Introduction to Python for Science

Release 1

Gaël Varoquaux

November 24, 2009

Contents

Why Python

- Efficient coding: what is the point of very fast simulations, if it takes longer to write them than to run them?
- Full-fledge, non-specialized, programming language.
- Communication: code should read like a book.
- Code that we understand: developing an intuition, an understanding of the algorithms through exploratory coding and interaction.

Installing with distributions:

- EPD: http://www.enthought.com/products/epd.php
- Python(x,y): http://www.pythonxy.com

Resources

Simple

- **In French** Python for Science: http://dakarlug.org/pat/scientifique/html/index.html
- **Videos** http://www.archive.org/search.php?query=SciPy%202009%20tutorial
- The Python tutorial (excellent): http://docs.python.org/tutorial/

Advanced

- http://docs.scipy.org/
- *Python Scripting for Computational Science*, Hans Petter Langtangen, Springer
- *Python Cookbook*, David Ascher, Matt Margolin, Alex Martelli, O'Reilly

CHAPTER 1

The workflow: IPython and a text editor

Interactive work to test and understand algorithm

Python is a general-purpose language. As such, there is not one blessed environement to work into, and not only one way of using it. Although this makes it harder for beginners to find there way in the beginning, it makes it possible for Python to be used to write programs, in web servers, or embedded devices. In this introductory chapter, we describe an interactive workflow with IPython that is handy to explore and understand algorithms.

Note: Reference document for this section:

IPython user manual: http://ipython.scipy.org/doc/manual/html/

1.1 Command line interaction

Start *ipython*:

```
In [1]: print('Hello world')
Hello world
```

Getting help:

```
In [2]: print?
Type:               builtin_function_or_method
Base Class:         <type 'builtin_function_or_method'>
String Form:        <built-in function print>
Namespace:          Python builtin
Docstring:
    print(value, ..., sep=' ', end='\n', file=sys.stdout)

    Prints the values to a stream, or to sys.stdout by default.
    Optional keyword arguments:
    file: a file-like object (stream); defaults to the current sys.stdout.
    sep:  string inserted between values, default a space.
    end:  string appended after the last value, default a newline.
```

1.2 Elaboration of the algorithm in an editor

Create a file *my_file.py* in a text editor. Under EPD, you can use *Scite*, available from the start menu. Under Ubuntu, if you don't already have your favorite editor, I would advise installing *Stani's Python editor*. In the file, add the following lines:

```
s = 'Hello world'
print(s)
```

Now, you can run it in ipython and explore the resulting variables:

```
In [3]: %run my_file.py
Hello word

In [4]: s
Out[4]: 'Hello word'

In [5]: %whos
Variable   Type    Data/Info
----------------------------
s          str     Hello word
```

From a script to functions

- A script is not reusable, functions are.
- Thinking in terms of functions helps breaking the problem in small blocks.

CHAPTER 2

Introduction to the Python language

Note: Reference document for this section:

Python tutorial: http://docs.python.org/tutorial/

2.1 Basic types

2.1.1 Numbers

- IPython as a calculator:

```
In [1]: 1 + 1
Out[1]: 2

In [2]: 2**10
Out[2]: 1024

In [3]: (1 + 1j)*(1 - 1j)
Out[3]: (2+0j)
```

- scalar types: int, float, complex

```
In [4]: type(1)
Out[4]: <type 'int'>

In [5]: type(1.)
Out[5]: <type 'float'>

In [6]: type(1 + 0j)
Out[6]: <type 'complex'>
```

Warning: Integer division

```
In [7]: 3/2
Out[7]: 1

In [8]: from __future__ import division

In [9]: 3/2
Out[9]: 1.5
```

Trick: Use floats

```
In [10]: 3./2
Out[10]: 1.5
```

- Type conversion:

```
In [11]: float(1)
Out[11]: 1.
```

Exercise:

Compare two approximations of pi: 22/7 and 355/113
(pi = 3.14159265...)

2.1.2 Collections

Collections: list, dictionaries (and strings, tuples, sets, ...)

Lists

```
In [12]: l = [1, 2, 3, 4, 5]
```

- Indexing:

```
In [13]: l[2]
Out[13]: 3
```

Counting from the end:

```
In [14]: l[-1]
Out[14]: 5
```

- Slicing:

```
In [15]: l[3:]
Out[15]: [4, 5]

In [16]: l[:3]
Out[16]: [1, 2, 3]
```



```
In [17]: l[::2]
Out[17]: [1, 3, 5]

In [18]: l[-3:]
Out[18]: [3, 4, 5]
```

Syntax: *start:stop:stride*

- Operations on lists:

Reverse *l*:

```
In [19]: r = l[::-1]

In [20]: r
Out[20]: [5, 4, 3, 2, 1]
```

Append an item to *r*:

```
In [21]: r.append(3.5)

In [22]: r
Out[22]: [5, 4, 3, 2, 1, 3.5]
```

Extend a list with another list (in-place):

```
In [23]: l.extend([6, 7])

In [24]: l
Out[24]: [1, 2, 3, 4, 5, 6, 7]
```

Concatenate two lists:

```
In [25]: r + l
Out[25]: [5, 4, 3, 2, 1, 3.5, 1, 2, 3, 4, 5, 6, 7]
```

Sort *r*:

```
In [26]: r.sort()

In [27]: r
Out[27]: [1, 2, 3, 3.5, 4, 5]
```

Note: Methods:

r.sort: *sort* is a method of *r*: a special function to is applied to *r*.

Warning: Mutables:
Lists are mutable types: *r.sort* modifies in place *r*.

Note: Discovering methods:

In IPython: tab-completion (press tab)

```
In [28]: r.
r.__add__            r.__iadd__           r.__setattr__
r.__class__          r.__imul__           r.__setitem__
r.__contains__       r.__init__           r.__setslice__
r.__delattr__        r.__iter__           r.__sizeof__
r.__delitem__        r.__le__             r.__str__
r.__delslice__       r.__len__            r.__subclasshook__
r.__doc__            r.__lt__             r.append
r.__eq__             r.__mul__            r.count
r.__format__         r.__ne__             r.extend
r.__ge__             r.__new__            r.index
r.__getattribute__   r.__reduce__         r.insert
r.__getitem__        r.__reduce_ex__      r.pop
r.__getslice__       r.__repr__           r.remove
r.__gt__             r.__reversed__       r.reverse
r.__hash__           r.__rmul__           r.sort
```

Dictionaries

Dictionaries are a mapping between keys and values:

```
In [29]: d = {'a': 1, 'b':1.2, 'c':1j}

In [30]: d['b']
Out[30]: 1.2

In [31]: d['d'] = 'd'

In [32]: d
Out[32]: {'a': 1, 'b': 1.2, 'c': 1j, 'd': 'd'}

In [33]: d.keys()
Out[33]: ['a', 'c', 'b', 'd']

In [34]: d.values()
Out[34]: [1, 1j, 1.2, 'd']
```

Warning: Keys are not ordered

Note: Dictionnaries are an essential data structure

For instance to store precomputed values.

Strings

- Different string syntaxes:

```
a = 'Mine'
a = "Chris's"
a = '''Mine
       and not his'''
a = """Mine
       and Chris's"""
```


- Strings are collections too:

```
In [35]: s = 'Python is cool'

In [36]: s[-4:]
Out[36]: 'cool'
```

- And they have many useful methods:

```
In [37]: s.replace('cool', 'powerful')
Out[37]: 'Python is powerful'
```

Warning: Strings are not mutable

- String substitution:

```
In [38]: 'An integer: %i; a float: %f; another string: %s' % (1, 0.1, 'string')
Out[38]: 'An integer: 1; a float: 0.100000; another string: string'
```

More collection types

- **Sets:** non ordered, unique items:

```
In [39]: s = set(('a', 'b', 'c', 'a'))

In [40]: s
Out[40]: set(['a', 'b', 'c'])

In [41]: s.difference(('a', 'b'))
Out[41]: set(['c'])
```

Sets cannot be indexed:

```
In [42]: s[1]
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)

TypeError: 'set' object does not support indexing
```

- **Tuples:** non-mutable lists:

```
In [43]: t = 1, 2

In [44]: t
Out[44]: (1, 2)

In [45]: t[1]
Out[45]: 2

In [46]: t[1] = 2
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)

TypeError: 'tuple' object does not support item assignment
```

2.2 Control Flow

Controls the order in which the code is executed.

2.2.1 if/else

```
In [1]: if 2**2 == 4:
   ...:     print('Totology')
   ...:
Totology
```

Blocks are delimited by indentation

```
In [2]: a = 10

In [3]: if a == 1:
   ...:     print(1)
   ...: elif a == 2:
   ...:     print(2)
   ...: else:
   ...:     print('A lot')
   ...:
A lot
```

2.2.2 for/range

Iterating with an index:

```
In [4]: for i in range(4):
   ...:     print(i)
   ...:
0
1
2
3
```

But most often, it is more readable to iterate over values:

```
In [5]: for word in ('cool', 'powerful', 'readable'):
   ...:     print('Python is %s' % word)
   ...:
Python is cool
Python is powerful
Python is readable
```

2.2.3 while/break/continue

Typical C-style while loop (Mandelbrot problem):

Introduction to Python for Science, Release 1

```
In [6]: z = 1 + 1j

In [7]: while abs(z) < 100:
   ...:     z = z**2 + 1
   ...:

In [8]: z
Out[8]: (-134+352j)
```

break out of enclosing for/while loop:

```
In [9]: z = 1 + 1j

In [10]: while abs(z) < 100:
   ....:     if z.imag == 0:
   ....:         break
   ....:     z = z**2 + 1
   ....:
   ....:
```

Rmk: *continue* the next iteration of a loop.

2.2.4 Conditional Expressions

- *if object*

  Evaluates to True:

  - any non-zero value
  - any sequence with a length > 0

  Evaluates to False:

  - any zero value
  - any empty sequence

- *a == b*

  Tests equality, with logics:

  ```
  In [19]: 1 == 1.
  Out[19]: True
  ```

- *a is b*

  Tests identity: both objects are the same

  ```
  In [20]: 1 is 1.
  Out[20]: False

  In [21]: a = 1

  In [22]: b = 1

  In [23]: a is b
  Out[23]: True
  ```

- *a in b*

  For any collection *b*: *b* contains *a*

  If *b* is a dictionary, this tests that *a* is a key of *b*.

2.2.5 Advanced iteration

Iterate over any *sequence*

- You can iterate over any sequence (string, list, dictioary, file, ...)

```
In [11]: vowels = 'aeiouy'

In [12]: for i in 'powerful':
   ....:     if i in vowels:
   ....:         print(i),
   ....:
   ....:
o e u
```

Warning: Not safe to modify the sequence you are iterating over.

Keeping track of enumeration number

Common task is to iterate over a sequence while keeping track of the item number.

- Could use while loop with a counter as above. Or a for loop:

```
In [13]: for i in range(0, len(words)):
   ....:     print(i, words[i])
   ....:
   ....:
0 cool
1 powerful
2 readable
```

- But Python provides **enumerate** for this:

```
In [14]: for index, item in enumerate(words):
   ....:     print(index, item)
   ....:
   ....:
0 cool
1 powerful
2 readable
```

Looping over a dictionary

Use **iteritems**:


```
In [15]: d = {'a': 1, 'b':1.2, 'c':1j}

In [15]: for key, val in d.iteritems():
   ....:     print('Key: %s has value: %s' % (key, val))
   ....:
   ....:
Key: a has value: 1
Key: c has value: 1j
Key: b has value: 1.2
```

2.2.6 List Comprehensions

```
In [16]: [i**2 for i in range(4)]
Out[16]: [0, 1, 4, 9]
```

Exercise

Compute the decimals of Pi using the Wallis formula:

$$\pi = 2 \prod_{i=1}^{\infty} \frac{4i^2}{4i^2 - 1}$$

The Pi Wallis Solution

2.3 Defining functions

2.3.1 Function definition

```
In [56]: def foo():
   ....:     print('in foo function')
   ....:
   ....:

In [57]: foo()
in foo function
```

2.3.2 Return statement

Functions can *optionally* return values.

```
In [6]: def area(radius):
   ...:     return 3.14 * radius * radius
```

```
   ...:

In [8]: area(1.5)
Out[8]: 7.0649999999999995
```

Note: By default, functions return `None`.

2.3.3 Parameters

Mandatory parameters (positional arguments)

```
In [81]: def double_it(x):
   ....:     return x * 2
   ....:

In [82]: double_it(3)
Out[82]: 6

In [83]: double_it()
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)

/Users/cburns/src/scipy2009/scipy_2009_tutorial/source/<ipython console> in <module>()

TypeError: double_it() takes exactly 1 argument (0 given)
```

Optional parameters (keyword or named arguments)

```
In [84]: def double_it(x=2):
   ....:     return x * 2
   ....:

In [85]: double_it()
Out[85]: 4

In [86]: double_it(3)
Out[86]: 6
```

Keyword arguments allow you to specify *default values*.

Warning: Default values are evaluated when the function is defined, not when it is called.

```
In [124]: bigx = 10

In [125]: def double_it(x=bigx):
   .....:     return x * 2
   .....:

In [126]: bigx = 1e9  # No big

In [128]: double_it()
Out[128]: 20
```

More involved example implementing python's slicing:

Introduction to Python for Science, Release 1

```
In [98]: def slicer(seq, start=None, stop=None, step=None):
   ....:     """Implement basic python slicing."""
   ....:     return seq[start:stop:step]
   ....:

In [101]: seuss = 'one fish, two fish, red fish, blue fish'.split()

In [102]: seuss
Out[102]: ['one', 'fish,', 'two', 'fish,', 'red', 'fish,', 'blue', 'fish']

In [103]: slicer(seuss)
Out[103]: ['one', 'fish,', 'two', 'fish,', 'red', 'fish,', 'blue', 'fish']

In [104]: slicer(seuss, step=2)
Out[104]: ['one', 'two', 'red', 'blue']

In [105]: slicer(seuss, 1, step=2)
Out[105]: ['fish,', 'fish,', 'fish,', 'fish']

In [106]: slicer(seuss, start=1, stop=4, step=2)
Out[106]: ['fish,', 'fish,']
```

2.3.4 Passed by value

Parameters to functions are passed by value.

When you pass a variable to a function, python passes the object to which the variable refers (the **value**). Not the variable itself.

If the **value** is immutable, the function does not modify the caller's variable. If the **value** is mutable, the function modifies the caller's variable.

```
In [1]: def foo(x, y):
   ...:     x = 23
   ...:     y.append(42)
   ...:     print('x is %d' % x)
   ...:     print('y is %d' % y)
   ...:

In [2]: a = 77    # immutable variable

In [3]: b = [99]  # mutable variable

In [4]: foo(a, b)
x is 23
y is [99, 42]

In [5]: print a
77

In [6]: print b    # mutable variable 'b' was modified
[99, 42]
```

Functions have a local variable table. Called a *local namespace*.

The variable `x` only exists within the function *foo*.

2.3.5 Global variables

Variables declared outside the function can be referenced within the function:

```
In [114]: x = 5

In [115]: def addx(y):
   .....:     return x + y
   .....:

In [116]: addx(10)
Out[116]: 15
```

But these "global" variables cannot be modified within the function, unless declared **global** in the function.

This doesn't work:

```
In [117]: def setx(y):
   .....:     x = y
   .....:     print('x is %d' % x)
   .....:
   .....:

In [118]: setx(10)
x is 10

In [120]: x
Out[120]: 5
```

This works:

```
In [121]: def setx(y):
   .....:     global x
   .....:     x = y
   .....:     print('x is %d' % x)
   .....:
   .....:

In [122]: setx(10)
x is 10

In [123]: x
Out[123]: 10
```

2.3.6 Variable number of parameters

Special forms of parameters:

- *args: any number of positional arguments packed into a tuple
- **kwargs: any number of keyword arguments packed into a dictionary

```
In [35]: def variable_args(*args, **kwargs):
   ....:     print 'args is', args
   ....:     print 'kwargs is', kwargs
   ....:
```



```
In [36]: variable_args('one', 'two', x=1, y=2, z=3)
args is ('one', 'two')
kwargs is {'y': 2, 'x': 1, 'z': 3}
```

2.3.7 Docstrings

Documention about what the function does and it's parameters. General convention:

```
In [67]: def funcname(params):
   ....:     """Concise one-line sentence describing the function.
   ....:
   ....:     Extended summary which can contain multiple paragraphs.
   ....:     """
   ....:     # function body
   ....:     pass
   ....:

In [68]: funcname?
Type:               function
Base Class: <type 'function'>
String Form:        <function funcname at 0xeaa0f0>
Namespace:  Interactive
File:               /Users/cburns/src/scipy2009/.../<ipython console>
Definition: funcname(params)
Docstring:
    Concise one-line sentence describing the function.

    Extended summary which can contain multiple paragraphs.
```

2.3.8 Functions are objects

Functions are first-class objects, which means they can be:

- assigned to a variable
- an item in a list (or any collection)
- passed as an argument to another function.

```
In [38]: va = variable_args

In [39]: va('three', x=1, y=2)
args is ('three',)
kwargs is {'y': 2, 'x': 1}
```

2.3.9 Methods

Methods are functions attached to objects. You've seen these in our examples on **lists**, **dictionaries**, **strings**, etc...

Exercise

Implement the quicksort algorithm, as defined by wikipedia:

```
function quicksort(array)
    var list less, greater
    if length(array)  1
        return array
    select and remove a pivot value pivot from array
    for each x in array
        if x  pivot then append x to less
        else append x to greater
    return concatenate(quicksort(less), pivot, quicksort(greater))
```

The Quicksort Solution

2.4 Exceptions handling in Python

2.4.1 Exceptions

Exceptions are raised by errors in Python:

```
In [1]: 1/0
---------------------------------------------------------------------------
ZeroDivisionError: integer division or modulo by zero

In [2]: 1 + 'e'
---------------------------------------------------------------------------
TypeError: unsupported operand type(s) for +: 'int' and 'str'

In [3]: d = {1:1, 2:2}

In [4]: d[3]
---------------------------------------------------------------------------
KeyError: 3

In [5]: l = [1, 2, 3]

In [6]: l[4]
---------------------------------------------------------------------------
IndexError: list index out of range

In [7]: l.foobar
---------------------------------------------------------------------------
AttributeError: 'list' object has no attribute 'foobar'
```

Different types of exceptions for different errors.

2.4.2 Catching exceptions

try/except

```
In [8]: while True:
 ....:     try:
 ....:         x = int(raw_input('Please enter a number: '))
 ....:         break
 ....:     except ValueError:
 ....:         print('That was no valid number.  Try again...')
 ....:
 ....:
Please enter a number: a
That was no valid number.  Try again...
Please enter a number: 1

In [9]: x
Out[9]: 1
```

try/finally

```
In [10]: try:
 ....:    x = int(raw_input('Please enter a number: '))
 ....: finally:
 ....:    print('Thank you for your input')
 ....:
 ....:
Please enter a number: a
Thank you for your input
---------------------------------------------------------------------------
ValueError: invalid literal for int() with base 10: 'a'
```

Important for resource management (e.g. closing a file)

Easier to ask for forgiveness than for permission

Don't enforce contracts before hand.

```
In [11]: def print_sorted(collection):
   ....:     try:
   ....:         collection.sort()
   ....:     except AttributeError:
   ....:         pass
   ....:     print(collection)
   ....:
   ....:

In [12]: print_sorted([1, 3, 2])
[1, 2, 3]

In [13]: print_sorted(set((1, 3, 2)))
set([1, 2, 3])
```

```
In [14]: print_sorted('132')
132
```

2.4.3 Raising exceptions

- Capturing and reraising an exception:

```
In [15]: def filter_name(name):
   ....:     try:
   ....:         name = name.encode('ascii')
   ....:     except UnicodeError, e:
   ....:         if name == 'Gaël':
   ....:             print('OK, Gaël')
   ....:         else:
   ....:             raise e
   ....:     return name
   ....:

In [16]: filter_name('Gaël')
OK, Gaël
Out[16]: 'Ga\xc3\xabl'

In [17]: filter_name('Stéfan')
---------------------------------------------------------------------------
UnicodeDecodeError: 'ascii' codec can't decode byte 0xc3 in position 2: ordinal not in range(128
```

- Exceptions to pass messages between parts of the code:

```
In [17]: def achilles_arrow(x):
   ....:     if abs(x - 1) < 1e-3:
   ....:         raise StopIteration
   ....:     x = 1 - (1-x)/2.
   ....:     return x
   ....:

In [18]: x = 0

In [19]: while True:
   ....:     try:
   ....:         x = achilles_arrow(x)
   ....:     except StopIteration:
   ....:         break
   ....:
   ....:

In [20]: x
Out[20]: 0.9990234375
```

Use exceptions to notify certain conditions are met (e.g. StopIteration) or not (e.g. custom error raising)

Warning: Capturing and not raising exception can lead to difficult debuging.

2.5 Reusing code

2.5.1 Importing objects

```
In [1]: import os

In [2]: os
Out[2]: <module 'os' from '/usr/lib/python2.6/os.pyc'>

In [3]: os.listdir('.')
Out[3]:
['conf.py',
 'basic_types.rst',
 'control_flow.rst',
 'functions.rst',
 'python_language.rst',
 'reusing.rst',
 'file_io.rst',
 'exceptions.rst',
 'workflow.rst',
 'index.rst']
```

And also:

```
In [4]: from os import listdir
```

Importing shorthands:

```
In [5]: import numpy as np
```

Warning:

```
from os import *
```

Do not do it.

- Makes the code harder to read and understand: where do symbols come from?
- Makes it impossible to guess the functionality by the context and the name (hint: *os.name* is the name of the OS), and to profit usefully from tab completion.
- Restricts the variable names you can use: *os.name* might override *name*, or vise-versa.
- Creates possible name clashes between modules.
- Makes the code impossible to statically check for undefined symbols.

A whole set of new functionnality!

```
In [6]: from __future__ import braces
```

2.5.2 Creating modules

File *demo.py*:

```
" A demo module. "

def print_b():
    " Prints b "
    print('b')

def print_a():
    " Prints a "
    print('a')


c = 2
d = 3
```

Importing it in IPython:

```
In [6]: import demo

In [7]: demo ?
Type:               module
Base Class: <type 'module'>
String Form:        <module 'demo' from 'demo.py'>
Namespace:  Interactive
File:               /home/varoquau/Projects/Python_talks/scipy_2009_tutorial/source/demo.py
Docstring:
    A demo module.


In [8]: demo.print_a()
a

In [9]: demo.print_b()
b
```

Warning: Module caching

Modules are cached: if you modify *demo.py* and re-import it in the old session, you will get the old one.

Solution:

```
In [10]: reload(demo)
```

2.5.3 '__main__' and module loading

File *demo2.py*:

```
def print_a():
    " Prints a "
    print('a')

print "Start"

if __name__ == '__main__':
    print_a()
```


Importing it:

```
In [11]: import demo2
b

In [12]: import demo2
```

Running it:

```
In [13]: %run demo2
b
a
```

2.5.4 Standalone scripts

- Running a script from the command line:

```
$ python demo2.py
b
a
```

- On Unix, make the file executable:
  - 'chmod uog+x demo2.py'
  - add at the top of the file:

```
#!/usr/bin/env python
```

- Command line arguments:

```
import sys
print sys.argv
```

```
$ python file.py test arguments
['file.py', 'test', 'arguments']
```

Note: Don't implement option parsing yourself. Use modules such as *optparse*.

Exercise

Implement a script that takes a directory name as argument, and returns the list of '.py' files, sorted by name length.

Hint: try to understand the docstring of list.sort

The Directory Listing Solution

2.6 File I/O in Python

2.6.1 Reading from a file

Open a file with the `open` function:

```
In [67]: fp = open("holy_grail.txt")

In [68]: fp
Out[68]: <open file 'holy_grail.txt', mode 'r' at 0xea1ec0>

In [69]: fp.
fp.__class__         fp.__new__           fp.fileno            fp.readline
fp.__delattr__       fp.__reduce__        fp.flush             fp.readlines
fp.__doc__           fp.__reduce_ex__     fp.isatty            fp.seek
fp.__enter__         fp.__repr__          fp.mode              fp.softspace
fp.__exit__          fp.__setattr__       fp.name              fp.tell
fp.__getattribute__  fp.__str__           fp.newlines          fp.truncate
fp.__hash__          fp.close             fp.next              fp.write
fp.__init__          fp.closed            fp.read              fp.writelines
fp.__iter__          fp.encoding          fp.readinto          fp.xreadlines
```

Close a file with the `close` method:

```
In [73]: fp.close()

In [74]: fp.closed
Out[74]: True
```

Can read one line at a time:

```
In [69]: first_line = fp.readline()

In [70]: first_line
Out[70]: "GUARD: 'Allo, daffy English kaniggets and Monsieur Arthur-King, who is\n"
```

Or we can read the entire file into a list:

```
In [75]: fp = open("holy_grail.txt")

In [76]: all_lines = fp.readlines()

In [77]: all_lines
Out[77]:
["GUARD: 'Allo, daffy English kaniggets and Monsieur Arthur-King, who is\n",
 '      afraid of a duck, you know!  So, we French fellows out-wit you a\n',
 '      second time!\n',
 ' \n',
...
 ' \n']

In [78]: all_lines[0]
Out[78]: "GUARD: 'Allo, daffy English kaniggets and Monsieur Arthur-King, who is\n"
```


2.6.2 Iterate over a file

Files are sequences, we can iterate over them:

```
In [81]: fp = open("holy_grail.txt")

In [82]: for line in fp:
   ....:     print line
   ....:
GUARD: 'Allo, daffy English kaniggets and Monsieur Arthur-King, who is

      afraid of a duck, you know!  So, we French fellows out-wit you a

      second time!
```

2.6.3 File modes

- Read-only: `r`
- Write-only: `w`
  - Note: Create a new file or *overwrite* existing file.
- Append a file: `a`
- Read and Write: `r+`
- Binary mode: `b`
  - Note: Use for binary files, especially on Windows.

2.6.4 Writing to a file

Use the `write` method:

```
In [83]: fp = open('newfile.txt', 'w')

In [84]: fp.write("I am not a tiny-brained wiper of other people's bottoms!")

In [85]: fp.close()

In [86]: fp = open('newfile.txt')

In [87]: fp.read()
Out[87]: "I am not a tiny-brained wiper of other people's bottoms!"
```

Update a file:

```
In [104]: fp = open('newfile.txt', 'r+')

In [105]: line = fp.read()

In [111]: line = "CHRIS: " + line + "\n"

In [112]: line
Out[112]: "CHRIS: I am not a tiny-brained wiper of other people's bottoms!\n"
```

```
In [113]: fp.seek(0)

In [114]: fp.write(line)

In [115]: fp.tell()
Out[115]: 64L

In [116]: fp.seek(0)

In [117]: fp.read()
Out[117]: "CHRIS: I am not a tiny-brained wiper of other people's bottoms!"

In [132]: fp.write("GAEL: I've met your children dear sir, yes you are!\n")

In [136]: fp.seek(0)

In [137]: fp.readlines()
Out[137]:
["CHRIS: I am not a tiny-brained wiper of other people's bottoms!\n",
 "GAEL: I've met your children dear sir, yes you are!\n"]
```

2.6.5 File processing

Often want to open the file, grab the data, then close the file:

```
In [54]: fp = open("holy_grail.txt")

In [60]: try:
   ....:     for line in fp:
   ....:         print line
   ....: finally:
   ....:     fp.close()
   ....:
GUARD: 'Allo, daffy English kaniggets and Monsieur Arthur-King, who is

      afraid of a duck, you know!  So, we French fellows out-wit you a

      second time!
```

With Python 2.5 use the `with` statement:

```
In [65]: from __future__ import with_statement

In [66]: with open('holy_grail.txt') as fp:
   ....:     for line in fp:
   ....:         print line
   ....:
GUARD: 'Allo, daffy English kaniggets and Monsieur Arthur-King, who is

      afraid of a duck, you know!  So, we French fellows out-wit you a

      second time!
```

This has the advantage that it closed the file properly, even if an exception is raised, and is more concise than the `try-finally`.

Note: The `from __future__` line isn't required in Python 2.6

Exercise

Write a function that will load the column of numbers in `data.txt` and calculate the min, max and sum values.

The Data File I/O Solution

2.7 Standard Library

Note: Reference document for this section:

- The Python Standard Library documentation: http://docs.python.org/library/index.html
- Python Essential Reference, David Beazley, Addison-Wesley Professional

2.7.1 `os` module: operating system functionality

"A portable way of using operating system dependent functionality."

Directory and file manipulation

Current directory:

```
In [17]: os.getcwd()
Out[17]: '/Users/cburns/src/scipy2009/scipy_2009_tutorial/source'
```

List a directory:

```
In [31]: os.listdir(os.curdir)
Out[31]:
['.index.rst.swo',
 '.python_language.rst.swp',
 '.view_array.py.swp',
 '_static',
 '_templates',
 'basic_types.rst',
 'conf.py',
 'control_flow.rst',
 'debugging.rst',
 ...
```

Make a directory:

```
In [32]: os.mkdir('junkdir')

In [33]: 'junkdir' in os.listdir(os.curdir)
Out[33]: True
```

Rename the directory:

```
In [36]: os.rename('junkdir', 'foodir')

In [37]: 'junkdir' in os.listdir(os.curdir)
Out[37]: False

In [38]: 'foodir' in os.listdir(os.curdir)
Out[38]: True

In [41]: os.rmdir('foodir')

In [42]: 'foodir' in os.listdir(os.curdir)
Out[42]: False
```

Delete a file:

```
In [44]: fp = open('junk.txt', 'w')

In [45]: fp.close()

In [46]: 'junk.txt' in os.listdir(os.curdir)
Out[46]: True

In [47]: os.remove('junk.txt')

In [48]: 'junk.txt' in os.listdir(os.curdir)
Out[48]: False
```

`os.path`: path manipulations

`os.path` provides common operations on pathnames.

```
In [70]: fp = open('junk.txt', 'w')

In [71]: fp.close()

In [72]: a = os.path.abspath('junk.txt')

In [73]: a
Out[73]: '/Users/cburns/src/scipy2009/scipy_2009_tutorial/source/junk.txt'

In [74]: os.path.split(a)
Out[74]: ('/Users/cburns/src/scipy2009/scipy_2009_tutorial/source',
          'junk.txt')

In [78]: os.path.dirname(a)
Out[78]: '/Users/cburns/src/scipy2009/scipy_2009_tutorial/source'

In [79]: os.path.basename(a)
Out[79]: 'junk.txt'

In [80]: os.path.splitext(os.path.basename(a))
Out[80]: ('junk', '.txt')

In [84]: os.path.exists('junk.txt')
Out[84]: True
```



```
In [86]: os.path.isfile('junk.txt')
Out[86]: True

In [87]: os.path.isdir('junk.txt')
Out[87]: False

In [88]: os.path.expanduser('~/local')
Out[88]: '/Users/cburns/local'

In [92]: os.path.join(os.path.expanduser('~'), 'local', 'bin')
Out[92]: '/Users/cburns/local/bin'
```

Running an external command

```
In [8]: os.system('ls *')
conf.py   debug_file.py  demo2.py~  demo.py   demo.pyc          my_file.py~
conf.py~  demo2.py      demo2.pyc  demo.py~  my_file.py  pi_wallis_image.py
```

Walking a directory

`os.path.walk` generates a list of filenames in a directory tree.

```
In [10]: for dirpath, dirnames, filenames in os.walk(os.curdir):
   ....:     for fp in filenames:
   ....:         print os.path.abspath(fp)
   ....:
   ....:
/Users/cburns/src/scipy2009/scipy_2009_tutorial/source/.index.rst.swo
/Users/cburns/src/scipy2009/scipy_2009_tutorial/source/.view_array.py.swp
/Users/cburns/src/scipy2009/scipy_2009_tutorial/source/basic_types.rst
/Users/cburns/src/scipy2009/scipy_2009_tutorial/source/conf.py
/Users/cburns/src/scipy2009/scipy_2009_tutorial/source/control_flow.rst
...
```

Environment variables:

```
In [9]: import os

In [11]: os.environ.keys()
Out[11]:
['_',
 'FSLDIR',
 'TERM_PROGRAM_VERSION',
 'FSLREMOTECALL',
 'USER',
 'HOME',
 'PATH',
 'PS1',
 'SHELL',
 'EDITOR',
 'WORKON_HOME',
 'PYTHONPATH',
```

```
...

In [12]: os.environ['PYTHONPATH']
Out[12]: '.:/Users/cburns/src/utils:/Users/cburns/src/nitools:
/Users/cburns/local/lib/python2.5/site-packages/:
/usr/local/lib/python2.5/site-packages/:
/Library/Frameworks/Python.framework/Versions/2.5/lib/python2.5'

In [16]: os.getenv('PYTHONPATH')
Out[16]: '.:/Users/cburns/src/utils:/Users/cburns/src/nitools:
/Users/cburns/local/lib/python2.5/site-packages/:
/usr/local/lib/python2.5/site-packages/:
/Library/Frameworks/Python.framework/Versions/2.5/lib/python2.5'
```

2.7.2 `shutil`: high-level file operations

The `shutil` provides useful file operations:

- `shutil.rmtree`: Recursively delete a directory tree.
- `shutil.move`: Recursively move a file or directory to another location.
- `shutil.copy`: Copy files or directories.

2.7.3 `glob`: Pattern matching on files

The `glob` module provides convenient file pattern matching.

Find all files ending in `.txt`:

```
In [18]: import glob

In [19]: glob.glob('*.txt')
Out[19]: ['holy_grail.txt', 'junk.txt', 'newfile.txt']
```

2.7.4 `sys` module: system-specific information

System-specific information related to the Python interpreter.

- Which version of python are you running and where is it installed:

```
In [117]: sys.platform
Out[117]: 'darwin'

In [118]: sys.version
Out[118]: '2.5.2 (r252:60911, Feb 22 2008, 07:57:53) \n
          [GCC 4.0.1 (Apple Computer, Inc. build 5363)]'

In [119]: sys.prefix
Out[119]: '/Library/Frameworks/Python.framework/Versions/2.5'
```

- List of command line arguments passed to a Python script:

```
In [100]: sys.argv
Out[100]: ['/Users/cburns/local/bin/ipython']
```


`sys.path` is a list of strings that specifies the search path for modules. Initialized from PYTHONPATH:

```
In [121]: sys.path
Out[121]:
['',
 '/Users/cburns/local/bin',
 '/Users/cburns/local/lib/python2.5/site-packages/grin-1.1-py2.5.egg',
 '/Users/cburns/local/lib/python2.5/site-packages/argparse-0.8.0-py2.5.egg',
 '/Users/cburns/local/lib/python2.5/site-packages/urwid-0.9.7.1-py2.5.egg',
 '/Users/cburns/local/lib/python2.5/site-packages/yolk-0.4.1-py2.5.egg',
 '/Users/cburns/local/lib/python2.5/site-packages/virtualenv-1.2-py2.5.egg',
 ...
```

2.7.5 `pickle`: easy persistence

Useful to store arbritrary objects to a file. Not safe or fast!

```
In [1]: import pickle

In [2]: l = [1, None, 'Stan']

In [3]: pickle.dump(l, file('test.pkl', 'w'))

In [4]: pickle.load(file('test.pkl'))
Out[4]: [1, None, 'Stan']
```

Exercise

Write a program to search your PYTHONPATH for the module `site.py`.

The PYTHONPATH Search Solution

CHAPTER 3

Core scientific modules

Context

- Numerical algorithms are not a special case of computing, the need for them arises simultaneously with the need for other tools.
- Exploratory coding, easy reading!
- Visualization: don't play with numbers without plotting, or you probably won't understand what you are doing.

Core scientific libraries

numpy	http://www.scipy.org/Download
ipython	http://ipython.scipy.org/
matplotlib	http://matplotlib.sourceforge.net/
scipy	http://www.scipy.org/Download
mayavi	http://code.enthought.com/projects/mayavi

Use distributions

- Python(x,y): http://www.pythonxy.com
- EPD: http://www.enthought.com/products/epd.php

Ressources

- http://docs.scipy.org/
- *numpy.lookfor*
- *Python: Les fondamentaux du langage -*

  La programmation pour Les scientifiques, Matthieu BRUCHER, editions ENI.
- *Python Scripting for Computational Science*, Hans Petter Langtangen, Springer
- *Beginning Python visualization*, Shai Vaingast, Apress

3.1 Numpy: array computing

Conventions

```
>>> import numpy as np
>>> import scipy as sp
>>> import pylab as pl
```

3.1.1 Array computing

Python	numpy
List: *a = [1, 2, 3]*	Array: *a = np.array([1, 2, 3])*

Doing operations on many numbers

- Standard numerical computing = loops

```
def square(data):
    for i in range(len(data)):
        data[i] = data[i]**2
    return data
```

```
In [1]: %timeit data = range(1000) ; square(data)
1000 loops, best of 3: 314 us per loop
```

- Vector computing: loops are replaced by vector operations, on arrays

```
def square(data):
    return data**2
```

```
In [2]: %timeit data=np.arange(1000) ; square(data)
100000 loops, best of 3: 10.6 us per loop
```

Multidimensional arrays

```
>>> a = np.arange(10)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> b = np.reshape(a, (2, 5))
>>> b
array([[0, 1, 2, 3, 4],
       [5, 6, 7, 8, 9]])
>>> b[:, 1]
array([1, 6])
```

Creating arrays

- With constants:

```
>>> np.ones((2, 3))
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
```

- Arrays contain typed entries:

```
>>> np.ones(3, dtype=np.int)
array([1, 1, 1])
```

- Creating a grid:

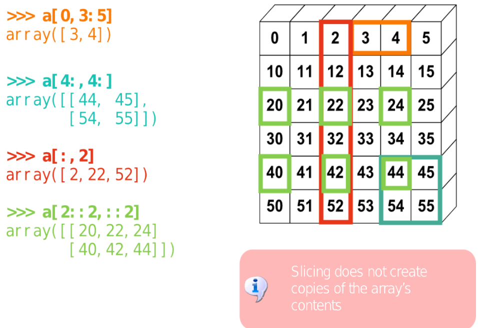
```
>>> x, y = np.indices((2, 2))
>>> x
array([[0, 0],
       [1, 1]])
>>> y
array([[0, 1],
       [0, 1]])
>>> x+1j*y
array([[ 0.+0.j,  0.+1.j],
       [ 1.+0.j,  1.+1.j]])
```

Views and copies

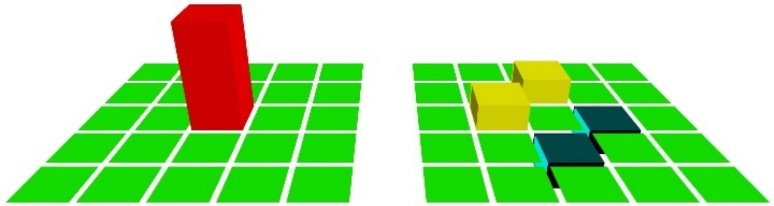
```
>>> x = np.zeros(10)
array([ 0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.])
>>> x[0] = 1
>>> x
array([ 1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.])
>>> y = x.copy()
>>> y[0] = 2
>>> x
array([ 1.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.,  0.])
```

Slicing

Multidimensional traversing of arrays

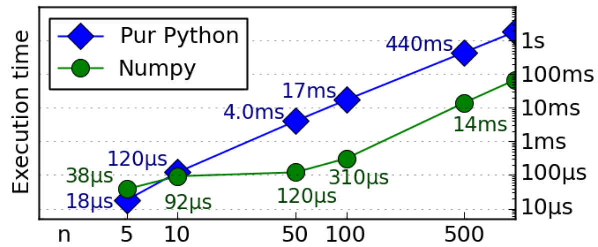


An example: calculating the laplacian



```
image[1:-1, 1:-1] = (image[:-2, 1:-1] - image[2:, 1:-1] +
                     image[1:-1, :-2] - image[1:-1, 2:])*0.25
```

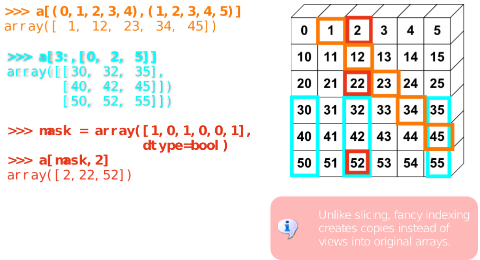
```
In [3]: import pylab as pl
In [4]: l = sp.lena()
In [5]: pl.imshow(l, cmap=pl.cm.gray)
In [6]: e = l[:-2, 1:-1] - l[2:, 1:-1] + l[1:-1, :-2] - l[1:-1, 2:]
In [7]: pl.imshow(e, cmap=pl.cm.gray)
```



Timing ratio

3.1.2 Advanced indexing

With integers or masks



With integer arrays

- Example: sorting a vector with another one:

```
>>> a, b = np.random.random_integers(10, size=(2, 4))
>>> a
array([8, 6, 2, 9])
>>> b
array([ 8,  9,  3, 10])
>>> a_order = np.argsort(a)
>>> a_order
array([2, 1, 0, 3])
>>> b[a_order]
array([ 3,  9,  8, 10])
```

Using masks

- Zeroing out all the even elements of a table:

```
>>> a = np.arange(10)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> a[(a % 2) == 1] = 0
>>> a
array([1, 3, 5, 7, 9])
```

- Applying a mask to a grid to select the center of an image:

```
In [8]: n, m = l.shape
In [9]: x, y = np.indices((n, m))
In [10]: distance = np.sqrt((x - 0.5*n)**2 + (y - 0.5*m)**2)
In [11]: l[distance > 200] = 255
In [12]: pl.imshow(l, cmap=pl.cm.gray)
```


3.1.3 Broadcasting

Multidimensional operations

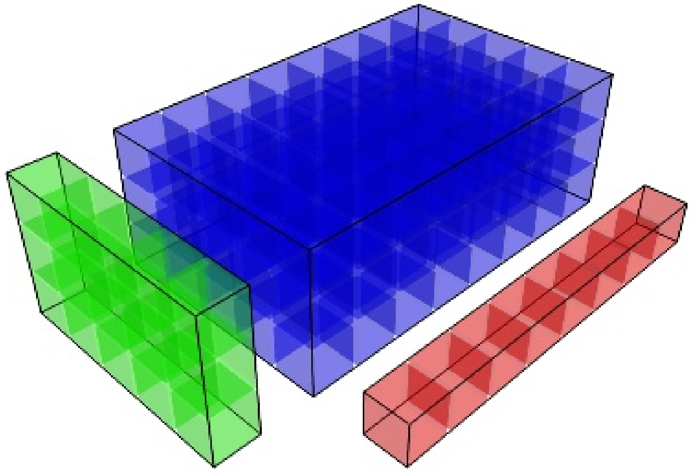
- You can add a numer to an array:

```
>>> a = np.ones((3, ))
>>> a
array([ 1.,  1.,  1.])
>>> a + 1
array([ 2.,  2.,  2.])
```

- And what if we add two arrays of different shapes?

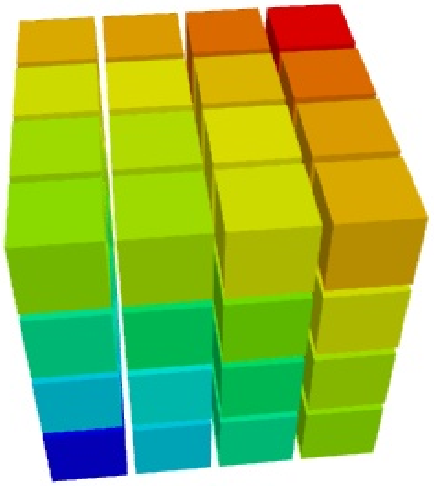
```
>>> b = 2*np.ones((2, 1))
>>> b
array([[ 2.],
       [ 2.]])
>>> a + b
array([[ 3.,  3.,  3.],
       [ 3.,  3.,  3.]])
```

- Dimensions are matched:

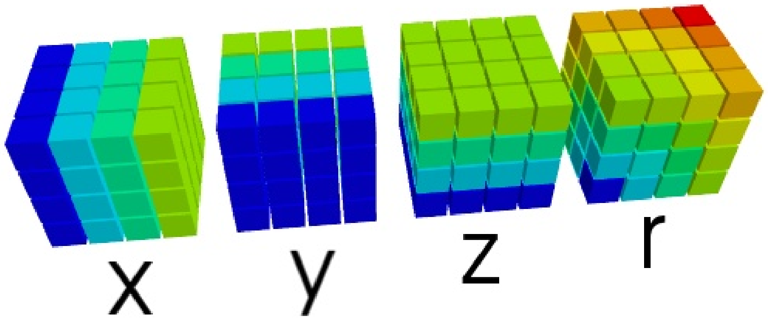


Using broadcasting for performance

- Creating a 3D grid



```
np.sqrt(x**2 + y**2 + z**2)
```

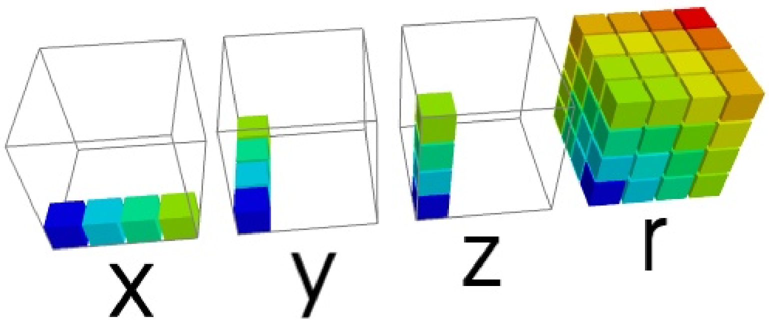
Without broadcasting

```
>>> x, y, z = np.mgrid[-100:100, -100:100, -100:100]
>>> print x.shape, y.shape, z.shape
(200, 200, 200) (200, 200, 200) (200, 200, 200)
>>> r = np.sqrt(x**2 + y**2 + z**2)
```

- Timing: **2.3s**: creating *x*, *y*, *z*: 0.5s, calculation of *r*: 1.8s
- Memory : 64Mo per array, 6 arrays, (*x*, *y*, *z*, *r*) and 2 temporary arrays

  => **400Mb**
- 200^3 floating point operations per array:

  48 million operations.



With broadcasting

```
>>> x, y, z = np.ogrid[-100:100, -100:100, -100:100]
>>> print x.shape, y.shape, z.shape
(200, 1, 1) (1, 200, 1) (1, 1, 200)
>>> r = np.sqrt(x**2 + y**2 + z**2)
```

- Timing: **1.1s**: creating *x*, *y*, *z*: 6ms
- Memory: *x*, *y*, *z* : 1.6Kb. *r* : 64Mo, and one 64Mo temporary array

  => 120Mb
- **16 million operations**

***numpy*: a structured view on memory, with associated operations**

- identical data type (*dtype*)
- fast indexing
- views and copies
- costless reshape
- shape-aware operations (broadcasting)

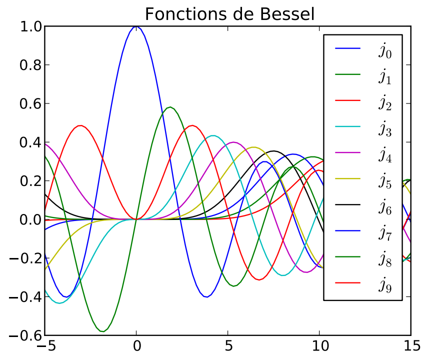
3.2 Matplotlib : scientific 2D plotting

Matplotlib: provides a matlab-like plotting interface, *pylab*

Note: Reference: the documentation is excellent: http://matplotlib.sourceforge.net/

3.2.1 Lines

```
import numpy as np
import pylab as pl
from scipy.special import jn
x = np.linspace(-5, 15, 100)

for i in range(10):
    y = jn(i, x)
    pl.plot(x, y, label='$j_%i$' % i)

pl.title('Fonctions de Bessel')
pl.legend()
```

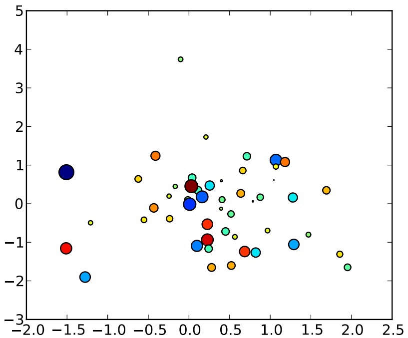


3.2.2 2D arrays

```
import scipy as sp
import pylab as pl
l = sp.lena()
pl.imshow(l, cmap=pl.cm.gray)
pl.axis('off')
```

3.2.3 Points

```
import numpy as np
import pylab as pl
x, y, value = np.random.normal(size=(3, 50))
pl.scatter(x, y, np.abs(50*value), c=value)
```

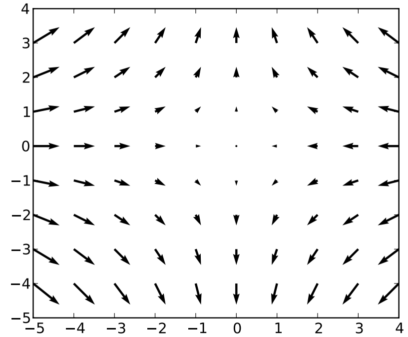


3.2.4 Vectors

```
import numpy as np
import pylab as pl
x, y = np.mgrid[-5:5, -5:5]
u = -x
```



```
v = y
pl.quiver(x, y, u, v)
```



3.3 Scipy: numerical and scientific toolbox

scipy is mainly composed of task-specific sub-modules:

cluster	Vector quantization / Kmeans
fftpack	Fourier transform
integrate	Integration routines
interpolate	Interpolation
io	Data input and output
linalg	Linear algebra routines
maxentropy	Routines for fitting maximum entropy models
ndimage	n-dimensional image package
odr	Orthogonal distance regression
optimize	Optimization
signal	Signal processing
sparse	Sparse matrices
spatial	Spatial data structures and algorithms
special	Any special mathematical functions
stats	Statistics

3.3.1 IO

- Load and save matlab files:

```
>>> from scipy import io
>>> struct = io.loadmat('file.mat', struct_as_record=True)
>>> io.savemat('file.mat', struct)
```

See also:

- Load text files:

```
np.loadtxt/np.savetxt
```

- Clever loading of text/csv files:

```
np.genfromtxt/np.recfromcsv
```

- Fast an efficient binary format:

```
np.save/np.load
```

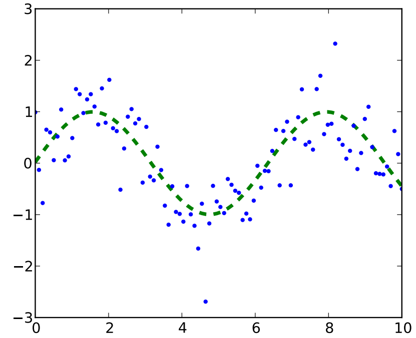
3.3.2 Optimization

- Finding zeros of a function:

```
>>> def f(x):
...     return x**3 - x**2 - 10
>>> from scipy import optimize
>>> optimize.fsolve(f, 1)
2.5445115283877615
```

- Curve fitting:

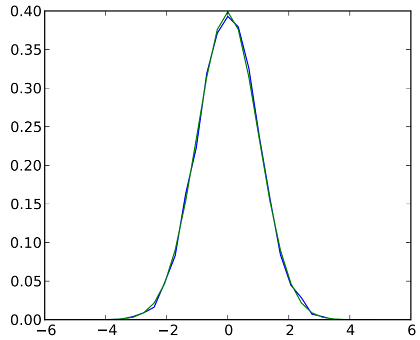
```
import numpy as np
import pylab as pl
from scipy import optimize

x = np.linspace(0, 10, 100)
y = np.sin(x) + 0.5*np.random.normal(size=100)

pl.plot(x, y, '.')

def test_func(x, a, f, phi):
    return a*np.sin(f*x+phi)

(a, f, phi), _ = optimize.curve_fit(test_func, x, y)
pl.plot(x, test_func(x, a, f, phi), '--', linewidth=3)
```

3.3.3 Statistics and random numbers

```
>>> a = np.random.normal(size=1000)
>>> bins = np.arange(-4, 5)
>>> bins
array([-4, -3, -2, -1,  0,  1,  2,  3,  4])
>>> histogram = np.histogram(a, bins=bins)
>>> bins = 0.5*(bins[1:] + bins[:-1])
>>> bins
array([-3.5, -2.5, -1.5, -0.5,  0.5,  1.5,  2.5,  3.5])
>>> from scipy import stats
>>> b = stats.norm.pdf(bins)
```

```
In [1]: pl.plot(bins, histogram)
In [2]: pl.plot(bins, b)
```

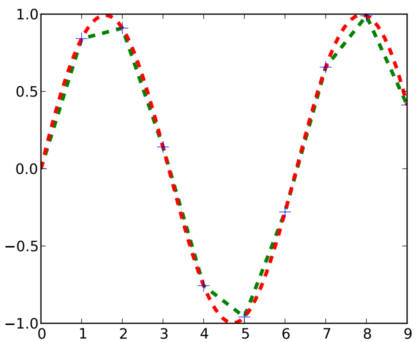


3.3.4 Image processing

```
from scipy import ndimage
l = sp.lena()
pl.imshow(ndimage.gaussian_filter(l, 5), cmap=pl.cm.gray)
pl.imshow(ndimage.gaussian_gradient_magnitude(l, 3), cmap=pl.cm.gray)
```

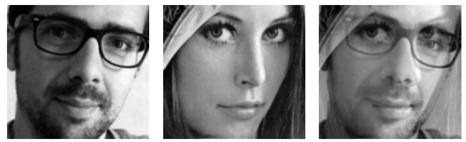
3.3.5 Interpolation

```
x = np.arange(10)
y = np.sin(x)

pl.plot(x, y, '+', markersize=10)

from scipy import interpolate

f = interpolate.interp1d(x, y)
X = np.linspace(0, 9, 100)
pl.plot(X, f(X), '--')

f = interpolate.interp1d(x, y, kind='cubic')
X = np.linspace(0, 9, 100)
pl.plot(X, f(X), '--')
```



3.3.6 Interlude

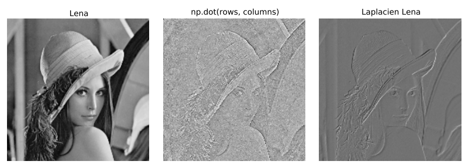
```
import scipy as sp
import numpy as np
import pylab as pl

l = sp.lena()
l = l[235:235+153, 205:162+205]

t = pl.imread('tarek.jpg')
t = t[::-1, ...]
t = t.sum(axis=-1)

pl.figure()
pl.imshow(t, cmap=pl.cm.gray)
pl.axis('off')

pl.figure()
pl.imshow(l, cmap=pl.cm.gray)
pl.axis('off')

t = t.astype(np.float)
t /= t.max()

l = l.astype(np.float)
l /= l.max()

pl.figure()
pl.imshow(t + l, cmap=pl.cm.gray)
pl.axis('off')
```



3.3.7 Lineaire Algebra

"whitening" Lena:

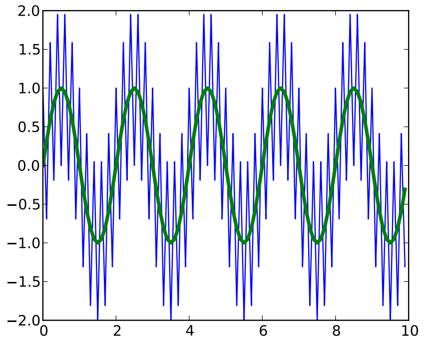
```
rows, weight, columns = np.linalg.svd(l, full_matrices=False)
l_ = np.dot(rows, columns)
```



3.3.8 FFT

Low pass filtering:

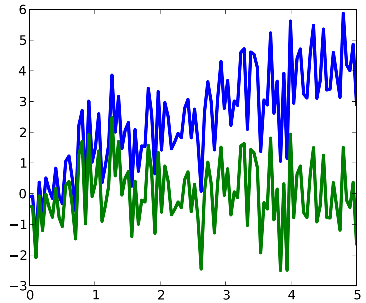
```
import numpy as np
import pylab as pl
from scipy import fftpack

t = np.arange(0, 10, 0.1)

s = np.sin(np.pi*t) + np.cos(10*np.pi*t)

pl.plot(t, s)

freq = fftpack.fftfreq(len(s), d=.1)
fft = fftpack.fft(s)
fft[np.abs(freq) > 1] = 0
s_ = fftpack.ifft(fft)

pl.plot(t, s_, linewidth=3)
```



3.3.9 Signal processing

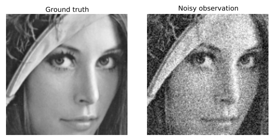
- Detrend:

```
import numpy as np
import pylab as pl
from scipy import signal
t = np.linspace(0, 5, 100)
x = t + np.random.normal(size=100)

pl.plot(t, x, linewidth=3)
pl.plot(t, signal.detrend(x), linewidth=3)
```

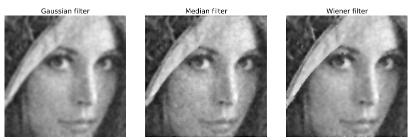



- Filtering:

Ground truth:	`l = sp.lena()[200:-100, 150:-150]` `l = l/float(l.max())`
Noisy observation:	`g = l + .1*np.random.normal(size=l.shape)`



Gaussian filter:	`ndimage.gaussian_filter(g, 1.6)`
Median filter:	`signal.medfilt2d(g, 5)`
Wiener filter:	`signal.wiener(g, (5, 5))`



CHAPTER 4

Python patterns in neuro image

4.1 Images and Mask

An fMRI dataset: 4D array, (x, y, z, t)

```
im = np.random.random((8, 9, 10, 11))
```

A mask (ROI, or brain): 3D array, (x, y, z)

```
mask = (np.random.random((8, 9, 10)) > .5)
```

Corresponding time series: 2D array, (voxel, t)

```
time_series = im[mask]
```

4.2 Memory management

- In place operations:

```
time_series -= time_series.mean(axis=-1)[:, np.newaxis]
time_series /= time_series.std(axis=-1)[:, np.newaxis]
```

- For loops rather than axis:

```
from scipy import signal

for time_serie in time_series:
    time_serie[:] = signal.detrend(time_serie)
```

Note: *time_serie* is a view on *time_series*. *time_serie[:]* gives an in-place operation.

- memmapping (np.load):

```
np.save('time_series.npy', time_series)
time_series = np.load('time_series.npy', mmap_mode='r')
```


Warning: memmap object: read-only

4.3 Masked arrays

Data, with many dimensions/parameters: subject, session, ROI, time:

```
data = np.ones((3, 4, 10)) # subject, ROI, time
```

But: **missing data**, **crapy data**, (babies anyone?):

```
bad_data = np.zeros(data.shape, dtype=np.bool)
# For subject 0, ROI 1 is outside of brain
bad_data[0, 1, :] = True
# Subject 1 moved between time 3 and 5:
bad_data[1, :, 3:6] = True
```

"Mask" the bad data: masked arrays (*np.ma*):

```
good_data = np.ma.masked_array(data, mask=bad_data)
```

How many useful ROIs:

```
>>> good_data.sum(axis=1)
masked_array(data =
[[3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0 3.0]
[4.0 4.0 4.0 -- -- -- 4.0 4.0 4.0 4.0]
[4.0 4.0 4.0 4.0 4.0 4.0 4.0 4.0 4.0 4.0]],
      mask =
[[False False False False False False False False False False]
[False False False  True  True  True False False False False]
[False False False False False False False False False False]],
      fill_value = 1e+20)
```

What's the mean across time, not counting bad data:

```
masked_array(data =
  [[1.0 -- 1.0 1.0]
  [1.0 1.0 1.0 1.0]
  [1.0 1.0 1.0 1.0]],
            mask =
  [[False  True False False]
  [False False False False]
  [False False False False]],
        fill_value = 1e+20)
```

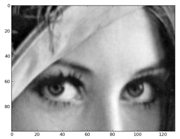
Note: Much better than NaNs, the above would not be possible.

Note: Also good for thresholding maps.

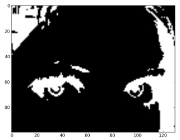
4.4 Dealing with labels

- ndimage.labels:

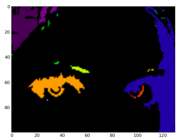
```
l = sp.lena()[200:300, 230:360]
pl.imshow(l, cmap=pl.cm.gray)
```



```
blacks = l < 80
pl.imshow(blacks, cmap=pl.cm.gray)
```



```
from scipy import ndimage
label_im, labels = ndimage.label(blacks)
imshow(label_im, cmap=pl.cm.spectral)
```

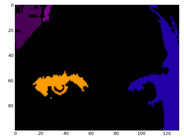


- ndimage.mean, ndimage.maximum, ndimage.maximum_position...:

```
means = ndimage.mean(l, labels=label_im, index=range(labels))
```

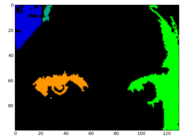
Clean up small connect components:

```
labels = np.arange(labels)
size = ndimage.sum(blacks, labels=label_im, index=labels)
for s, index in zip(size, labels):
    if s < 40:
        label_im[label_im == index] = 0
```

- Reassign labels np.searchsorted:

```
labels = np.unique(label_im)
label_im = np.searchsorted(labels, label_im)
```

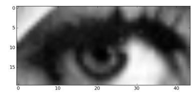


- ndimage.center_of_mass:

```
>>> ndimage.center_of_mass(label_im.astype(np.float),
                        label_im.astype(np.float), index=labels)
[(nan, nan),
(14.303212851405622, 8.6425702811244989),
(6.0357142857142856, 24.910714285714285),
(62.170854271356781, 33.984924623115575),
(nan, nan),
(nan, nan)]
```

- ndimage.find_objects:

```
slice_x, slice_y = ndimage.find_objects(label_im==4)[0]
eye = l[slice_x, slice_y]
pl.imshow(eye, cmap=pl.cm.gray)
```

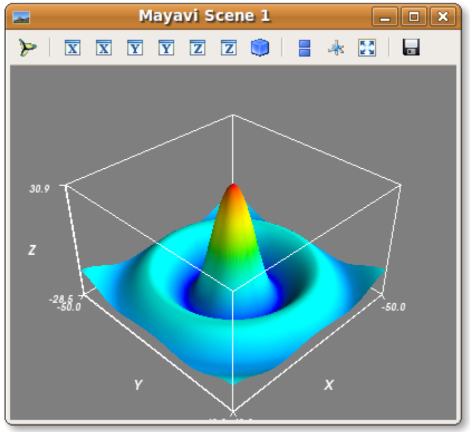


CHAPTER 5

3D plotting with Mayavi

5.1 A simple example

Warning: Start *ipython -wthread*



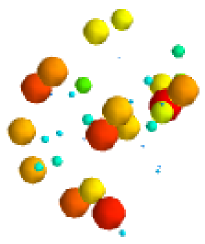

```
import numpy as np

x, y = np.mgrid[-10:10:100j, -10:10:100j]
r = np.sqrt(x**2 + y**2)
z = np.sin(r)/r

from enthought.mayavi import mlab
mlab.surf(z, warp_scale='auto')

mlab.outline()
mlab.axes()
```

np.mgrid[-10:10:100j, -10:10:100j]: Create an x,y grid, going from -10 to 10, with 100 steps in each directions.

5.2 3D plotting functions

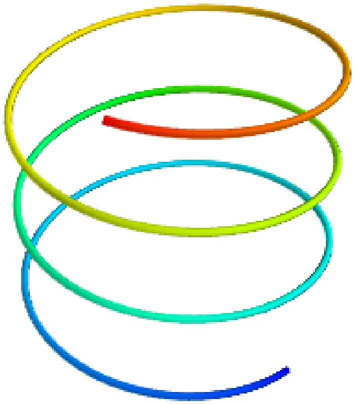
5.2.1 Points

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

In [2]: from enthought.mayavi import mlab

In [3]: x, y, z, value = np.random.random((4, 40))

In [4]: mlab.points3d(x, y, z, value)
Out[4]: <enthought.mayavi.modules.glyph.Glyph object at 0xc3c795c>
```



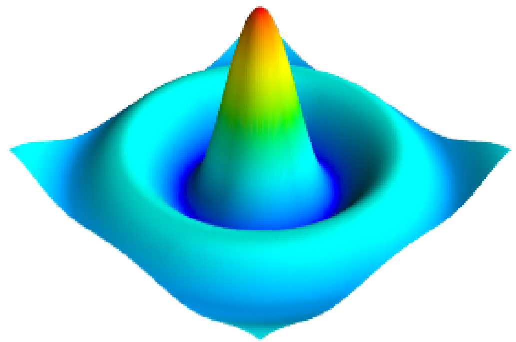
5.2.2 Lines

```
In [5]: mlab.clf()

In [6]: t = np.linspace(0, 20, 200)

In [7]: mlab.plot3d(np.sin(t), np.cos(t), 0.1*t, t)
Out[7]: <enthought.mayavi.modules.surface.Surface object at 0xcc3e1dc>
```



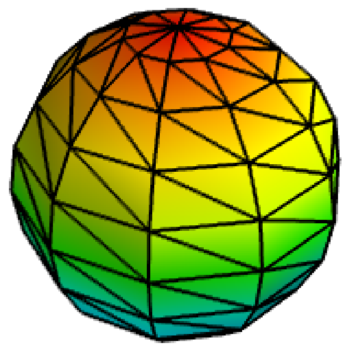
5.2.3 Elevation surface

```
In [8]: mlab.clf()

In [9]: x, y = np.mgrid[-10:10:100j, -10:10:100j]

In [10]: r = np.sqrt(x**2 + y**2)

In [11]: z = np.sin(r)/r

In [12]: mlab.surf(z, warp_scale='auto')
Out[12]: <enthought.mayavi.modules.surface.Surface object at 0xcdb98fc>
```

5.2.4 Arbitrary regular mesh

```
In [13]: mlab.clf()

In [14]: phi, theta = np.mgrid[0:pi:11j, 0:2*pi:11j]

In [15]: x = sin(phi)*cos(theta)

In [16]: y = sin(phi)*sin(theta)

In [17]: z = cos(phi)

In [18]: mlab.mesh(x, y, z)

In [19]: mlab.mesh(x, y, z, representation='wireframe', color=(0, 0, 0))
Out[19]: <enthought.mayavi.modules.surface.Surface object at 0xce1017c>
```



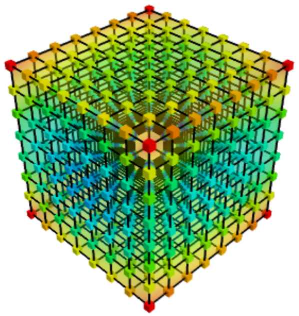
Note: A surface is defined by points **connected** to form triangles or polygones. In *mlab.func* and *mlab.mesh*, the connectivity is implicity given by the layout of the arrays. See also *mlab.triangular_mesh*.

Our data is often more than points and values: it needs some connectivity information

5.2.5 Volumetric data

```
In [20]: mlab.clf()

In [21]: x, y, z = np.mgrid[-5:5:64j, -5:5:64j, -5:5:64j]

In [22]: values = x*x*0.5 + y*y + z*z*2.0

In [23]: mlab.contour3d(values)
Out[24]: <enthought.mayavi.modules.iso_surface.IsoSurface object at 0xcfe392c>
```

This function works with a regular orthogonal grid:



5.3 Figures and decorations

5.3.1 Figure management

Get the current figure:	*mlab.gcf()*
Clear the current figure:	*mlab.clf()*
Set the current figure:	*mlab.figure(1, bgcolor=(1, 1, 1), fgcolor=(0.5, 0.5, 0.5)*
Save figure to image file:	*mlab.savefig('foo.png', size=(300, 300))*
Change the view:	mlab.view(azimuth=45, elevation=54, distance=1.)

5.3.2 Changing plot properties

Example docstring: ***mlab.mesh***

Plots a surface using grid-spaced data supplied as 2D arrays.
Function signatures:

```
mesh(x, y, z, ...)
```

x, y, z are 2D arrays, all of the same shape, giving the positions of the vertices of the surface. The connectivity between these points is implied by the connectivity on the arrays.
For simple structures (such as orthogonal grids) prefer the surf function, as it will create more efficient data structures.
Keyword arguments:

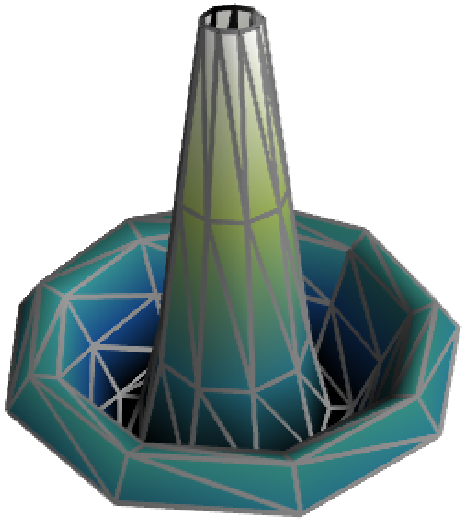
color the color of the vtk object. Overides the colormap, if any, when specified. This is specified as a triplet of float ranging from 0 to 1, eg (1, 1, 1) for white.
colormap type of colormap to use.
extent [xmin, xmax, ymin, ymax, zmin, zmax] Default is the x, y, z arrays extents. Use this to change the extent of the object created.
figure Figure to populate.
line_width The with of the lines, if any used. Must be a float. Default: 2.0
mask boolean mask array to suppress some data points.
mask_points If supplied, only one out of 'mask_points' data point is displayed. This option is usefull to reduce the number of points displayed on large datasets Must be an integer or None.
mode the mode of the glyphs. Must be '2darrow' or '2dcircle' or '2dcross' or '2ddash' or '2ddiamond' or '2dhooked_arrow' or '2dsquare' or '2dthick_arrow' or '2dthick_cross' or '2dtriangle' or '2dvertex' or 'arrow' or 'cone' or 'cube' or 'cylinder' or 'point' or 'sphere'. Default: sphere
name the name of the vtk object created.
representation the representation type used for the surface. Must be 'surface' or 'wireframe' or 'points' or 'mesh' or 'fancymesh'. Default: surface
resolution The resolution of the glyph created. For spheres, for instance, this is the number of divisions along theta and phi. Must be an integer. Default: 8
scalars optional scalar data.
scale_factor scale factor of the glyphs used to represent the vertices, in fancy_mesh mode. Must be a float. Default: 0.05
scale_mode the scaling mode for the glyphs ('vector', 'scalar', or 'none').
transparent make the opacity of the actor depend on the scalar.
tube_radius radius of the tubes used to represent the lines, in mesh mode. If None, simple lines are used.
tube_sides number of sides of the tubes used to represent the lines. Must be an integer. Default: 6
vmax vmax is used to scale the colormap If None, the max of the data will be used
vmin vmin is used to scale the colormap If None, the min of the data will be used

Example:

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

In [2]: r, theta = np.mgrid[0:10, -np.pi:np.pi:10j]

In [3]: x = r*np.cos(theta)

In [4]: y = r*np.sin(theta)

In [5]: z = np.sin(r)/r
```

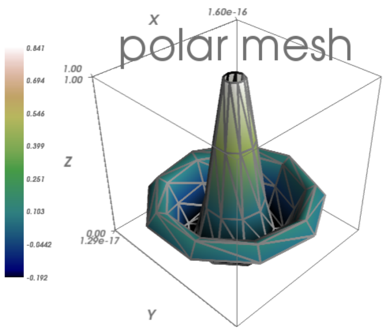


```
In [6]: from enthought.mayavi import mlab

In [7]: mlab.mesh(x, y, z, colormap='gist_earth', extent=[0, 1, 0, 1, 0, 1])
Out[7]: <enthought.mayavi.modules.surface.Surface object at 0xde6f08c>

In [8]: mlab.mesh(x, y, z, extent=[0, 1, 0, 1, 0, 1],
   ...: representation='wireframe', line_width=1, color=(0.5, 0.5, 0.5))
Out[8]: <enthought.mayavi.modules.surface.Surface object at 0xdd6a71c>
```



5.3.3 Decorations

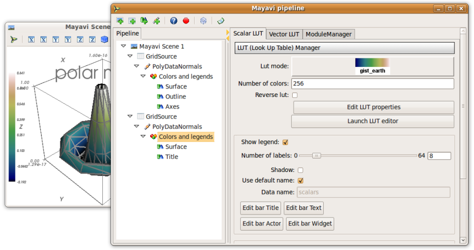
```
In [9]: mlab.colorbar(Out[7], orientation='vertical')
Out[9]: <tvtk_classes.scalar_bar_actor.ScalarBarActor object at 0xd897f8c>

In [10]: mlab.title('polar mesh')
Out[10]: <enthought.mayavi.modules.text.Text object at 0xd8ed38c>

In [11]: mlab.outline(Out[7])
Out[11]: <enthought.mayavi.modules.outline.Outline object at 0xdd21b6c>

In [12]: mlab.axes(Out[7])
Out[12]: <enthought.mayavi.modules.axes.Axes object at 0xd2e4bcc>
```



Warning: **extent:** If we specified extents for a plotting object, *mlab.outline' and 'mlab.axes* don't get them by default.

5.4 Interaction

Click on the 'Mayavi' button in the scene, and you can control properties of objects with dialogs.



Click on the red button, and it generates lines of code.

CHAPTER 6

Debugging

The python debugger `pdb`: http://docs.python.org/library/pdb.html

6.1 Coding best practices to avoid getting in trouble

Brian Kernighan

"Everyone knows that debugging is twice as hard as writing a program in the first place. So if you're as clever as you can be when you write it, how will you ever debug it?"

- We all write buggy code. Accept it. Deal with it.
- Write your code with testing and debugging in mind.
- Keep It Simple, Stupid (KISS).
  - What is the simplest thing that could possibly work?
- Don't Repeat Yourself (DRY).
  - Every piece of knowledge must have a single, unambiguous, authoritative representation within a system.
  - Constants, algorithms, etc...
- Try to limit interdependencies of your code. (Loose Coupling)
- Give your variables, functions and modules meaningful names.

6.2 The debugger

A debugger allows you to inspect your code interactively.

Specifically it allows you to:

- View the source code.
- Walk up and down the call stack.
- Inspect values of variables.

- Modify values of variables.
- Set breakpoints.

Ways to launch the debugger:

1. Postmortem, launch debugger after module errors.
2. Enable debugger in ipython and automatically drop into debug-mode on error.
3. Launch the module with the debugger.

6.2.1 Postmortem

Situation: You're working in ipython and you get a traceback.

Type `%debug` and drop into the debugger.

```
In [6]: run index_error.py
---------------------------------------------------------------------------
IndexError                                Traceback (most recent call last)

/Users/cburns/src/scipy2009/scipy_2009_tutorial/source/index_error.py in <module>()
      6
      7 if __name__ == '__main__':
----> 8     index_error()
      9
     10

/Users/cburns/src/scipy2009/scipy_2009_tutorial/source/index_error.py in index_error()
      3 def index_error():
      4     lst = list('foobar')
----> 5     print lst[len(lst)]
      6
      7 if __name__ == '__main__':

IndexError: list index out of range
WARNING: Failure executing file: <index_error.py>

In [7]: %debug
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/index_error.py(5)index_error()
      4     lst = list('foobar')
----> 5     print lst[len(lst)]
      6

ipdb> list
      1 """Small snippet to raise an IndexError."""
      2
      3 def index_error():
      4     lst = list('foobar')
----> 5     print lst[len(lst)]
      6
      7 if __name__ == '__main__':
      8     index_error()

ipdb> len(lst)
6
ipdb> print lst[len(lst)-1]
r
```



```
ipdb> quit

In [8]:
```

6.2.2 Debugger launch

Situation: You believe a bug exists in a module but are not sure where.

Launch the module with the debugger and step through the code in the debugger.

```
In [38]: run -d debug_file.py
*** Blank or comment
*** Blank or comment
Breakpoint 1 at /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py:3
NOTE: Enter 'c' at the ipdb>  prompt to start your script.
> <string>(1)<module>()
```

Step into code with `s(tep)`:

```
ipdb> step
--Call--
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(4)<module>()
1     3 Data is stored in data.txt.
----> 4 """
      5
```

Set a breakpoint at the `load_data` function:

```
ipdb> break load_data
Breakpoint 2 at /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py:12
ipdb> break
Num Type         Disp Enb   Where
1   breakpoint   keep yes   at /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py:
2   breakpoint   keep yes   at /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py:
```

List the code with `l(ist)`:

```
ipdb> list
      1 """Script to read in a column of numbers and calculate the min, max and sum.
      2
1     3 Data is stored in data.txt.
----> 4 """
      5
      6 def parse_data(data_string):
      7     data = []
      8     for x in data_string.split('.'):
      9         data.append(x)
     10     return data
     11

ipdb> list
2    12 def load_data(filename):
     13     fp = open(filename)
     14     data_string = fp.read()
     15     fp.close()
     16     return parse_data(data_string)
```

```
     17
     18 if __name__ == '__main__':
     19     data = load_data('exercises/data.txt')
     20     print('min: %f' % min(data)) # 10.20
     21     print('max: %f' % max(data)) # 61.30
```

Continue execution to next breakpoint with `c(ont(inue))`:

```
ipdb> continue
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(13)load_data()
2    12 def load_data(filename):
---> 13     fp = open(filename)
     14     data_string = fp.read()
```

I don't want to debug python's `open` function, so use the `n(ext)` command to continue execution on the next line:

```
ipdb> next
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(14)load_data()
     13     fp = open(filename)
---> 14     data_string = fp.read()
     15     fp.close()

ipdb> next
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(15)load_data()
     14     data_string = fp.read()
---> 15     fp.close()
     16     return parse_data(data_string)

ipdb> next
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(16)load_data()
     15     fp.close()
---> 16     return parse_data(data_string)
     17
```

Step into `parse_data` function with `s(tep)` command:

```
ipdb> step
--Call--
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(6)parse_data()
      5
----> 6 def parse_data(data_string):
      7     data = []

ipdb> list
      1 """Script to read in a column of numbers and calculate the min, max and sum.
      2
1     3 Data is stored in data.txt.
      4 """
      5
----> 6 def parse_data(data_string):
      7     data = []
      8     for x in data_string.split('.'):
      9         data.append(x)
     10     return data
     11
```

Continue stepping through code and print out values with the `p(rint)` command:


```
ipdb> step
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(9)parse_data()
      8     for x in data_string.split('.'):
----> 9         data.append(x)
     10     return data

ipdb> p x
'10'
ipdb> s
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(8)parse_data()
      7     data = []
----> 8     for x in data_string.split('.'):
      9         data.append(x)

ipdb> s
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(9)parse_data()
      8     for x in data_string.split('.'):
----> 9         data.append(x)
     10     return data

ipdb> p x
'2\n43'
```

You can also walk up and down the call stack with `u(p)` and `d(own)`:

```
ipdb> list
      4 """
      5
      6 def parse_data(data_string):
      7     data = []
      8     for x in data_string.split('.'):
----> 9         data.append(x)
     10     return data
     11
2    12 def load_data(filename):
     13     fp = open(filename)
     14     data_string = fp.read()

ipdb> up
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(16)load_data()
     15     fp.close()
---> 16     return parse_data(data_string)
     17

ipdb> list
     11
2    12 def load_data(filename):
     13     fp = open(filename)
     14     data_string = fp.read()
     15     fp.close()
---> 16     return parse_data(data_string)
     17
     18 if __name__ == '__main__':
     19     data = load_data('exercises/data.txt')
     20     print('min: %f' % min(data)) # 10.20
     21     print('max: %f' % max(data)) # 61.30
```

```
ipdb> down
> /Users/cburns/src/scipy2009/scipy_2009_tutorial/source/debug_file.py(9)parse_data()
      8     for x in data_string.split('.'):
----> 9         data.append(x)
     10     return data

ipdb> list
      4 """
      5
      6 def parse_data(data_string):
      7     data = []
      8     for x in data_string.split('.'):
----> 9         data.append(x)
     10     return data
     11
2    12 def load_data(filename):
     13     fp = open(filename)
     14     data_string = fp.read()

ipdb>
```

6.3 print

Yes, `print` statements do work as a debugging tool.

6.4 Debugging strategies

1. Make it fail reliably. Find a test case that makes the code fail every time.
2. Divide and Conquer. Once you have a failing test case, isolate the failing code.

- Which module.
- Which function.
- Which line of code.

1. Change one thing at a time and re-run the failing test case.
2. Take notes. It may take a while.
3. Be patient. It may take a while.
4. Purposely raise an exception where you believe the problem is, to inspect the code via the debuger (eg '%debug' in IPython)

CHAPTER 7

Profiling Python code

No optimization without measuring!

- **Measure:** profiling, timing
- "Premature optimization is the root of all evil"

7.1 Timeit

In IPython, to time elementatry operations:

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

In [2]: a = np.arange(1000)

In [3]: %timeit a**2
100000 loops, best of 3: 5.73 us per loop

In [4]: %timeit a**2.1
1000 loops, best of 3: 154 us per loop

In [5]: %timeit a*a
100000 loops, best of 3: 5.56 us per loop
```

7.2 Profiler

Useful when you have a large program to profile.

```
import numpy as np
from scipy import linalg
from ica import fastica

@profile
```

```python
def test():
    data = np.random.random((5000, 100))
    u, s, v = linalg.svd(data)
    pca = np.dot(u[:10, :], data)
    results = fastica(pca.T, whiten=False)

test()
```

```
 In [1]: %run -t demo.py

 IPython CPU timings (estimated):
     User  :    14.3929 s.
     System:   0.256016 s.

 In [2]: %run -p demo.py

      916 function calls in 14.551 CPU seconds

Ordered by: internal time

ncalls  tottime  percall  cumtime  percall filename:lineno(function)
     1   14.457   14.457   14.479   14.479 decomp.py:849(svd)
     1    0.054    0.054    0.054    0.054 {method 'random_sample' of 'mtrand.RandomState' objects}
     1    0.017    0.017    0.021    0.021 function_base.py:645(asarray_chkfinite)
    54    0.011    0.000    0.011    0.000 {numpy.core._dotblas.dot}
     2    0.005    0.002    0.005    0.002 {method 'any' of 'numpy.ndarray' objects}
     6    0.001    0.000    0.001    0.000 ica.py:195(gprime)
     6    0.001    0.000    0.001    0.000 ica.py:192(g)
    14    0.001    0.000    0.001    0.000 {numpy.linalg.lapack_lite.dsyevd}
    19    0.001    0.000    0.001    0.000 twodim_base.py:204(diag)
     1    0.001    0.001    0.008    0.008 ica.py:69(_ica_par)
     1    0.001    0.001   14.551   14.551 {execfile}
   107    0.000    0.000    0.001    0.000 defmatrix.py:239(__array_finalize__)
     7    0.000    0.000    0.004    0.001 ica.py:58(_sym_decorrelation)
     7    0.000    0.000    0.002    0.000 linalg.py:841(eigh)
   172    0.000    0.000    0.000    0.000 {isinstance}
     1    0.000    0.000   14.551   14.551 demo.py:1(<module>)
    29    0.000    0.000    0.000    0.000 numeric.py:180(asarray)
    35    0.000    0.000    0.000    0.000 defmatrix.py:193(__new__)
    35    0.000    0.000    0.001    0.000 defmatrix.py:43(asmatrix)
    21    0.000    0.000    0.001    0.000 defmatrix.py:287(__mul__)
    41    0.000    0.000    0.000    0.000 {numpy.core.multiarray.zeros}
    28    0.000    0.000    0.000    0.000 {method 'transpose' of 'numpy.ndarray' objects}
     1    0.000    0.000    0.008    0.008 ica.py:97(fastica)
    25    0.000    0.000    0.000    0.000 {abs}
    19    0.000    0.000    0.000    0.000 {numpy.core.multiarray.arange}
    21    0.000    0.000    0.000    0.000 defmatrix.py:527(getT)
     7    0.000    0.000    0.000    0.000 linalg.py:64(_commonType)
    41    0.000    0.000    0.000    0.000 {len}
    13    0.000    0.000    0.000    0.000 {max}
     9    0.000    0.000    0.000    0.000 {method 'view' of 'numpy.ndarray' objects}
    28    0.000    0.000    0.000    0.000 {method 'get' of 'dict' objects}
    14    0.000    0.000    0.000    0.000 linalg.py:36(isComplexType)
    23    0.000    0.000    0.000    0.000 {issubclass}
     7    0.000    0.000    0.000    0.000 linalg.py:92(_fastCopyAndTranspose)
    14    0.000    0.000    0.000    0.000 {method 'astype' of 'numpy.ndarray' objects}
    14    0.000    0.000    0.000    0.000 linalg.py:49(_realType)
```



```
     7    0.000    0.000    0.000    0.000 {numpy.core.multiarray._fastCopyAndTranspose}
     7    0.000    0.000    0.000    0.000 linalg.py:31(_makearray)
     7    0.000    0.000    0.000    0.000 linalg.py:110(_assertSquareness)
     1    0.000    0.000    0.000    0.000 lapack.py:63(get_lapack_funcs)
     1    0.000    0.000    0.000    0.000 lapack.py:48(find_best_lapack_type)
     7    0.000    0.000    0.000    0.000 linalg.py:104(_assertRank2)
    15    0.000    0.000    0.000    0.000 {min}
     7    0.000    0.000    0.000    0.000 {method '__array_wrap__' of 'numpy.ndarray' objects}
     6    0.000    0.000    0.000    0.000 defmatrix.py:521(getA)
```

7.3 Line-profiler

```python
@profile
def test():
    data = np.random.random((5000, 100))
    u, s, v = linalg.svd(data)
    pca = np.dot(u[:10, :], data)
    results = fastica(pca.T, whiten=False)
```

```
~ $ kernprof.py -l -v demo.py

Wrote profile results to demo.py.lprof
Timer unit: 1e-06 s

File: demo.py
Function: test at line 5
Total time: 14.2793 s

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
     5                                           @profile
     6                                           def test():
     7         1        19015  19015.0      0.1      data = np.random.random((5000, 100))
     8         1     14242163 14242163.0   99.7      u, s, v = linalg.svd(data)
     9         1        10282  10282.0      0.1      pca = np.dot(u[:10, :], data)
    10         1         7799   7799.0      0.1      results = fastica(pca.T, whiten=False)
```

The SVD is taking all the time. We need to optimise this ligne.

```
In [3]: %timeit np.linalg.svd(data)
1 loops, best of 3: 14.5 s per loop

In [4]: from scipy import linalg

In [5]: %timeit linalg.svd(data)
1 loops, best of 3: 14.2 s per loop

In [6]: %timeit linalg.svd(data, full_matrices=False)
1 loops, best of 3: 295 ms per loop

In [7]: %timeit np.linalg.svd(data, full_matrices=False)
1 loops, best of 3: 293 ms per loop
```

CHAPTER 8

Advanced numpy

Optimising numpy code

1. avoiding loops
2. algorithmic optimisation (eg. not doing the same thing more than once)
3. memory/number of operations minimization and trade-off

Avoiding loops

- *Fancy indexing*
- Know the numpy library well
- *Reshaping, striding*
- Think different

Algorithmic optimisation

- See the forest, not the trees:
  - Think before you code
  - Refactor
- Know the standard scientific library (scipy)
  - http://docs.scipy.org/
  - *numpy.lookfor*
- Know your math:

wrong:

```
import numpy as np
_, singular_values, _ = np.linalg.svd(np.dot(X.T, X))
```

harder, better, faster stronger:

```
from scipy import linalg
singular_values = sp.linalg.eigvalsh(np.dot(X.T, X))
```

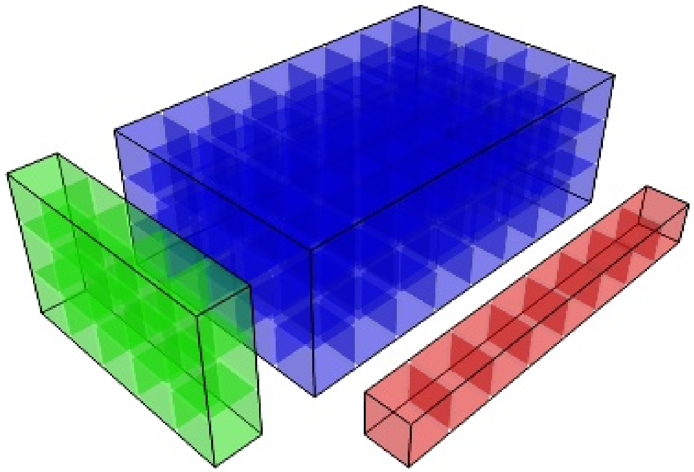
Minimize memory/number of operations

Table of Contents

8.1 Broadcasting

8.1.1 Broadcasting definition

Applying operators on arrays of different shapes:



- Adding a scalar and an array of course works:

```
>>> import numpy as np
>>> a = np.ones((3, ))
>>> a
array([ 1.,  1.,  1.])
>>> a + 1
array([ 2.,  2.,  2.])
```

- What about adding (or multiplying) two arrays of different shape?

```
>>> b = 2*np.ones((2, 1))
>>> b
array([[ 2.],
       [ 2.]])
```

```
>>> a + b
array([[ 3.,  3.,  3.],
       [ 3.,  3.,  3.]])
```

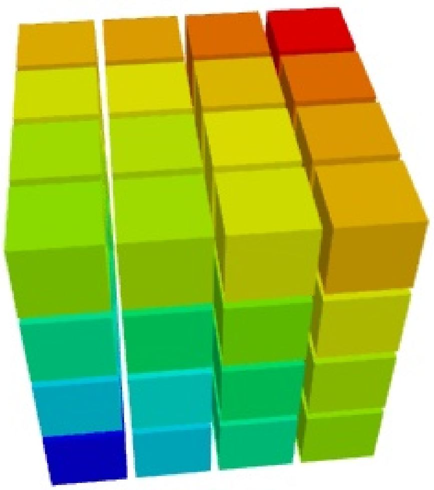
Broadcasting rules:

- Element-wize operations on arrays:
- Compare dimensions, starting from last
- Dimension of size 1 are extrapolated.

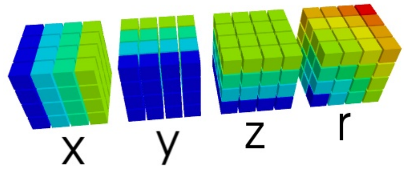
8.1.2 Applications

- Yet another way of avoiding loops
- Decreases memory consumption

Creating a 3D grid of size n



```
np.sqrt(x**2 + y**2 + z**2)
```

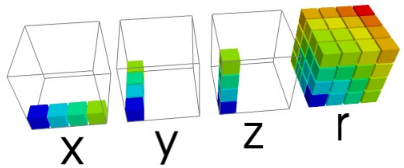
Without broadcasting

```
>>> x, y, z = np.mgrid[-100:100, -100:100, -100:100]
>>> print x.shape, y.shape, z.shape
(200, 200, 200) (200, 200, 200) (200, 200, 200)
>>> r = np.sqrt(x**2 + y**2 + z**2)
```

These three lines take **2.3s**: the creation of *x*, *y*, *z* takes 0.5s, and the calculation of *r* takes 1.8s.

The total memory used is 64Mb per array. There are 4 named arrays (*x*, *y*, *z*) and at least 2 temporary arrays are created. Thus around **400Mb** are used.

Squaring each array take 200^3 operations, as well as the two additions, and the call to *np.sqrt*. Thus a total of **48 million operations**.



With broadcasting

```
>>> x, y, z = np.ogrid[-100:100, -100:100, -100:100]
>>> print x.shape, y.shape, z.shape
(200, 1, 1) (1, 200, 1) (1, 1, 200)
>>> r = np.sqrt(x**2 + y**2 + z**2)
```

These lines take **1.1s** second, with only 6ms to create the arrays.

The three input arrays take only 1.6Kb. The output array 64Mb, and there is not more than a 64Mb and a 320kb temporary array created. Around **120Mb** are used.

Squaring each array takes 200 operations, the first addition is 200^2 = 40 thousands operations, and the second, as well as the call to *np.sqrt*, is 200^3 = 8 million operations. Thus around **16 million operations** are performed.

Looking at the relative timings between non-broadcasted and broadcasted versions, we can see that they do not scale proportionally to the number of operations. Broadcasting does take some time.

Monte-Carlo density evaluation

Density evaluation of *f = A sin(k1 X) + B sin(k2 Y)* using the probability distribution of *A*, *B*, *X* and *Y*.

Strategy: sample *f* with huge arrays of the random variables, and build an histogram of the results.

With broadcasting, sample *n* values for each *A*, *B*, *X* and *Y*, along a different direction each time. *n^4* samples for *f*.

Warning: Unwanted correlations are introduced between the random variables.

8.2 Views and strides

8.2.1 Views and copies

Views

Two arrays can point to the same data:

```
>>> import numpy as np
>>> a = np.arange(10)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> b = a[3:7]
>>> b
array([3, 4, 5, 6])
>>> b[0] = 0
>>> b
array([0, 4, 5, 6])
>>> a
array([0, 1, 2, 0, 4, 5, 6, 7, 8, 9])
```

a was also modified.

No memory duplication

How to tell: inspecting the data buffer

-
  ```
  >>> np.may_share_memory(a, b)
  True
  ```
- The *base* attribute of the array:
  ```
  >>> b.base is a
  True
  ```
- Look at the base pointer of the data buffer, and the extent:
  ```
  a.ctypes.data
  140052096
  a.ctypes.data + len(a.data)
  140052136
  b.ctypes.data
  140052108
  b.ctypes.data + len(b.data)
  140052124
  ```
- Look at the 'OWNDATA' flag to tell if the array owns its data:


```
>>> b.flags
  C_CONTIGUOUS : True
  F_CONTIGUOUS : True
  OWNDATA : False
  WRITEABLE : True
  ALIGNED : True
  UPDATEIFCOPY : False
```

But this does not mean another array shares the data:

```
>>> del a
>>> b.flags
  C_CONTIGUOUS : True
  F_CONTIGUOUS : True
  OWNDATA : False
  WRITEABLE : True
  ALIGNED : True
  UPDATEIFCOPY : False
```

The base data container is not cleared as long as there are views opened on it.

Applications

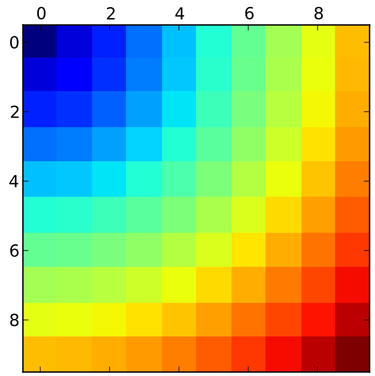
- **With a mask:**
  ```
  >>> a = np.arange(10)
  >>> a
  array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
  >>> a[(a % 2) == 0] = 0
  >>> a
  array([0, 1, 0, 3, 0, 5, 0, 7, 0, 9])
  ```
  A view was created: an array of shape (5,), and all the elements were set to zero (through *Broadcasting* of 0 to a (5,)-shaped array).
- **In loops:**
  ```
  >>> a = np.arange(30).reshape((3, 10))
  >>> a
  array([[ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9],
         [10, 11, 12, 13, 14, 15, 16, 17, 18, 19],
         [20, 21, 22, 23, 24, 25, 26, 27, 28, 29]])
  >>> from scipy.signal import detrend
  >>> for line in a:
  ...     line[:] = detrend(line)
  >>> a
  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, 0, 0, 0, 0, 0, 0]])
  ```

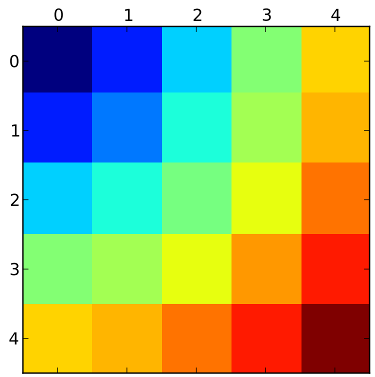
8.2.2 Reshaping, striding

Reshaping can be a special case of views.

- You can do unusual operations on arrays along certain strides:

```
import numpy as np
import pylab as pl

x, y = np.ogrid[0:10, 0:10]
r = np.sqrt(x**2 + y**2)
pl.matshow(r)

r_binned = r.reshape((5, 2, 5, 2)).sum(axis=-1).sum(axis=1)
pl.matshow(r_binned)
```



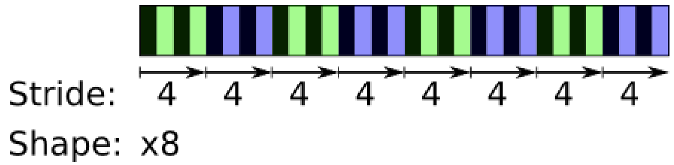


- To understand this better, let us consider what happens to the first line:


```
>>> r[:, 0]
array([ 0.,   1.,   2.,   3.,   4.,   5.,   6.,   7.,   8.,   9.])
>>> r[:, 0].reshape((5, 2))
array([[ 0.,  1.],
       [ 2.,  3.],
       [ 4.,  5.],
       [ 6.,  7.],
       [ 8.,  9.]])
>>> r[:, 0].reshape((5, 2)).sum(axis=-1)
array([  1.,   5.,   9.,  13.,  17.])
```

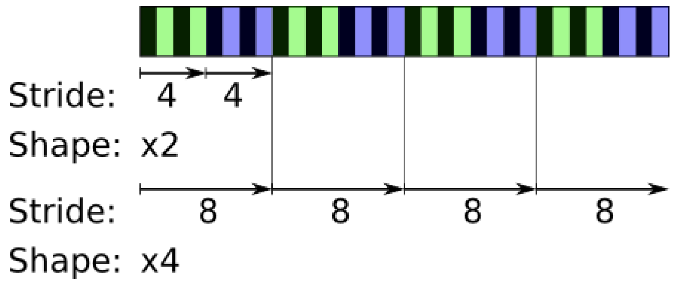
- Reshaping is (when possible) just a matter of changing the stride and shape for a flat array:

```
>>> r = np.arange(8)
>>> r.strides
(4,)
>>> r.shape
(8,)
```



After reshape:

```
>>> r2 = r.reshape((4, 2))
>>> r2.strides
(8, 4)
>>> r2.shape
(4, 2)
```



And when slicing backwards:

```
>>> r3 = r[::-1]
>>> r3.strides
(-4,)
```

Take home message:

You can apply operations with 'a certain regularity' on an array by finding the view that gives you the right striding and shape.

8.2.3 In place operations

- Inplace operators (*=)
- All ufuncs take an out arguments.

Without inplace operations

```
>>> x = np.linspace(-100, 100, 1e6)
>>> y = np.linspace(-100, 100, 1e6)
>>> r = np.sqrt(x**2 + y**2)
```

Time of the calculation of *r*: **2s**

Using inplace operations All *ufunc* take an *out* argument:

```
>>> x **= 2
>>> y **= 2
>>> x += y
>>> r = np.sqrt(x, x)
```

Total time: **1.4s**

Memory consumption twice as small.

In conclusion:

views (eventually strided) avoid memory consumption, and open the door to interesting array manipulations

8.3 Fancy indexing

8.3.1 Rules

Indexing with integer arrays

```
>>> import numpy as np
>>> a = np.arange(30).reshape((3, -1))
>>> a
array([[ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9],
       [10, 11, 12, 13, 14, 15, 16, 17, 18, 19],
       [20, 21, 22, 23, 24, 25, 26, 27, 28, 29]])
>>> a[:, (1, 3)]
array([[ 1,  3],
       [11, 13],
       [21, 23]])
```


Shape is given by (shape of indexing array) * slices:

```
>>> a[:, ((1, 3), (2, 4))].shape
(3, 2, 2)
```

If multiple integer arrays for indexing, they are broadcasted together:

```
>>> a[(1, 2), ((1, ), (2, ))]
array([[11, 21],
       [12, 22]])
```

Indexing with boolean arrays

```
>>> a[(a%2)==0]
array([ 0,  2,  4,  6,  8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28])
```

Flat shape. Slicing not used:

```
>>> a[:, (a%2)==0]
array([ 0,  2,  4,  6,  8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28])
```

8.3.2 Applications

Rearranging vectors

We have a vector family:

```
>>> vectors = np.random.randint(10, size=(4, 5))
>>> vectors
array([[2, 8, 2, 1, 7],
       [5, 9, 2, 4, 6],
       [0, 8, 6, 5, 3],
       [1, 1, 6, 1, 1]])
```

We want to rearrange them by variance:

```
>>> variance = np.var(vectors, axis=0)
>>> variance
array([  3.5    ,  10.25   ,   4.     ,   3.1875,   5.6875])
>>> rearranged = vectors[:, np.argsort(variance)]
>>> np.var(rearranged, axis=0)
array([  3.1875,   3.5    ,   4.     ,   5.6875,  10.25  ])
```

Bootstrapping

We have a vector *a*:

```
>>> a = np.arange(20).reshape((2, 10))
>>> a
array([[ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9],
       [10, 11, 12, 13, 14, 15, 16, 17, 18, 19]])
```

We want to drawn three times 10 vectors out of *a*:

```
>>> indices = np.random.randint(a.shape[-1], size=(3, 10))
>>> indices
array([[3, 6, 5, 4, 8, 9, 1, 7, 9, 6],
       [8, 0, 5, 0, 9, 6, 2, 0, 5, 2],
       [6, 3, 7, 0, 9, 0, 3, 2, 3, 1]])
>>> bootstrap = a[:, indices]
>>> bootstrap
array([[[ 3,  6,  5,  4,  8,  9,  1,  7,  9,  6],
        [ 8,  0,  5,  0,  9,  6,  2,  0,  5,  2],
        [ 6,  3,  7,  0,  9,  0,  3,  2,  3,  1]],
<BLANKLINE>
       [[13, 16, 15, 14, 18, 19, 11, 17, 19, 16],
        [18, 10, 15, 10, 19, 16, 12, 10, 15, 12],
        [16, 13, 17, 10, 19, 10, 13, 12, 13, 11]]])
```

Now we can do vectorized computations easily on the bootstraped sample.

Extracting a cut of volume along a horizon

We have an image (volumetric data):

```
>>> image = np.random.randint(10, size=(5, 5))
>>> image
array([[3, 1, 3, 7, 1],
       [7, 4, 0, 5, 1],
       [5, 9, 9, 4, 0],
       [9, 8, 8, 6, 8],
       [6, 3, 1, 2, 5]])
```

And a horizon: the coordinates of a curve in the image:

```
>>> horizon = np.array([3, 2, 1, 3, 2])
```

We can extract the value on the horizon:

```
>>> image[horizon, np.arange(5)]
array([9, 9, 0, 6, 0])
```

Local average along a horizon

This time, we want to extract the voxels in the 3-voxels-wide region around the horizon:

```
>>> image[horizon + np.arange(-1, 2)[:, np.newaxis], np.arange(5)]
array([[5, 4, 3, 4, 1],
       [9, 9, 0, 6, 0],
       [6, 8, 9, 2, 8]])
```

Two broadcastings: one in x coordinates *horizon + np.arange(-1, 2)[:, np.newaxis]*, and the second one between the x and the y coordinates.

Drawback of these techniques: costly in memory

8.4 Robert (Kern)'s nasty stride trick

Warning: Parents guidance: not for underaged children

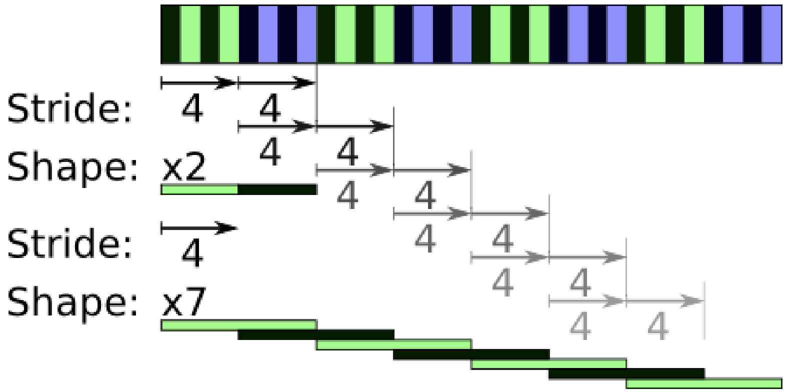
Problem Sliding average, but we don't want copies.

We want to take a sliding average of a, on a window of size 2:

```
>>> import numpy as np
>>> a = np.arange(8)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7])
>>> a.strides
(4,)
```

We are going to create improbable strides and shapes (numpy 1.2):

```
>>> from numpy.lib import stride_tricks
>>> b = stride_tricks.as_strided(a, shape=(2, 7), strides=(4, 4))
>>> b
array([[0, 1, 2, 3, 4, 5, 6],
       [1, 2, 3, 4, 5, 6, 7]])
```



Overlapping dimensions!

Easy, now all we have to do is sum along the axis 0:

```
>>> b.sum(axis=0)
array([ 1,  3,  5,  7,  9, 11, 13])
```

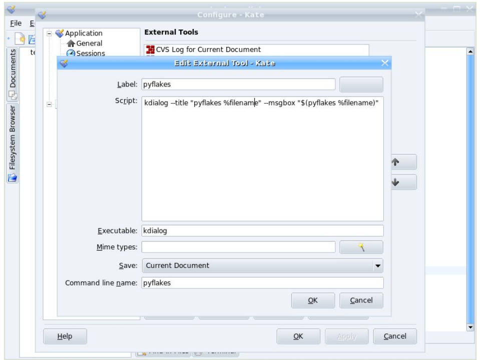
CHAPTER 9

pyflakes: fast static analysis

- **Fast, simple**
- Detects syntax errors, missing imports, typos on names.

9.1 In kate

Menu: ‘settings -> configure kate -> External Tools’, add *pyflakes*:



9.2 In vim

In your *.vimrc* (binds F5 to *pyflakes*):

```
autocmd FileType python let &mp = 'echo "*** running % ***" ; pyflakes %'
autocmd FileType tex,mp,rst,python imap <Esc>[15~ <C-O>:make!^M
autocmd FileType tex,mp,rst,python map  <Esc>[15~ :make!^M
autocmd FileType tex,mp,rst,python set autowrite
```


9.3 In emacs

In your *.emacs* (binds F5 to *pyflakes*):

```
(defun pyflakes-thisfile () (interactive)
       (compile (format "pyflakes %s" (buffer-file-name)))
)

(define-minor-mode pyflakes-mode
    "Toggle pyflakes mode.
    With no argument, this command toggles the mode.
    Non-null prefix argument turns on the mode.
    Null prefix argument turns off the mode."
    ;; The initial value.
    nil
    ;; The indicator for the mode line.
    " Pyfalkes"
    ;; The minor mode bindings.
    '( ([f5] . pyflakes-thisfile) )
)

(add-hook 'python-mode-hook (lambda () (pyflakes-mode t)))
```