

Scientific Python Tutorial

Scientific Python

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This Tutorial

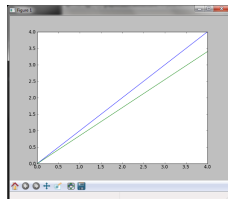
- This tutorial is for someone with basic python experience.
- First:
 - 1 matplotlib - plotting library, like Matlab
 - 2 numpy - fast arrays manipulation
 - 3 scipy - math methods galore.
 - 4 ipython - better interactive python
- Then I will cover a few intermediate details about python programming in general

Plotting in scripts

- `matplotlib` is a package that has many modules, `pyplot` is the main driver.
- `matplotlib` is designed for both interactive and script-based use.

Plotting in scripts

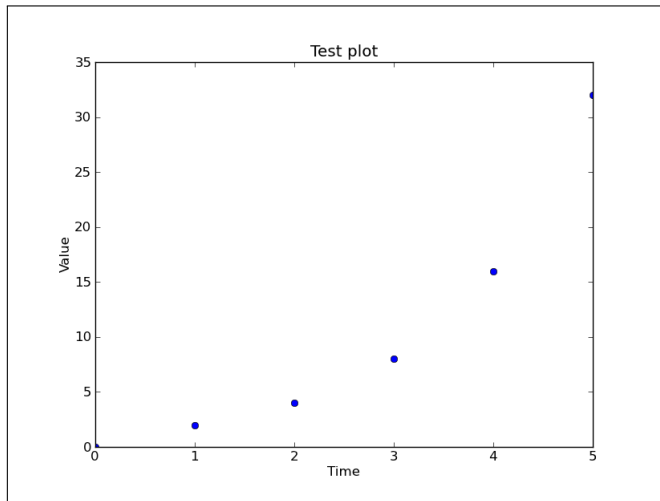
- `matplotlib` is a package that has many modules, `pyplot` is the main driver.
- `matplotlib` is designed for both interactive and script-based use.
- a `Figure` can contain many `Axes`, which contain many plots.
- `pyplot` creates a default `Figure` and `Axes` if you just want get to plotting things quickly.



Basic Example

```
1 from matplotlib import pyplot
2
3 pyplot.plot([0, 2, 4, 8, 16, 32], "o")
4
5 pyplot.ylabel("Value")
6 pyplot.xlabel("Time")
7 pyplot.title("Test plot")
8
9 pyplot.show()
```

Basic Plot - Results



World Population - Practice Part 1

Explaining what's there

practice/world_population.py

```
3 def get_data():
4     data = file("world_population.txt", "r").readlines()
5     dates = []
6     populations = []
7     for point in data:
8         date, population = point.split()
9         dates.append(date)
10        populations.append(population)
11    return dates, populations
```

1 We read in the data

World Population - Practice Part 1

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- 1 We read in the data
- 2 For each line ('point') we need to separate the date from population

World Population - Practice Part 1

Explaining what's there

practice/world_population.py

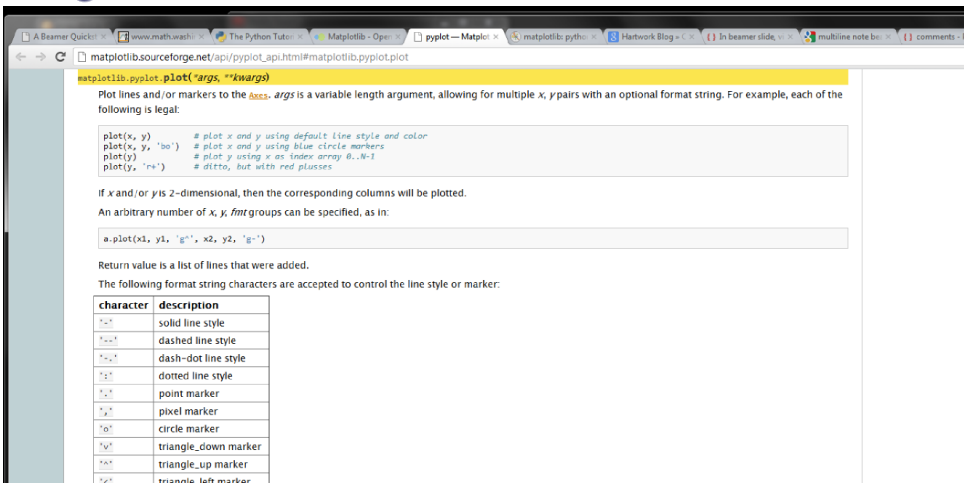
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4     data = file("world_population.txt", "r").readlines()
5     dates = []
6     populations = []
7     for point in data:
8         date, population = point.split()
9         dates.append(date)
10        populations.append(population)
11    return dates, populations
```

- 1 We read in the data
- 2 For each line ('point') we need to separate the date from population
- 3 `split()` splits text at any whitespace, by default.

World Population - Getting Help

How to read online docs

- 1 Google "matplotlib" and pick first choice
- 2 "Quick Search" (on right side) for "pyplot.plot"
- 3 Select result entitled "matplotlib.pyplot.plot"



The screenshot shows a web browser with multiple tabs. The active tab is titled "matplotlib.pyplot.plot" and displays the API documentation for the `matplotlib.pyplot.plot` function. The page content includes:

- A yellow header bar with the text `matplotlib.pyplot.plot(*args, **kwargs)`.
- A paragraph explaining that `plot` takes lines and/or markers to the `Axes`, with `args` being a variable length argument for multiple `x, y` pairs and an optional format string.
- A code block showing four examples of `plot` usage:

```
plot(x, y)           # plot x and y using default line style and color
plot(x, y, 'bo')      # plot x and y using blue circle markers
plot(y)              # plot y using x as index array 0..N-1
plot(y, 'r+')         # ditto, but with red plusses
```
- A paragraph stating that if `x` and/or `y` is 2-dimensional, the corresponding columns will be plotted.
- A paragraph stating that an arbitrary number of `x, y, fmt` groups can be specified, as in:

```
a.plot(x1, y1, 'g^', x2, y2, 'g-')
```
- A paragraph stating that the return value is a list of lines that were added.
- A paragraph stating that the following format string characters are accepted to control the line style or marker.
- A table with 2 columns: "character" and "description".

character	description
"-"	solid line style
"--"	dashed line style
"-."	dash-dot line style
":"	dotted line style
"."	point marker
"x"	pixel marker
"o"	circle marker
"v"	triangle_down marker
"^"	triangle_up marker
"<"	triangle_left marker

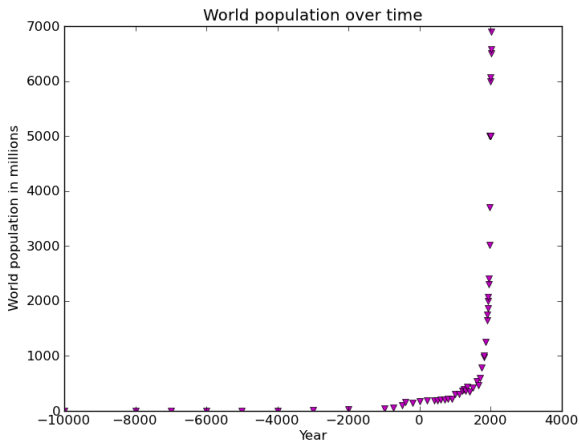
World Population - Practice Part 2

Your Assignment

```
13 def plot_world_pop(dates, populations):  
14     pass  
15  
16 dates, populations = get_data()  
17 plot_world_pop(dates, populations)  
18 pyplot.show()
```

- 1 Make a plot of population (y) vs dates (x)
- 2 Title: "World population over time"
- 3 Y-axis: "World population in millions"
- 4 X-axis: "Year"
- 5 Set the plot type to a
Magenta, downward-triangle

World Population - Final



Life Expectancy - Practice Part 1

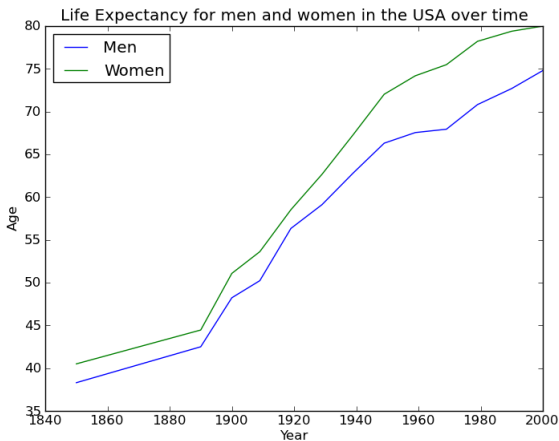
practice/life_expectancies_usa.py

```
1 from matplotlib import pyplot
2
3 def get_data():
4     # each line: year,men,women
5     data = file("life_expectancies_usa.txt", "r").readlines()
6     dates = []
7     men = []
8     women = []
9     # finish me!
10    return dates, men, women
11
12 def plot_expectancies(dates, men, women):
13     pass
14
15 dates, men, women = get_data()
16 plot_expectancies(dates, men, women)
17 pyplot.show()
```

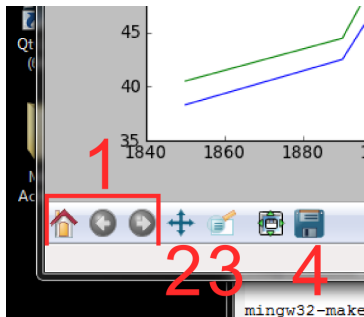
Life Expectancy - Practice Part 2

- 1 Use `split(',')` to split strings at commas
- 2 Add a label to each plot (look at documentation)
- 3 Label Axes and give a title.
- 4 Call `plot 2x` to plot two lines
- 5 Add a legend: `pyplot.legend`
 - ▶ “Quick Search” again
 - ▶ search for “`pyplot.legend`”

Life Expectancy - Results

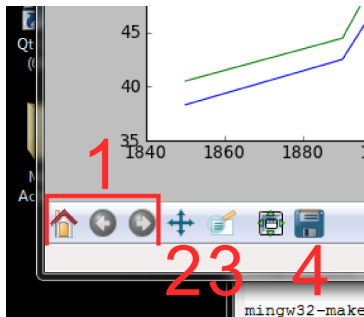


Plotting Interactively



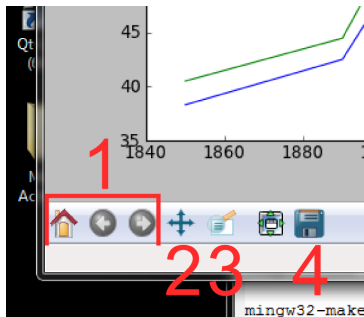
- 1 **Home - Backward - Forward** - Control edit history

Plotting Interactively



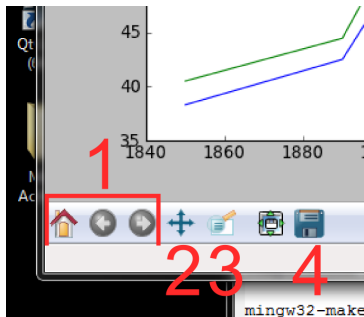
- 1 **Home - Backward - Forward** - Control edit history
- 2 **Pan - Zoom** - Left click + drag shifts center, right click + drag changes zoom

Plotting Interactively



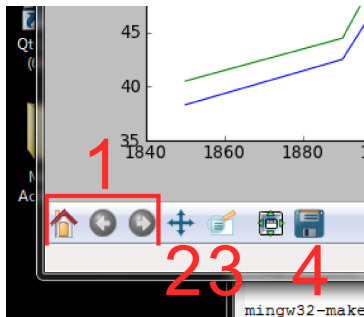
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Plotting Interactively



- ① **Home - Backward - Forward** - Control edit history
- ② **Pan - Zoom** - Left click + drag shifts center, right click + drag changes zoom
- ③ **Zoom** - Select zoom region
- ④ **Save**

Plotting Interactively



- 1 **Home - Backward - Forward** - Control edit history
- 2 **Pan - Zoom** - Left click + drag shifts center, right click + drag changes zoom
- 3 **Zoom** - Select zoom region
- 4 **Save**

`pyplot.savefig('filename')` is an alternative to `pyplot.show()` when you are using pyplot non-interactively.

Matplotlib Resources

- **Possibilities:**

`matplotlib.org/gallery.html`

`http://matplotlib.org/basemap/users/examples.html`

- **Guide/Tutorial:**

`matplotlib.org/users/index.html`

- **Questions:**

`stackoverflow.com`

Or contact us: `help@scv.bu.edu`

- **Source for tutorial:**

`openhatch.org/wiki/Matplotlib`

Array Creation

- By convention: `import numpy as np`
- `x = np.array([1,2,3], int)`; `x` is a Numpy array
- `x` is like a list, but certain operations are much faster

Array Creation

A 2D array:

```
1 A = np.array(((1,0,0),  
2               (0, 0, -1),  
3               (0, 1, 0)))
```

Array Creation

- `np.ones(5)` makes `array([ 1., 1., 1., 1., 1.])`
- `np.zeros` same thing for zeroes

Array Creation

- `np.ones(5)` makes `array([ 1., 1., 1., 1., 1.])`
- `np.zeros` same thing for zeroes
- `np.zeros((2,2))` makes `array([[0., 0.], [0., 0.]])`
that is a 2D, 2x2 array of zeros

Array Creation

- `np.arange`, numpy's version of built-in `range` method
- `np.linspace` is similar to `np.arange` but you pass the number of elements, *not* step size

Array Basics - Results

```
4 >>> import numpy as np
5 >>> x = np.array(((1, 2, 3), (4, 5, 6)))
6 >>> x.size # total number of elements
7 6
8 >>> x.ndim # number of dimensions
9 2
10 >>> x.shape # number of elements in each dimension
11 (2L, 3L)
12 >>> x[1,2] # first index is the rows, then the column
13 6
14 >>> x[1] # give me '1' row
15 array([4, 5, 6])
16 >>> x[1][2]
17 6
18 >>> x.dtype
19 dtype('int32')
```

Basic Operations

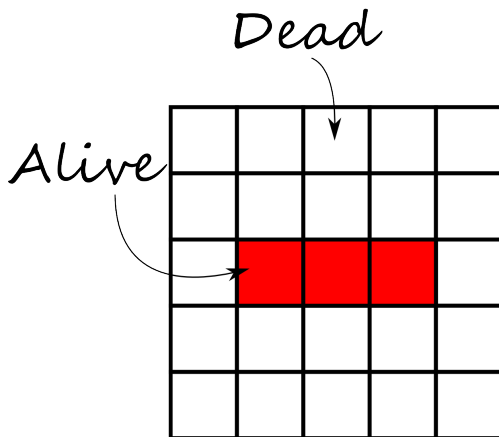
```
14 x = np.array([0, np.pi/4, np.pi/2])
15 np.sin(x)
16 np.dot([2, 2, 2], [2, 2, 2])
```

Basic Operations

```
14 x = np.array([0, np.pi/4, np.pi/2])
15 np.sin(x)
16 np.dot([2, 2, 2], [2, 2, 2])
```

```
22 >>> x = np.array([0, np.pi/4, np.pi/2])
23 >>> np.sin(x)
24 array([ 0.          ,  0.70710678,  1.          ])
25 >>> np.dot([2, 2, 2], [2, 2, 2])
26 12
```

It's a Simple Game

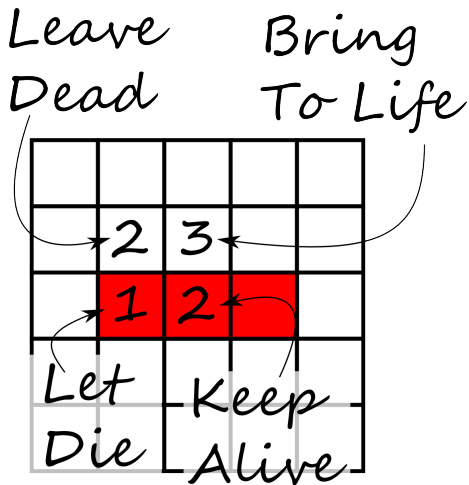


Calculating Neighbors

Neighbors
Number

0	0	0	0	0
1	2	3	2	1
1	1	2	1	1
1	2	3	2	1
0	0	0	0	0

Use the Neighbors to Update



A Practice Problem

In the `practice` directory:

1 `conway.py` is a program; try it out.

A Practice Problem

In the `practice` directory:

- 1 `conway.py` is a program; try it out.
- 2 `conway_work.py` is an assignment; try to do it.
- 3 `test_conway.py` is a program to test your work.

Remember, the `shape` attribute:

```
1 a = np.array(((1,2),(3,4),(5,6))) # make a 3x2
2 print a.shape[0] # prints 3
3 print a.shape[1] # prints 2
```

Conway's Game of Life

`np.roll(a, 1, axis=0)` returns a new array that cycles the values.

```
1 >>> a
2 array([[0, 1, 2],
3        [3, 4, 5],
4        [6, 7, 8]])
5 >>> np.roll(a, 1, axis=0)
6 array([[6, 7, 8],
7        [0, 1, 2],
8        [3, 4, 5]])
```

This can be used to make the `neighbors` function.

Conway's Game of Life

`np.where(b == 0)` returns a series of indices where it's true.

`np.where(b == 0, -1, b)` to replace 0's with -1's.

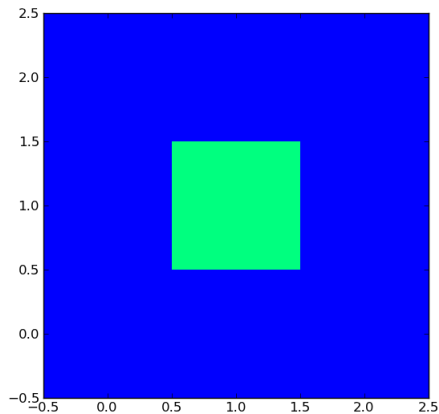
```
1 >>> b
2 array([[ 0.,  0.,  0.],
3        [ 2.,  2.,  2.],
4        [ 0.,  3.,  0.]])
5 >>> np.where(b == 0)
6 (array([0, 0, 0, 2, 2]), array([0, 1, 2, 0, 2]))
7 >>> np.where(b == 0, -1, b)
8 array([[ -1.,  -1.,  -1.],
9        [  2.,   2.,   2.],
10       [ -1.,   3.,  -1.]])
```

Look up the `np.logical_or` method; this and `np.where` can be used to redefine the `update` function.

Matplotlib Imshow

```
0 import matplotlib.pyplot as plt
1 import numpy as np
2 a = np.zeros((3,3))
3 a[1,1] = 1
4 plt.imshow(a,
5             interpolation='nearest',
6             cmap=plt.winter(),
7             origin='lower')
```

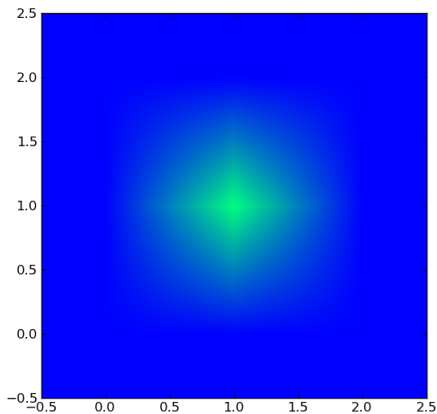
Nearest Neighbors



Matplotlib Imshow

```
11 plt.imshow(a,  
12 #           interpolation='nearest',  
13           cmap=plt.winter(),  
14           origin='lower')  
15 plt.show()
```

Default: usually 'bilinear'



Plenty More

- `www.scipy.org/Tentative_NumPy_Tutorial`
- "Universal Functions" section
- PyTrieste Numpy Tutorial

scipy: Many Useful Scientific Tools

<http://docs.scipy.org/doc/scipy/reference/tutorial/index.html>

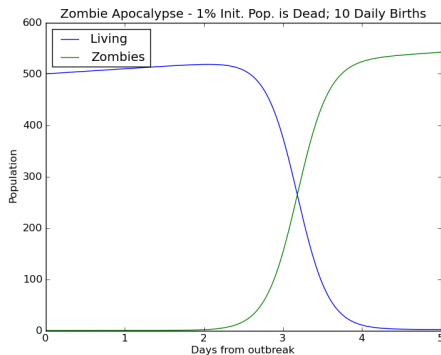
- Numpy
- Integration
- Optimization
- Interpolation
- FFT
- Linear Algebra
- Statistics
- And much more....

Constants

```
4 >>> from scipy import constants
5 >>> constants.c # speed of light
6 299792458.0
7 >>> # physical constants: value, units, uncertainty
8 >>> constants.physical_constants["electron mass"]
9 (9.10938291e-31, 'kg', 4e-38)
10 >>> # look-up constants, only first 3 !
11 >>> masses = constants.find("mass")[:3]
12 >>> for val in masses:
13 ...     print "'{}' is available".format(val)
14 ...
15 'Planck mass' is available
16 'Planck mass energy equivalent in GeV' is available
17 'alpha particle mass' is available
```

Zombie Apocalypse - ODEINT

http://www.scipy.org/Cookbook/Zombie_Apocalypse_ODEINT



Zombie Apocalypse - ODEINT

generated/scipy.integrate.odeint.html

on » SciPy v0.11.dev Reference Guide (DRAFT) » Integration and ODEs (scipy.integrate) » previous | next | modules | modules | index

scipy.integrate.odeint

```
scipy.integrate.odeint(func, y0, t, args=(), Dfun=None, col_deriv=0, full_output=0, ml=None, mu=None,
    rtol=None, atol=None, tcrit=None, h0=0.0, hmax=0.0, hmin=0.0, ixpr=0, mxstep=0, mxhnil=0, mxordn=12,
    mxords=5, printmessg=0)
```

[\[source\]](#)

Integrate a system of ordinary differential equations.

Solve a system of ordinary differential equations using lsoda from the FORTRAN library odepack.

Solves the initial value problem for stiff or non-stiff systems of first order ode-s:

```
dy/dt = func(y, t0, ...)
```

where y can be a vector.

Parameters :

func : callable(y, t0, ...)

Computes the derivative of y at t0.

y0 : array

Initial condition on y (can be a vector).

t : array

A sequence of time points for which to solve for y. The initial value point should be the first element of this sequence.

args : tuple

Zombie Apocalypse - ODEINT

Look at `examples\zombie.py`

```
5 def calc_rate(P=0, d=0.0001, B=0.0095, G=0.0001, A=0.0001, S0=500):
6     def f(y, t):
7         Si = y[0]
8         Zi = y[1]
9         Ri = y[2]
10        # the model equations (see Munz et al. 2009)
11        f0 = P - B*Si*Zi - d*Si
12        f1 = B*Si*Zi + G*Ri - A*Si*Zi
13        f2 = d*Si + A*Si*Zi - G*Ri
14        return [f0, f1, f2]
15    Z0 = 0 # initial zombie population
16    R0 = 0 # initial death population
17    y0 = [S0, Z0, R0] # initial condition vector
18    t = np.linspace(0, 5., 1000) # time grid
19    # solve the DEs
20    soln = odeint(f, y0, t)
21    S = soln[:, 0]
22    Z = soln[:, 1]
23    R = soln[:, 2]
24    return t, S, Z
```

ipython - plotting

Amazing interactive python.

Using the '-pylab' flag, you can get plotting for free

```
1 % ipython -pylab
2 ...
3 In [1]: plot(range(10))
```

ipython - Magic Functions

Amazing interactive python.

It provides “Magic” functions:

- `cd` - like unix change directory
- `ls` - list directory
- `timeit` - time execution of statement
- and so on ...

ipython - Logging

Amazing interactive python.

You can log an interactive session:

```
1 In [1]: logstart mylogfile.py
```

- Everything you type will be recorded to mylogfile.py
- `logon` and `logoff` turn it on and off
- `logstop` turns it off and saves file
- To re-run it in ipython, us the **run** command:

```
1 In [1]: run -i mylogfile.py
```

ipython - Misc.

Amazing interactive python.

- You can use `?` instead of `help()`.

In [1]: `len?` and Enter will print help

In fact you get even more information than the standard `help()`

- Tab-completion
- Start typing a method, and "pop-up" help is shown
You need a newer version than Katana's, and
you need to type `ipython qtconsole`

Simple Parallelized Python

`multiprocessing` is a module that allows you to easily start other processes. They do **not** share memory, but `multiprocess` helps them communicate info/data.

Pool

`multiprocessing.Pool` creates a pool of processes that you give tasks to perform. See in

`examples/mp_vowels_pool.py`

```
16     nproc = multiprocessing.cpu_count()
17     task_pool = multiprocessing.Pool(
18         processes=nproc,
19         initializer=start_proc)
20
21     words = "Mary had a little lamb".split()
```

map

`task_pool.map` takes a function and a list of arguments, and applies that function to each argument, in parallel.

```
24 map_results = task_pool.map(count_vowels, words)
```

The `map` method is blocking. The code progresses when all tasks are complete.

apply_async

`task_pool.apply_async` takes a function and a sequence of arguments and applies that function to that argument.

```
27     async_results = []
28     for word in words:
29         async_results.append(
30             task_pool.apply_async(count_vowels,
31                                   (word,)))
32
33     task_pool.close() # no more tasks
34     task_pool.join() # wait here until all
```

This is not blocking

apply_async, getting results

`task_pool.map` just returns a list of results

```
39     for word, nvowels in zip(words, map_results):
40         print "'{word:s}' has {nvowels:d} vowels".format(word=word,
41                                                         nvowels=nvowels)
```

But `task_pool.apply_async` returns an object from which you can `get` results.

```
45     for word, result in zip(words, async_results):
46         print "'{word:s}' has {nvowels:d} vowels".format(word=word,
47                                                         nvowels=result.get())
```

Outline for section 2

1 Scientific Python

2 Beyond the Basics

- Super Scripting
- More on Functions
- String Formatting
- Files
- External Programs
- Command line arguments

3 Solving Laplace's Equation

- `pass` is python's way of saying
“Keep moving, nothing to see here...”.

- `pass` is python's way of saying "Keep moving, nothing to see here..." .
- It's used for yet unwritten function.
- If you try to call a function that doesn't exist, you get an error.

- `pass` is python's way of saying "Keep moving, nothing to see here..."
- It's used for yet unwritten function.
- If you try to call a function that doesn't exist, you get an error.
- `pass` just creates a function that does nothing.
- Great for planning work!

```
1 def step1():  
2     pass  
3 step1() # no error!  
4 step2() # error, darn!
```

- `None` is Python's formal value for “nothing”
- Use this as a default value for a variable,
- or as a return value when things don't work, and you don't want a catastrophic error.

- `None` is Python's formal value for “nothing”
- Use this as a default value for a variable,
- or as a return value when things don't work, and you don't want a catastrophic error.
- Test if something `is None`, to see if you need to handle these special cases

```
1 name=None
2 if name is None:
3     name = 'Johnny'
```

```
"__main__"
```

- Every module has a name, which is stored in `__name__`
- The script/console that you are running is called `"__main__"`.

`"__main__"`

- Every module has a name, which is stored in `__name__`
- The script/console that you are running is called `"__main__"`.
- Use this to make a file both a module *and* a script.

```
1 # module greeting.py
2 def hey_there(name):
3     print "Hi!", name, "... How's it going?"
4
5 hey_there('Joey')
6 if __name__ == "__main__":
7     hey_there('Timmy')
```

`python greeting.py` → "Hi! Timmy ... How's it going?"

The Docstring

- This is an un-assigned string that is used for documentation.
- It can be at the top of a file, documenting a script or module
- or the first thing inside a function, documenting it.

The Docstring

- This is an un-assigned string that is used for documentation.
- It can be at the top of a file, documenting a script or module
- or the first thing inside a function, documenting it.
- This is what `help()` uses...

```
1 def dot_product(v1, v2):
2     """Perform the dot product of v1 and v2.
3
4     'v1' is a three element vector.
5     'v2' is a three element vector.
6     """
7     sum = 0 #....
```

Keyword Arguments

- Arguments that have default values.
- In the function signature, `keyword=default_value`
- `None` is a good default if you want to make a decision

```
1 def hello(name='Joe', repeat=None):  
2     if repeat is None:  
3         repeat=len(name)  
4     print 'Hi!', name*repeat
```

Returning Values

- A function can return multiple values.
- Formally this creates a **Tuple** - an *immutable* list

Returning Values

- A function can return multiple values.
- Formally this creates a **Tuple** - an *immutable* list
- You can collect the returned values as a Tuple, or as individual values.

```
1 def pows(val):  
2     return val, val*val, val*val*val  
3 two, four, eight = pows(2)  
4 ones = pows(1)  
5 print ones[0], ones[1], ones[2] # 1 1 1
```

```
‘string’.format()
```

- Strings can be paired with values to control printing.

```
4 >>> "Hi there {}".format('Yann')
5 'Hi there Yann!'
6 >>> "Coords: {}, {}".format(-1, 2)
7 'Coords: -1, 2;'
8 >>> "{1}, the cost is {0:.2f}".format(1125.747025, 'Y
9 'Yann, the cost is 1125.75'
```

Keyword arguments to format

- It's sometimes tricky to format many values
- You can name some of the format targets

```
9 email = """
10 Subject: {subject}
11 Date: {mon:2d}/{day:2d}/{year:2d}
12 Message: {msg}
13 """
14 print email.format(mon=10, year=12, day=31,
15                  subject='Happy Halloween',
16                  msg='Booh')
```

Keyword arguments to format – result

```
13 >>> email = """
14 ... Subject: {subject}
15 ... Date: {mon:2d}/{day:2d}/{year:2d}
16 ... Message: {msg}
17 ... """
18 >>> print email.format(mon=10, year=12, day=31,
19 ...                     subject='Happy Halloween',
20 ...                     msg='Booh ')
21
22 Subject: Happy Halloween
23 Date: 10/31/12
24 Message: Booh
```

More features at:

<http://docs.python.org/library/string.html>

csv reader and writer

- For reading and writing comma-separated-values
- `csv.reader` for reading, `csv.writer` for writing
- Dialects option correspond to predefined formats
- 'excel' for excel output without needing to know the separator and quote characters

```
1 reader = csv.reader(file)
2 for row in reader:
3     # row is a list
4 writer = csv.writer(file)
5 writer.writerow([1,2,3])
```


subprocess – running external programs

```
1 import subprocess
2 output = subprocess.call(['ls', '-l'])
3 print "output = ", output
```

- `subprocess` provides many tools
- The most basic is the `call` function.
- It takes a list that is joined and executed.
- `output` just holds the exit code (0 if successful)
- `check_output` is like `call` but 1) returns output and 2) causes an error if program fails

argparse – easy command line arguments

- `argparse` module is the easiest way.
- You first create a `ArgumentParser` object
- You define the allowable arguments with the `add_argument` function
- You can add required or optional arguments
- `sys.argv` is a list of arguments passed to the program/script.
- Pass this list to `parse_args` function to process and get an object with your parameters defined.

argparse – example

Look over `examples\argparse_ex.py`

```
1 import sys
2 import argparse
3 parser = argparse.ArgumentParser(description='Plot zombie statistics')
4 parser.add_argument('prefix', help='the prefix for the plot filename')
5 parser.add_argument('-p', dest='pop', default=500, type=int,
6                     help='Set the starting population')
7 parser.add_argument('-s', dest='show',
8                     help='Show the figure', action='store_true')
9 parser.add_argument('city', help='Plot information for a specific city',
10                    nargs='?', default=None)
11
12 args = sys.argv[1:]
13 params = parser.parse_args(args)
14
15 print "prefix = ", params.prefix
16 print "pop = ", params.pop
17 if params.city is not None:
18     print "city = ", params.city
19 print "show? "
20 if params.show:
21     print "yes!"
22 else:
23     print "no :-(
```

Solve Laplace's Equation 1a

- Solve $\nabla^2 u = 0$

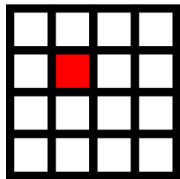
Solve Laplace's Equation 1a

- Solve $\nabla^2 u = 0$
- Solve iteratively, each time changing u with following equation:
$$u_{j,l}^{n+1} = 1/4(u_{j+1,l}^n + u_{j-1,l}^{n+1} + u_{j,l+1}^n + u_{j,l-1}^{n+1})$$
- Just an averages of the neighboring points.

Solve Laplace's Equation 1a

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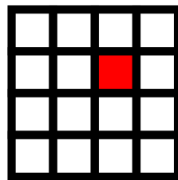
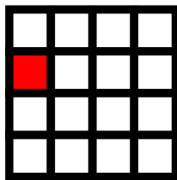
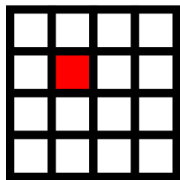
$$U_{j,l}^{n+1} = 1/4 ($$



Solve Laplace's Equation 1b

- Solve $\nabla^2 u = 0$
- Solve iteratively, each time changing u with following equation:
$$u_{j,l}^{n+1} = 1/4(u_{j+1,l}^n + u_{j-1,l}^n + u_{j,l+1}^n + u_{j,l-1}^n)$$
- Just an averages of the neighboring points.

$$U_{j,l}^{n+1} = 1/4 (U_{j-1,l}^n + U_{j+1,l}^n + \dots$$



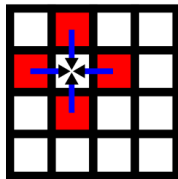
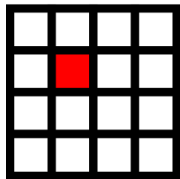
Solve Laplace's Equation 1c

- Solve $\nabla^2 u = 0$
- Solve iteratively, each time changing u with following equation:

$$u_{j,l}^{n+1} = 1/4(u_{j+1,l}^n + u_{j-1,l}^{n+1} + u_{j,l+1}^n + u_{j,l-1}^{n+1})$$

- Just an averages of the neighboring points.

$$U_{j,l}^{n+1} = 1/4 (\quad \dots \quad)$$



Solve Laplace's Equation 1d

- Solve $\nabla^2 u = 0$
- Solve iteratively, each time changing u with following equation:
$$u_{j,l}^{n+1} = 1/4(u_{j+1,l}^n + u_{j-1,l}^{n+1} + u_{j,l+1}^n + u_{j,l-1}^{n+1})$$
- Just an average of the neighboring points.
- Repeat this calculation until $\text{rms}(u^{n+1} - u^n) < \epsilon$, some threshold
- Set some limit on total number of iterations
- `practice/laplace.py`

Solve Laplace's Equation 2

First task:

```
19 def pure_python_step(u):
20     '''Pure python implementation of Gauss-Siedel method. Performs
21     iteration.'''
22     rms_err = 0
23     # use for loop to loop through each element in u
24     #     temporarily store old value to later calculate rms_err
25     #     update current u using 4 point averaging
26     #     update running value of rms_err
27     # when done looping complete rms_err calculation and return it
28     return rms_err
```

Slicing - 1

```
19 x = np.array((1, 2, 3, 4, 5, 6))
20 x[2]
21 x[2:5]
22 x[2:-1]
23 x[:5]
24 x[:5:2] = 10
25 x
```

Slicing - 2

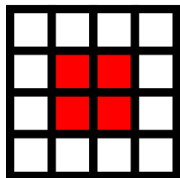
```
29 >>> x = np.array((1, 2, 3, 4, 5, 6))
30 >>> x[2]
31 3
32 >>> x[2:5]
33 array([3, 4, 5])
34 >>> x[2:-1]
35 array([3, 4, 5])
36 >>> x[:5]
37 array([1, 2, 3, 4, 5])
38 >>> x[:5:2] = 10
39 >>> x
40 array([10,  2, 10,  4, 10,  6])
```

Array Copying

```
43 >>> a = np.array((1,2,3,4))
44 >>> b = a
45 >>> b is a
46 True
47 >>> c = a.view()
48 >>> c.shape = 2,2
49 >>> c[1,1]=10
50 >>> c
51 array([[ 1,  2],
52        [ 3, 10]])
53 >>> a
54 array([ 1,  2,  3, 10])
55 >>> d = a.copy()
```

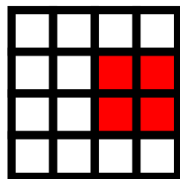
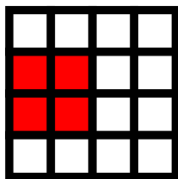
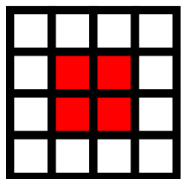
Solve Laplace's Equation 3a

$$U_{j,l}^{n+1} = 1/4 ($$



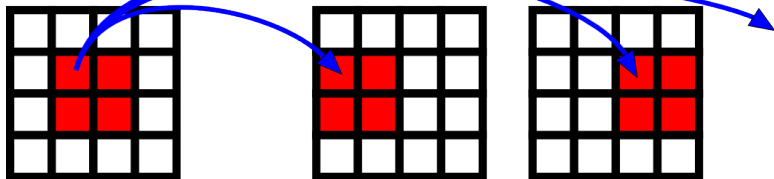
Solve Laplace's Equation 3b

$$U_{j,l}^{n+1} = 1/4 (U_{j-1,l}^n + U_{j+1,l}^n + \dots)$$



Solve Laplace's Equation 3c

$$U_{j,l}^{n+1} = 1/4 (U_{j-1,l}^n + U_{j+1,l}^n + \dots)$$



Solve Laplace's Equation 3d

Second task:

```
35 def numpy_step(u):
36     '''Numpy based Jacobi's method. Performs one iteration.'''
37     # make a copy so that you can calculate the error
38     u_old = u.copy()
39     # use slicing to shift array
40     # utmp = u[1:-1, 1:-1] makes a new array, so that utmp[0,0] is
41     # as u[1,1]
42     # then
43     # utmp = u[0:-2, 1:-1] makes a new array that leads to a shift
44     # because utmp[0,0] is the same as u[0, 1]
45     # use this concept to solve this equation in on line
46     # u = 1/4*(u_{j-1,i} + u_{j+1,i} + u_{j, i-1} + u_{j, i+1})
47     return calc_err(u, u_old)
```

Solve Laplace's Equation 4a

Third task:

```
4 def laplace_driver(u, stepper, maxit=100, err=1e3):
5     '''Repeatedly call stepper(u) to solve  $\nabla^2 u = 0$  until
6     rms error < err or maxit number of iterations is reached.
7
8     'u' - a numpy array
9     'stepper' - a function whose sole argument is u
10    '''
11    rms_err = 0
12    # take one step with stepper, to define initial rms_err
13    # loop until rms_err < err
14    #     check to see that number of iterations is less than maxit
15    #     perform single iteration using stepper method
16    # return rms_error
17    return rms_err
```

Solve Laplace's Equation 4b

```
59 def time_method(stepper):
60     '''Time how long a particular stepper takes to solve an ideal
61     u = set_bc(np.zeros((100,100)))
62     start = time.time()
63     err = laplace_driver(u, stepper)
64     return time.time()-start
65
66 if __name__ == "__main__":
67     pure_python_time = time_method(pure_python_step)
68     numpy_time = time_method(numpy_step)
69     print "Pure python method takes {:.3f} seconds".format(pure_python_time)
70     print "Numpy method takes {:.3f} seconds".format(numpy_time)
```

Solve Laplace's Results

```
1 Pure python method takes 3.624 seconds  
2 Numpy method takes 0.016 seconds
```

Resources

- [SCV help site](#)
- [Numpy Tutorial](#)
- [Scipy tutorial](#)
- [Scientific Python Tutorial](#)
- [Another Scientific Python Tutorial](#)
- [iPython Tutorial](#)

What I Didn't Cover

- [Exception Handling](#)
- [Duck Typing](#)
- [Virtualenv](#)
- [Pandas](#)
- [mpi4py](#)
- And many other useful things