, 1, 2, 3, 4, 5,
                [40, 41, 42, 43, 44, 45, 46, 47],
                [16, 17, 18, 19, 20, 21, 22, 23]])
In [49]: y[[0,2,5],[1,2,7]]
```

```
Out[49]: array([ 1, 18, 47])
  We can use a : to indicate we want all the values from a particular axis:
In [50]: y[0:8:2,[0,2]]
Out[50]: array([[ 0, 2],
                 [16, 18],
                 [32, 34],
                 [48, 50]])
  We can mix array selectors, boolean selectors, :s and ordinary array sequencers:
In [51]: z=x.reshape([4,4,4])
         print z
          File "<ipython-input-51-6c9969bdafa5>", line 2
        print z
    SyntaxError: Missing parentheses in call to 'print'
In [52]: z[:,[1,3],0:3]
        NameError
                                                      Traceback (most recent call last)
        <ipython-input-52-59cc1f632a34> in <module>()
    ---> 1 z[:,[1,3],0:3]
        NameError: name 'z' is not defined
  We can manipulate shapes by adding new indices in selectors with np.newaxis:
In [53]: z[:,np.newaxis,[1,3],0].shape
                                                      Traceback (most recent call last)
        NameError
        <ipython-input-53-bf45bf44fbc7> in <module>()
    ---> 1 z[:,np.newaxis,[1,3],0].shape
        NameError: name 'z' is not defined
```

When we use basic indexing with integers and : expressions, we get a **view** on the matrix so a copy is avoided:

```
In [54]: a=z[:,:,2]
         a[0,0] = -500
                                                       Traceback (most recent call last)
        NameError
         <ipython-input-54-7da219c5659e> in <module>()
    ----> 1 a=z[:,:,2]
          2 a[0,0] = -500
           3 z
        NameError: name 'z' is not defined
  We can also use ... to specify ": for as many as possible intervening axes":
In [55]: z[1]
        NameError
                                                       Traceback (most recent call last)
         <ipython-input-55-e7abb66cbb1e> in <module>()
    ---> 1 z[1]
        NameError: name 'z' is not defined
In [56]: z[...,2]
        NameError
                                                       Traceback (most recent call last)
        <ipython-input-56-14b38f39ea1c> in <module>()
    ----> 1 z[...,2]
        NameError: name 'z' is not defined
  However, boolean mask indexing and array filter indexing always causes a copy.
  Let's try again at avoiding doing unnecessary work by using new arrays containing the reduced data
instead of a mask:
```

```
diverged_at_count=np.zeros(position.shape)
             while limit>0:
                 limit-=1
                 value=value**2+positions
                 diverging_now=value*np.conj(value)>4
                 diverging_now_indices=indices[:,diverging_now]
                 carry_on=np.logical_not(diverging_now)
                 value=value[carry_on]
                 indices=indices[:,carry_on]
                 positions=positions[carry_on]
                 diverged_at_count[diverging_now_indices[0,:],
                                   diverging_now_indices[1,:]]=limit
             return diverged_at_count
In [58]: data9=mandel7(values)
In [59]: plt.imshow(data9,interpolation='none')
Out[59]: <matplotlib.image.AxesImage at 0x2b896b2a2b00>
```



Still slower. Probably due to lots of copies – the point here is that you need to *experiement* to see which optimisations will work. Performance programming needs to be empirical.

8.4 Cython

Cython can be viewed as an extension of Python where variables and functions are annotated with extra information, in particular types. The resulting Cython source code will be compiled into optimized C or C++ code, and thereby yielding substantial speed-up of slow Python code. In other word, cython provides a way of writting Python with comparable performance to that of C/C++.

8.4.1 Start Coding in Cython

Cython code must, unlike Python, be compiled. This happens in the following stages:

- The cython code in .pyx file will be translated to a C file.
- The C file will be compiled by a C compiler into a shared library, which will be directly loaded into Python.

In ipython notebook, everything is a lot easier. One need only to load Cython extension (%load_ext Cython) at the beginning and put %%cython mark in front of cells of cython code. Cells with cython mark will be treated as a .pyx code and consequently, compiled into C.

For details, please see Building Cython Code.

Pure python Mandelbrot set:

2157

```
In [1]: xmin=-1.5
        ymin=-1.0
        xmax=0.5
        ymax=1.0
        resolution=300
        xstep=(xmax-xmin)/resolution
        ystep=(ymax-ymin)/resolution
        xs=[(xmin+(xmax-xmin)*i/resolution) for i in range(resolution)]
        ys=[(ymin+(ymax-ymin)*i/resolution) for i in range(resolution)]
In [2]: def mandel(position, limit=50):
            value=position
            while abs(value)<2:</pre>
                limit-=1
                value=value * *2+position
                if limit<0:</pre>
                    return 0
            return limit
  Compiled by Cython:
In [3]: %load_ext Cython
        ImportErrorTraceback (most recent call last)
        <ipython-input-3-1f34cad6ae68> in <module>()
    ---> 1 get_ipython().magic(u'load_ext Cython')
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
                    magic_name, _, magic_arg_s = arg_s.partition(' ')
       2156
```

magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)

```
-> 2158
                    return self.run_line_magic(magic_name, magic_arg_s)
       2159
       2160
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2077
                            kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
       2078
                        with self.builtin_trap:
    -> 2079
                            result = fn(*args,**kwargs)
       2080
                        return result
       2081
        <decorator-gen-62> in load_ext(self, module_str)
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
                # but it's overkill for just that one bit of state.
               def magic_deco(arg):
        187
                   call = lambda f, *a, **k: f(*a, **k)
    --> 188
        189
        190
                   if callable(arg):
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/extension.pyc is
                   if not module str:
         36
                        raise UsageError('Missing module name.')
    ---> 37
                   res = self.shell.extension_manager.load_extension(module_str)
         38
         39
                   if res == 'already loaded':
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/extensions.pyc in load
                        if module_str not in sys.modules:
         82
                            with prepended_to_syspath(self.ipython_extension_dir):
    ---> 83
                                __import___(module_str)
         84
                        mod = sys.modules[module str]
         85
                        if self._call_load_ipython_extension(mod):
        ImportError: No module named Cython
In [4]: %%cython
        def mandel_cython(position, limit=50):
            value=position
            while abs(value)<2:
                limit-=1
                value=value**2+position
                if limit<0:
                    return 0
            return limit
```

```
ERROR:root:Cell magic `%%cython` not found.
```

In [5]: from matplotlib import pyplot as plt

Let's verify the result

```
%matplotlib inline
        f, axarr = plt.subplots(1,2)
        axarr[0].imshow([[mandel(complex(x,y)) for x in xs] for y in ys],interpolation='no:
        axarr[0].set_title('Pure Python')
        axarr[1].imshow([[mandel(complex(x,y)) for x in xs] for y in ys],interpolation='nor
        axarr[1].set_title('Cython')
        ImportErrorTraceback (most recent call last)
        <ipython-input-5-434d46bb4f46> in <module>()
    ---> 1 from matplotlib import pyplot as plt
          2 get_ipython().magic(u'matplotlib inline')
          3 f, axarr = plt.subplots(1,2)
          4 axarr[0].imshow([[mandel(complex(x,y)) for x in xs] for y in ys], interpolations
          5 axarr[0].set_title('Pure Python')
        ImportError: No module named matplotlib
In [6]: timeit [[mandel(complex(x,y)) for x in xs] for y in ys] # pure python
        %timeit [[mandel_cython(complex(x,y)) for x in xs] for y in ys] # cython
1 loop, best of 3: 499 ms per loop
        NameErrorTraceback (most recent call last)
        <ipython-input-6-3fca44e9db1c> in <module>()
         1 get_ipython().magic(u'timeit [[mandel(complex(x,y)) for x in xs] for y in ys] =
    ----> 2 get_ipython().magic(u'timeit [[mandel_cython(complex(x,y)) for x in xs] for y
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2156
                   magic_name, _, magic_arg_s = arg_s.partition(' ')
      2157
                   magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
    -> 2158
                    return self.run_line_magic(magic_name, magic_arg_s)
      2159
       2160
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc in
       2077
                            kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
```

```
2078
                    with self.builtin_trap:
-> 2079
                        result = fn(*args, **kwargs)
  2080
                   return result
  2081
   <decorator-gen-58> in timeit(self, line, cell)
    /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
            # but it's overkill for just that one bit of state.
   187
           def magic_deco(arg):
               call = lambda f, *a, **k: f(*a, **k)
--> 188
   189
   190
               if callable (arg):
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
                    number = 1
  1042
  1043
                    for \_ in range(1, 10):
-> 1044
                        time_number = timer.timeit(number)
  1045
                        worst_tuning = max(worst_tuning, time_number / number)
  1046
                        if time_number >= 0.2:
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc in
   137
                gc.disable()
   138
               try:
--> 139
                    timing = self.inner(it, self.timer)
   140
                finally:
   141
                    if gcold:
    <magic-timeit> in inner(_it, _timer)
   NameError: global name 'mandel_cython' is not defined
```

We have improved the performance of a factor of 1.5 by just using the cython compiler, **without changing the code**!

8.4.2 Cython with C Types

But we can do better by telling Cython what C data type we would use in the code. Note we're not actually writing C, we're writing Python with C types.

typed variable

```
In [7]: %%cython
    def var_typed_mandel_cython(position, limit=50):
        cdef double complex value # typed variable
        value=position
        while abs(value)<2:
            limit-=1
            value=value**2+position</pre>
```

```
if limit<0:
                    return 0
            return limit
ERROR:root:Cell magic `%%cython` not found.
  typed function + typed variable
In [8]: %%cython
        cpdef call_typed_mandel_cython(double complex position,
                                        int limit=50): # typed function
            cdef double complex value # typed variable
            value=position
            while abs(value) < 2:
                limit-=1
                value=value**2+position
                if limit<0:</pre>
                    return 0
            return limit
ERROR:root:Cell magic `%%cython` not found.
  performance of one number:
In [9]: # pure python
        %timeit a=mandel(complex(0,0))
The slowest run took 5.41 times longer than the fastest. This could mean that an intermedia
100000 loops, best of 3: 10.7 \mus per loop
In [10]: # premitive cython
         %timeit a=mandel_cython(complex(0,0))
        NameErrorTraceback (most recent call last)
        <ipython-input-10-c0110f206180> in <module>()
          1 # premitive cython
    ----> 2 get_ipython().magic(u'timeit a=mandel_cython(complex(0,0))')
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2156
                    magic_name, _, magic_arg_s = arg_s.partition(' ')
       2157
                    magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
    -> 2158
                    return self.run_line_magic(magic_name, magic_arg_s)
       2159
       2160
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc in
```

kwargs['local_ns'] = sys._getframe(stack_depth).f_locals

2077

```
2078
                        with self.builtin_trap:
    -> 2079
                            result = fn(*args, **kwargs)
       2080
                        return result
       2081
        <decorator-gen-58> in timeit(self, line, cell)
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
                # but it's overkill for just that one bit of state.
        187
               def magic_deco(arg):
                   call = lambda f, *a, **k: f(*a, **k)
    --> 188
        189
        190
                   if callable(arg):
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
       1042
                        number = 1
       1043
                        for \_ in range(1, 10):
    -> 1044
                            time_number = timer.timeit(number)
      1045
                            worst_tuning = max(worst_tuning, time_number / number)
                            if time_number >= 0.2:
       1046
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc in
        137
                    gc.disable()
        138
                    try:
    --> 139
                        timing = self.inner(it, self.timer)
        140
                    finally:
        141
                        if gcold:
        <magic-timeit> in inner(_it, _timer)
        NameError: global name 'mandel_cython' is not defined
In [11]: # cython with C type variable
         %timeit a=var_typed_mandel_cython(complex(0,0))
        NameErrorTraceback (most recent call last)
        <ipython-input-11-9b72560222e9> in <module>()
         1 # cython with C type variable
    ----> 2 get_ipython().magic(u'timeit a=var_typed_mandel_cython(complex(0,0))')
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
                   magic_name, _, magic_arg_s = arg_s.partition(' ')
       2157
                    magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
```

```
-> 2158
                   return self.run_line_magic(magic_name, magic_arg_s)
       2159
      2160
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2077
                            kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
       2078
                       with self.builtin_trap:
    -> 2079
                            result = fn(*args,**kwargs)
      2080
                       return result
       2081
        <decorator-gen-58> in timeit(self, line, cell)
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
                # but it's overkill for just that one bit of state.
               def magic_deco(arg):
       187
                   call = lambda f, *a, **k: f(*a, **k)
    --> 188
       189
       190
                  if callable(arg):
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
      1042
                       number = 1
      1043
                       for \_ in range(1, 10):
    -> 1044
                           time_number = timer.timeit(number)
      1045
                            worst_tuning = max(worst_tuning, time_number / number)
      1046
                            if time_number >= 0.2:
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
       137
                   gc.disable()
       138
                   trv:
    --> 139
                       timing = self.inner(it, self.timer)
       140
                   finally:
       141
                       if gcold:
        <magic-timeit> in inner( it, timer)
       NameError: global name 'var_typed_mandel_cython' is not defined
In [12]: # cython with typed variable + function
         %timeit a=call_typed_mandel_cython(complex(0,0))
       NameErrorTraceback (most recent call last)
        <ipython-input-12-e8b23b7818f1> in <module>()
```

```
1 # cython with typed variable + function
----> 2 get_ipython().magic(u'timeit a=call_typed_mandel_cython(complex(0,0))')
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
               magic_name, _, magic_arg_s = arg_s.partition(' ')
   2156
               magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
  2157
-> 2158
               return self.run_line_magic(magic_name, magic_arg_s)
   2159
   2160
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
                        kwarqs['local_ns'] = sys._qetframe(stack_depth).f_locals
   2077
   2078
                    with self.builtin_trap:
-> 2079
                        result = fn(*args, **kwargs)
   2080
                   return result
   2081
   <decorator-gen-58> in timeit(self, line, cell)
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
            # but it's overkill for just that one bit of state.
   186
   187
           def magic deco(arg):
--> 188
               call = lambda f, *a, **k: f(*a, **k)
   189
   190
               if callable (arg):
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
                   number = 1
  1042
  1043
                   for \_ in range(1, 10):
-> 1044
                        time number = timer.timeit(number)
  1045
                        worst_tuning = max(worst_tuning, time_number / number)
  1046
                        if time number >= 0.2:
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
               qc.disable()
   138
--> 139
                   timing = self.inner(it, self.timer)
   140
                finally:
   141
                   if gcold:
    <magic-timeit> in inner(_it, _timer)
   NameError: global name 'call_typed_mandel_cython' is not defined
```

8.4.3 Cython with numpy ndarray

You can use NumPy from Cython exactly the same as in regular Python, but by doing so you are losing potentially high speedups because Cython has support for fast access to NumPy arrays.

```
In [13]: import numpy as np
         ymatrix, xmatrix=np.mgrid[ymin:ymax:ystep, xmin:xmax:xstep]
         values=xmatrix+1j*ymatrix
        ImportErrorTraceback (most recent call last)
        <ipython-input-13-6c79bcb1275c> in <module>()
    ----> 1 import numpy as np
          2 ymatrix, xmatrix=np.mgrid[ymin:ymax:ystep,xmin:xmax:xstep]
          3 values=xmatrix+1j*ymatrix
        ImportError: No module named numpy
In [14]: %%cython
         import numpy as np
         cimport numpy as np
         cpdef numpy_cython_1(np.ndarray[double complex, ndim=2] position,
                              int limit=50):
             cdef np.ndarray[long,ndim=2] diverged_at
             cdef double complex value
             cdef int xlim
             cdef int ylim
             cdef double complex pos
             cdef int steps
             cdef int x, y
             xlim=position.shape[1]
             ylim=position.shape[0]
             diverged_at=np.zeros([ylim, xlim], dtype=int)
             for x in xrange(xlim):
                 for y in xrange(ylim):
                      steps=limit
                      value=position[y,x]
                      pos=position[y,x]
                      while abs(value)<2 and steps>=0:
                         steps-=1
                         value=value**2+pos
                      diverged_at[y,x]=steps
             return diverged_at
ERROR:root:Cell magic `%%cython` not found.
```

Note the double import of numpy: the standard numpy module and a Cython-enabled version of numpy that ensures fast indexing of and other operations on arrays. Both import statements are necessary in code that uses numpy arrays. The new thing in the code above is declaration of arrays by np.ndarray.

```
In [15]: %timeit data_cy=[[mandel(complex(x,y)) for x in xs] for y in ys] # pure python
1 loop, best of 3: 494 ms per loop
In [16]: %timeit data_cy=[[call_typed_mandel_cython(complex(x,y)) for x in xs] for y in ys
        NameErrorTraceback (most recent call last)
        <ipython-input-16-8f986b5c4d0c> in <module>()
    ----> 1 get_ipython().magic(u'timeit data_cy=[[call_typed_mandel_cython(complex(x,y)) :
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
                    magic_name, _, magic_arg_s = arg_s.partition(' ')
       2156
       2157
                    magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
    -> 2158
                    return self.run_line_magic(magic_name, magic_arg_s)
       2159
       2160
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
                            kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
       2077
       2078
                       with self.builtin_trap:
    -> 2079
                            result = fn(*args, **kwargs)
       2080
                        return result
       2081
        <decorator-gen-58> in timeit(self, line, cell)
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
             # but it's overkill for just that one bit of state.
        186
        187
               def magic_deco(arg):
    --> 188
                    call = lambda f, *a, **k: f(*a, **k)
        189
        190
                   if callable (arg):
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
       1042
                        number = 1
       1043
                        for \_ in range(1, 10):
    -> 1044
                            time_number = timer.timeit(number)
       1045
                            worst_tuning = max(worst_tuning, time_number / number)
       1046
                            if time_number >= 0.2:
```

```
/opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
                    gc.disable()
        137
                    try:
        138
    --> 139
                        timing = self.inner(it, self.timer)
        140
                    finally:
                        if gcold:
        141
        <magic-timeit> in inner(_it, _timer)
        NameError: global name 'call_typed_mandel_cython' is not defined
In [17]: %timeit numpy_cython_1(values) # ndarray
        NameErrorTraceback (most recent call last)
        <ipython-input-17-208f4e765cd3> in <module>()
    ---> 1 get_ipython().magic(u'timeit numpy_cython_1(values) # ndarray')
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2156
                    magic_name, _, magic_arg_s = arg_s.partition(' ')
       2157
                    magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
    -> 2158
                    return self.run_line_magic(magic_name, magic_arg_s)
       2159
       2160
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2077
                            kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
       2078
                        with self.builtin_trap:
    -> 2079
                            result = fn(*args, **kwargs)
       2080
                        return result
       2081
        <decorator-gen-58> in timeit(self, line, cell)
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
        186
                # but it's overkill for just that one bit of state.
        187
                def magic_deco(arg):
    --> 188
                    call = lambda f, *a, **k: f(*a, **k)
        189
        190
                   if callable(arg):
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
       1042
                        number = 1
       1043
                        for \_ in range(1, 10):
```

```
-> 1044
                          time number = timer.timeit(number)
      1045
                          worst_tuning = max(worst_tuning, time_number / number)
                          if time number >= 0.2:
      1046
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
                  qc.disable()
                  try:
       138
   --> 139
                      timing = self.inner(it, self.timer)
       140
                  finally:
       141
                      if gcold:
       <magic-timeit> in inner(_it, _timer)
       NameError: global name 'numpy_cython_1' is not defined
  A trick of using np.vectorize
In [18]: numpy_cython_2=np.vectorize(call_typed_mandel_cython)
       NameErrorTraceback (most recent call last)
       <ipython-input-18-5b55612dbc49> in <module>()
   ---> 1 numpy_cython_2=np.vectorize(call_typed_mandel_cython)
       NameError: name 'np' is not defined
In [19]: %timeit numpy_cython_2(values) # vectorize
       NameErrorTraceback (most recent call last)
       <ipython-input-19-4cc36eea8568> in <module>()
   ----> 1 get_ipython().magic(u'timeit numpy_cython_2(values) # vectorize')
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
      2156
                  magic_name, _, magic_arg_s = arg_s.partition(' ')
      2157
                  magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
   -> 2158
                  return self.run_line_magic(magic_name, magic_arg_s)
      2159
      2160
               #-----
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
```

```
2077
                        kwarqs['local_ns'] = sys._qetframe(stack_depth).f_locals
  2078
                   with self.builtin_trap:
                        result = fn(*args,**kwargs)
-> 2079
  2080
                    return result
  2081
    <decorator-gen-58> in timeit(self, line, cell)
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
            # but it's overkill for just that one bit of state.
   186
   187
           def magic_deco(arg):
--> 188
               call = lambda f, *a, **k: f(*a, **k)
   189
   190
               if callable(arg):
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
  1042
                    number = 1
  1043
                    for \_ in range(1, 10):
-> 1044
                       time_number = timer.timeit(number)
  1045
                        worst_tuning = max(worst_tuning, time_number / number)
  1046
                        if time number >= 0.2:
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
   137
               gc.disable()
   138
               try:
--> 139
                   timing = self.inner(it, self.timer)
   140
               finally:
   141
                   if gcold:
    <magic-timeit> in inner(_it, _timer)
   NameError: global name 'numpy_cython_2' is not defined
```

8.4.4 Calling C functions from Cython

Example: compare sin() from Python and C library

```
In [21]: %%cython
        from libc.math cimport sin as csin # import from C library
        cpdef c sin():
            cdef int x
            cdef double y
            for x in xrange(1e7):
                y = csin(x)
ERROR:root:Cell magic `%%cython` not found.
In [22]: %timeit [math.sin(i) for i in xrange(int(1e7))] # python
       NameErrorTraceback (most recent call last)
       <ipython-input-22-038873be7cae> in <module>()
   ---> 1 get_ipython().magic(u'timeit [math.sin(i) for i in xrange(int(1e7))] # python'
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
      2156
                   magic_name, _, magic_arg_s = arg_s.partition(' ')
      2157
                   magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
    -> 2158
                   return self.run_line_magic(magic_name, magic_arg_s)
      2159
               #-----
      2160
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc in
                           kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
      2077
      2078
                       with self.builtin_trap:
    -> 2079
                          result = fn(*args, **kwargs)
      2080
                       return result
      2081
       <decorator-gen-58> in timeit(self, line, cell)
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
       186
               # but it's overkill for just that one bit of state.
       187
               def magic_deco(arg):
    --> 188
                  call = lambda f, *a, **k: f(*a, **k)
       189
       190
                  if callable (arg):
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
      1042
                       number = 1
      1043
                       for \_ in range(1, 10):
    -> 1044
                          time_number = timer.timeit(number)
      1045
                          worst_tuning = max(worst_tuning, time_number / number)
      1046
                          if time_number >= 0.2:
```

```
/opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
        137
                    gc.disable()
        138
                    try:
    --> 139
                       timing = self.inner(it, self.timer)
                    finally:
        140
                        if gcold:
        141
        <magic-timeit> in inner(_it, _timer)
        NameError: global name 'math' is not defined
In [23]: %timeit py_sin()
                                                         # cython call python library
        NameErrorTraceback (most recent call last)
        <ipython-input-23-cb320c027901> in <module>()
    ----> 1 get_ipython().magic(u'timeit py_sin()
                                                                                  # cython
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2156
                    magic_name, _, magic_arg_s = arg_s.partition(' ')
       2157
                    magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
    -> 2158
                    return self.run_line_magic(magic_name, magic_arg_s)
       2159
       2160
       /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc in
       2077
                            kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
       2078
                        with self.builtin_trap:
    -> 2079
                           result = fn(*args, **kwargs)
       2080
                        return result
       2081
        <decorator-gen-58> in timeit(self, line, cell)
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
             # but it's overkill for just that one bit of state.
        187
               def magic_deco(arg):
    --> 188
                   call = lambda f, *a, **k: f(*a, **k)
        189
        190
                   if callable (arg):
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
```

```
1042
                        number = 1
       1043
                        for \_ in range(1, 10):
    -> 1044
                            time number = timer.timeit(number)
       1045
                            worst_tuning = max(worst_tuning, time_number / number)
       1046
                            if time number >= 0.2:
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
        137
                    gc.disable()
        138
                    try:
    --> 139
                        timing = self.inner(it, self.timer)
                    finally:
        140
        141
                        if gcold:
        <magic-timeit> in inner(_it, _timer)
        NameError: global name 'py_sin' is not defined
In [24]: %timeit c_sin()
                                                          # cython call C library
        NameErrorTraceback (most recent call last)
        <ipython-input-24-le5fbbb18c42> in <module>()
    ----> 1 get_ipython().magic(u'timeit c_sin()
                                                                                    # cython
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2156
                    magic_name, _, magic_arg_s = arg_s.partition(' ')
       2157
                    magic_name = magic_name.lstrip(prefilter.ESC_MAGIC)
    -> 2158
                    return self.run_line_magic(magic_name, magic_arg_s)
       2159
       2160
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/interactiveshell.pyc is
       2077
                            kwargs['local_ns'] = sys._getframe(stack_depth).f_locals
       2078
                        with self.builtin_trap:
    -> 2079
                            result = fn(*args, **kwargs)
       2080
                        return result
       2081
        <decorator-gen-58> in timeit(self, line, cell)
        /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magic.pyc in <lambda>(
                # but it's overkill for just that one bit of state.
        186
        187
                def magic_deco(arg):
                    call = lambda f, \stara, \star \stark: f(\stara, \star \stark)
    --> 188
```

```
189
   190
               if callable(arg):
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
                    number = 1
   1042
  1043
                    for \_ in range(1, 10):
-> 1044
                        time_number = timer.timeit(number)
  1045
                        worst_tuning = max(worst_tuning, time_number / number)
                       if time_number >= 0.2:
  1046
   /opt/python/2.7.10/lib/python2.7/site-packages/IPython/core/magics/execution.pyc is
               gc.disable()
   137
   138
               try:
--> 139
                    timing = self.inner(it, self.timer)
   140
               finally:
   141
                   if gcold:
    <magic-timeit> in inner(_it, _timer)
   NameError: global name 'c_sin' is not defined
```

8.5 Scaling for containers and algorithms

We've seen that NumPy arrays are really useful. Why wouldn't we always want to use them for data which is all the same type?

```
In [3]: def time_append_to_list(count):
            return repeat('before.append(0)',
                           'before=[0] * '+str(count),
                           number=10000)
In [4]: counts=np.arange(1,100000,10000)
        NameErrorTraceback (most recent call last)
        <ipython-input-4-20e43b1696b6> in <module>()
    ----> 1 counts=np.arange(1,100000,10000)
        NameError: name 'np' is not defined
In [5]: plt.plot(counts, map(time_append_to_list, counts))
        plt.ylim(ymin=0)
        NameErrorTraceback (most recent call last)
        <ipython-input-5-20893a41b370> in <module>()
    ----> 1 plt.plot(counts, map(time_append_to_list, counts))
          2 plt.ylim(ymin=0)
        NameError: name 'plt' is not defined
In [6]: plt.plot(counts, map(time_append_to_ndarray, counts))
        plt.ylim(ymin=0)
        NameErrorTraceback (most recent call last)
        <ipython-input-6-de519676749d> in <module>()
    ---> 1 plt.plot(counts, map(time_append_to_ndarray, counts))
          2 plt.ylim(ymin=0)
        NameError: name 'plt' is not defined
  Both scale well for accessing the middle element:
In [7]: def time_lookup_middle_element_in_list(count):
            before=[0]*count
            def totime():
                x=before[count/2]
            return repeat(totime, number=10000)
```

```
In [8]: def time_lookup_middle_element_in_ndarray(count):
            before=np.ndarray(count)
            def totime():
                x=before[count/2]
            return repeat(totime, number=10000)
In [9]: plt.plot(counts, map(time_lookup_middle_element_in_list, counts))
        plt.ylim(ymin=0)
        NameErrorTraceback (most recent call last)
        <ipython-input-9-4adfdbbf4641> in <module>()
    ----> 1 plt.plot(counts, map(time_lookup_middle_element_in_list, counts))
          2 plt.ylim(ymin=0)
        NameError: name 'plt' is not defined
In [10]: plt.plot(counts, map(time_lookup_middle_element_in_ndarray, counts))
         plt.ylim(ymin=0)
        NameErrorTraceback (most recent call last)
        <ipython-input-10-7798b6541fe4> in <module>()
    ----> 1 plt.plot(counts, map(time_lookup_middle_element_in_ndarray, counts))
          2 plt.ylim(ymin=0)
        NameError: name 'plt' is not defined
  But a list performs badly for insertions at the beginning:
In [11]: x=range(5)
In [12]: x
Out[12]: [0, 1, 2, 3, 4]
In [13]: x[0:0] = [-1]
In [14]: x
Out[14]: [-1, 0, 1, 2, 3, 4]
In [15]: def time_insert_to_list(count):
             return repeat('before[0:0]=[0]','before=[0]*'+str(count),number=10000)
In [16]: plt.plot(counts, map(time_insert_to_list, counts))
         plt.ylim(ymin=0)
```

```
---> 1 plt.plot(counts, map(time_insert_to_list, counts))
          2 plt.ylim(ymin=0)
        NameError: name 'plt' is not defined
  There are containers in Python that work well for insertion at the start:
In [17]: from collections import deque
In [18]: def time_insert_to_deque(count):
             return repeat ('before.appendleft(0)','from collections import deque; before=de
In [19]: plt.plot(counts, map(time_insert_to_deque, counts))
         plt.ylim(ymin=0)
        NameErrorTraceback (most recent call last)
        <ipython-input-19-0104c063f223> in <module>()
    ---> 1 plt.plot(counts, map(time_insert_to_deque, counts))
          2 plt.ylim(ymin=0)
        NameError: name 'plt' is not defined
  But looking up in the middle scales badly:
In [20]: def time_lookup_middle_element_in_deque(count):
             before=deque([0]*count)
             def totime():
                  x=before[count/2]
             return repeat(totime, number=10000)
In [21]: plt.plot(counts, map(time_lookup_middle_element_in_deque, counts))
         plt.ylim(ymin=0)
        NameErrorTraceback (most recent call last)
        <ipython-input-21-fa19c4d72a30> in <module>()
    ----> 1 plt.plot(counts, map(time_lookup_middle_element_in_deque, counts))
          2 plt.ylim(ymin=0)
```

NameErrorTraceback (most recent call last)

<ipython-input-16-6d3166f1d4b3> in <module>()

```
NameError: name 'plt' is not defined
```

What is going on here?

Arrays are stored as contiguous memory. Anything which changes the length of the array requires the whole array to be copied elsewhere in memory.

This copy takes time proportional to the array size.

The Python list type is **also** an array, but it is allocated with **extra memory**. Only when that memory is exhausted is a copy needed.

If the extra memory is typically the size of the current array, a copy is needed every 1/N appends, and costs N to make, so **on average** copies are cheap. We call this **amortized constant time**.

The deque type works differently: each element contains a pointer to the next. Inserting elements is therefore very cheap, but looking up the Nth element requires traversing N such pointers.

8.5.1 Dictionary performance

For another example, let's consider the performance of a dictionary versus a couple of other ways in which we could implement an associative array.

```
In [22]: class evildict(object):
             def __init__(self, data):
                 self.data=data
             def ___getitem___(self,akey):
                 for key, value in self.data:
                     if key==akey:
                         return value
                 raise KevError()
In [23]: me=[["Name","James"],["Job","Programmer"],["Home","London"]]
In [24]: me_evil=evildict(me)
In [25]: me_evil["Job"]
Out [25]: 'Programmer'
In [26]: me_dict=dict(me)
In [27]: me_evil["Job"]
Out [27]: 'Programmer'
In [28]: x=["Hello", "Goodbye", "whatever", "something", "this", "apple"]
In [29]: sorted(x, key=lambda el: el.lower())
Out[29]: ['apple', 'Goodbye', 'Hello', 'something', 'this', 'whatever']
In [30]: class sorteddict(object):
             def __init__(self, data):
                 self.data=sorted(data, key = lambda x:x[0])
                 self.keys=map(lambda x:x[0],self.data)
             def getitem (self,akey):
                 from bisect import bisect_left
```

```
loc=bisect_left(self.keys, akey)
                 if loc!=len(self.data):
                     return self.data[loc][1]
                 raise KeyError()
In [31]: me_sorted=sorteddict(me)
In [32]: me_sorted["Job"]
Out[32]: 'Programmer'
In [33]: def time_dict_generic(ttype, count, number=10000):
             from random import randrange
             keys=range(count)
             values=[0]*count
             data=ttype(zip(keys, values))
             def totime():
                 x=data[keys[count/2]]
             return repeat (totime, number=10000)
In [34]: time_dict=lambda count: time_dict_generic(dict, count)
         time_sorted=lambda count: time_dict_generic(sorteddict, count)
         time_evil=lambda count: time_dict_generic(evildict, count)
In [35]: plt.plot(counts, map(time_sorted, counts))
         plt.ylim(ymin=0)
        NameErrorTraceback (most recent call last)
        <ipython-input-35-04b55b5c57dd> in <module>()
    ---> 1 plt.plot(counts, map(time_sorted, counts))
          2 plt.ylim(ymin=0)
        NameError: name 'plt' is not defined
```

We can't really see what's going on here for the sorted example as there's too much noise, but theoretically we should get **logarithmic** asymptotic performance. We write this down as $O(\ln N)$. This doesn't mean there isn't also a constant term, or a term proportional to something that grows slower (such as $\ln(\ln N)$): we always write down just the term that is dominant for large N. We saw before that list is O(1) for appends, O(N) for inserts. Numpy's array is O(N) for appends.

```
<ipython-input-36-8fd504b57827> in <module>()
----> 1 counts=np.arange(1,1000,100)
        2 plt.plot(counts,map(time_evil,counts))
        3 plt.ylim(ymin=0)

NameError: name 'np' is not defined
```

The simple check-each-in-turn solution is O(N) - linear time.

```
In [37]: counts=np.arange(1,100000,10000)
        plt.plot(counts,map(time_dict,counts))
        plt.ylim(ymin=0)

        NameErrorTraceback (most recent call last)

        <ipython-input-37-559ddc2048bc> in <module>()
----> 1 counts=np.arange(1,100000,10000)
        2 plt.plot(counts,map(time_dict,counts))
        3 plt.ylim(ymin=0)

        NameError: name 'np' is not defined
```

Python's built-in dictionary is, amazingly, O(1): the time is **independent** of the size of the dictionary. This uses a miracle of programming called the Hash Table: you can learn more about these issues here This material is pretty advanced, but, I think, really interesting!

Optional exercise: determine what the asymptotic performance for the Boids model in terms of the number of Boids. Make graphs to support this. Bonus: how would the performance scale with the number of dimensions?