



Python Scientific lecture notes

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EuroScipy tutorial team

Editors: Valentin Haenel, Emmanuelle Gouillart, Gaël Varoquaux

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Contents

I Authors	2
1 Editors	2
2 Chapter authors	2
3 Additional Contributions	2
II License	2
III Getting started with Python for science	4
4 Scientific computing with tools and workflow	5
4.1 Why Python?	5
4.2 Scientific Python building blocks	7
4.3 The interactive workflow: IPython and a text editor	8
5 The Python language	10
5.1 First steps	11
5.2 Basic types	11
5.3 Assignment operator	17
5.4 Control Flow	18
5.5 Defining functions	22
5.6 Reusing code: scripts and modules	27
5.7 Input and Output	34
5.8 Standard Library	34
5.9 Exceptions handling in Python	38
5.10 Object-oriented programming (OOP)	41
6 NumPy: creating and manipulating numerical data	42
6.1 Intro	42
6.2 1. Basics I	42
6.3 2. Basics II	58
6.4 3. Moving on	78
6.5 4. Under the hood	89
7 Getting help and finding documentation	93

8 Matplotlib	97	236
8.1 Introduction	97	237
8.2 IPython	97	238
8.3 pylab	97	240
8.4 Simple Plots	97	242
8.5 Properties	99	251
8.6 Text	101	257
8.7 Ticks	103	
8.8 Figures, Subplots, and Axes	104	
8.9 Other Types of Plots	106	
8.10 The Class Library	112	
9 Scipy : high-level scientific computing	115	266
9.1 Scipy builds upon Numpy	116	266
9.2 File input/output: <code>scipy.io</code>	116	267
9.3 Signal processing: <code>scipy.signal</code>	117	270
9.4 Special functions: <code>scipy.special</code>	118	273
9.5 Statistics and random numbers: <code>scipy.stats</code>	118	
9.6 Linear algebra operations: <code>scipy.linalg</code>	120	
9.7 Numerical integration: <code>scipy.integrate</code>	121	
9.8 Fast Fourier transforms: <code>scipy.fftpack</code>	124	
9.9 Interpolation: <code>scipy.interpolate</code>	127	
9.10 Optimization and fit: <code>scipy.optimize</code>	129	
9.11 Image processing: <code>scipy.ndimage</code>	130	
9.12 Summary exercises on scientific computing	135	
IV Advanced topics	149	289
10 Advanced Python Constructs	150	290
10.1 Iterators, generator expressions and generators	151	
10.2 Decorators	155	
10.3 Context managers	163	
11 Advanced Numpy	166	
11.1 Life of ndarray	167	
11.2 Universal functions	179	
11.3 Interoperability features	188	
11.4 Siblings: <code>chararray, maskedarray, matrix</code>	195	
11.5 Summary	196	
11.6 Contributing to Numpy/Scipy	196	
12 Debugging code	200	
12.1 Avoiding bugs	200	
12.2 Debugging workflow	202	
12.3 Using the Python debugger	203	
12.4 Debugging segmentation faults using <code>gdb</code>	207	
13 Optimizing code	210	
13.1 Optimization workflow	210	
13.2 Profiling Python code	211	
13.3 Making code go faster	213	
13.4 Writing faster numerical code	214	
14 Sparse Matrices in SciPy	216	
14.1 Introduction	216	
14.2 Storage Schemes	218	
14.3 Linear System Solvers	230	
14.4 Other Interesting Packages	234	
15 Image manipulation and processing using Numpy and Scipy	237	
15.1 Opening and writing to image files	237	
15.2 Displaying images	238	
15.3 Basic manipulations	240	
15.4 Image filtering	242	
15.5 Feature extraction	251	
15.6 Measuring objects properties	257	
16 3D plotting with Mayavi	266	
16.1 A simple example	266	
16.2 3D plotting functions	267	
16.3 Figures and decorations	270	
16.4 Interaction	273	
17 Sympy : Symbolic Mathematics in Python	274	
17.1 First Steps with SymPy	275	
17.2 Algebraic manipulations	276	
17.3 Calculus	277	
17.4 Equation solving	278	
17.5 Linear Algebra	279	
18 scikit-learn: machine learning in Python	281	
18.1 Loading an example dataset	282	
18.2 Supervised learning	283	
18.3 Clustering: grouping observations together	285	
18.4 Putting it all together : face recognition with Support Vector Machines	287	
Bibliography		
Index		

This document

Teaching material on the scientific Python ecosystem, a quick introduction to central tools and technics. The different chapters each correspond to a 1 to 2 hours course with increasing level of expertise, from beginner to expert.

Part I**Authors****CHAPTER 1****Editors**

- Valentin Haenel
- Emmanuelle Gouillart
- Gaël Varoquaux

CHAPTER 2**Chapter authors**

Listed by alphabetical order.

- Christopher Burns
- Christophe Combelles
- Adrian Chauve
- Robert Cimrman
- André Espaze
- Emmanuelle Gouillart
- Mike Müller
- Fabian Pedregosa
- Gaël Varoquaux

Contents

- Li Virtanen
- Zbigniew Jędrzejewski-Szmek

CHAPTER 3

Part III

Getting started with Python for science

CHAPTER 4

Scientific computing with tools and workflow

authors Fernando Perez, Emmanuelle Gouillart, Gaël Varoquaux

4.1 Why Python?

4.1.1 The scientist's needs

- Get data (simulation, experiment control)
- Manipulate and process data.
- Visualize results... to understand what we are doing!
- Communicate on results: produce figures for reports or publications, write presentations.

4.1.2 Specifications

- Rich collection of already existing **bricks** corresponding to classical numerical methods or basic actions: we don't want to re-program the plotting of a curve, a Fourier transform or a fitting algorithm. Don't reinvent the wheel!
- Easy to learn: computer science neither is our job nor our education. We want to be able to draw a curve, smooth a signal, do a Fourier transform in a few minutes.
- Easy communication with collaborators, students, customers, to make the code live within a labo or a company: the code should be as readable as a book. Thus, the language should contain as few syntax symbols or unneeded routines that would divert the reader from the mathematical or scientific understanding of the code.
- Efficient code that executes quickly... But needless to say that a very fast code becomes useless if we spend too much time writing it. So, we need both a quick development time and a quick execution time.
- A single environment/language for everything, if possible, to avoid learning a new software for each new problem.

4.1.3 Existing solutions

Which solutions do the scientists use to work?

Compiled languages: C, C++, Fortran, etc.

- Advantages:
 - Very fast. Very optimized compilers. For heavy computations, it's difficult to outperform these languages.
 - Some very optimized scientific libraries have been written for these languages. Ex: blas (vector/matrix operations)
- Drawbacks:
 - Painful usage: no interactivity during development, mandatory compilation steps, verbose syntax (&, ::, {}, ; etc.), manual memory management (tricky in C). These are **difficult languages** for non computer scientists.

Scripting languages: Matlab

- Advantages:
 - Very rich collection of libraries with numerous algorithms, for many different domains. Fast execution because these libraries are often written in a compiled language.
 - Pleasant development environment: comprehensive and well organized help, integrated editor, etc.
 - Commercial support is available.
- Drawbacks:
 - Base language is quite poor and can become restrictive for advanced users.
 - Not free.

Other script languages: Scilab, Octave, Igor, R, IDL, etc.

- Advantages:
 - Open-source, free, or at least cheaper than Matlab.
 - Some features can be very advanced (statistics in R, figures in Igor, etc.)
- Drawbacks:
 - fewer available algorithms than in Matlab, and the language is not more advanced.
 - Some software are dedicated to one domain. Ex: Gnuplot or xmgrace to draw curves. These programs are very powerful, but they are restricted to a single type of usage, such as plotting.

What about Python?

- Advantages:
 - Very rich scientific computing libraries (a bit less than Matlab, though)
 - Well-thought language, allowing to write very readable and well structured code: we “code what we think”.
 - Many libraries for other tasks than scientific computing (web server management, serial port access, etc.)
 - Free and open-source software, widely spread, with a vibrant community.
- Drawbacks:
 - less pleasant development environment than, for example, Matlab. (More geek-oriented).
 - Not all the algorithms that can be found in more specialized software or toolboxes.

4.2 Scientific Python building blocks

- **Python**, a generic and modern computing language
 - Python language: data types (string, int), flow control, data collections (lists, dictionaries), patterns, etc.
 - Modules of the standard library.
 - A large number of specialized modules or applications written in Python: web protocols, web framework, etc. ... and scientific computing.
 - Development tools (automatic tests, documentation generation)

```
Shell - Konsole <2>
In [6]: s.
s.capitalize  s.expandtabs  s.lower  s.rstrip  s.ti
s.center  s.encode  s.lstrip  s.replace  s.translate
s.count  s.index  s.partition  s.replace  s.splitlines  s.uq
s.decode  s.isalnum  s.lstrip  s.rfind  s.startswith
s.encode  s.isalpha  s.join  s.rindex  s.strip
s.endswith  s.isdigit  s.ljust  s.rjust  s.zfill
s.expandtabs  s.lowercase  s.lstrip  s.replace  s.zfill

In [7]: s.
Functions are automatically parenthesized, saving typing:

In [8]: s.replace('TAB', 'tab')
Out[8]: s.replace('TAB', 'tab')

In [9]: s.
    Python uses Tab for name completion. Hit Tab after the dot:

In [10]: s.replace TAB
          s.replace('TAB', 'tab')
Out[10]: IPython uses TAB for name completion. Hit TAB after the dot:
```

- **IPython**, an advanced Python shell

<http://ipython.scipy.org/moin/>

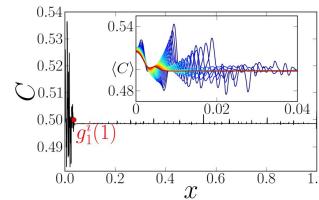
- **Numpy** : provides powerful **numerical arrays** objects, and routines to manipulate them.

<http://www.scipy.org/>

- **Scipy** : high-level data processing routines. Optimization, regression, interpolation, etc

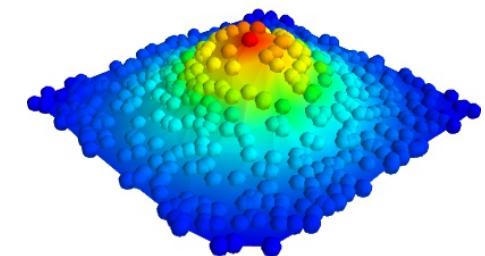
<http://www.scipy.org/>

- **Matplotlib** : 2-D visualization, “publication-ready” plots



<http://matplotlib.sourceforge.net/>

- **Mayavi** : 3-D visualization



<http://code.enthought.com/projects/mayavi/>

4.3 The interactive 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 environment to work into, and not only one way of using it. Although this makes it harder for beginners to find their way, it makes it possible for Python to be used to write programs, in web servers, or embedded devices. Here, 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/>

4.3.1 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.
```

4.3.2 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 Python(x,y), you can use Spyder. 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.

The Python language

authors Chris Burns, Christophe Combelle, Emmanuelle Gouillart, Gaël Varoquaux

Python for scientific computing

We introduce here the Python language. Only the bare minimum necessary for getting started with Numpy and Scipy is addressed here. To learn more about the language, consider going through the excellent tutorial <http://docs.python.org/tutorial>. Dedicated books are also available, such as <http://diveintopython.org/>.



Python is a **programming language**, as are C, Fortran, BASIC, PHP, etc. Some specific features of Python are as follows:

- an *interpreted* (as opposed to *compiled*) language. Contrary to e.g. C or Fortran, one does not compile Python code before executing it. In addition, Python can be used **interactively**: many Python interpreters are available, from which commands and scripts can be executed.
- a free software released under an **open-source** license: Python can be used and distributed free of charge, even for building commercial software.
- **multi-platform**: Python is available for all major operating systems, Windows, Linux/Unix, MacOS X, most likely your mobile phone OS, etc.
- a very readable language with clear non-verbose syntax
- a language for which a large variety of high-quality packages are available for various applications, from web frameworks to scientific computing.
- a language very easy to interface with other languages, in particular C and C++.
- Some other features of the language are illustrated just below. For example, Python is an object-oriented language, with dynamic typing (the same variable can contain objects of different types during the course of a program).

See <http://www.python.org/about/> for more information about distinguishing features of Python.

5.1 First steps

Start the **Ipython** shell (an enhanced interactive Python shell):

- by typing “ipython” from a Linux/Mac terminal, or from the Windows cmd shell,
- or by starting the program from a menu, e.g. in the [Python\(x,y\)](#) or [EPD](#) menu if you have installed one of these scientific-Python suites.

If you don't have Ipython installed on your computer, other Python shells are available, such as the plain Python shell started by typing “python” in a terminal, or the Idle interpreter. However, we advise to use the Ipython shell because of its enhanced features, especially for interactive scientific computing.

Once you have started the interpreter, type

```
>>> print "Hello, world!"
Hello, world!
```

The message “Hello, world!” is then displayed. You just executed your first Python instruction, congratulations!

To get yourself started, type the following stack of instructions

```
>>> a = 3
>>> b = 2*a
>>> type(b)
<type 'int'>
>>> print b
6
>>> a*b
18
>>> b = 'hello'
>>> type(b)
<type 'str'>
>>> b + b
'hellohello'
>>> 2*b
'hellohello'
```

Two variables `a` and `b` have been defined above. Note that one does not declare the type of a variable before assigning its value. In C, conversely, one should write:

```
int a = 3;
```

In addition, the type of a variable may change, in the sense that at one point in time it can be equal to a value of a certain type, and a second point in time, it can be equal to a value of a different type. `b` was first equal to an integer, but it became equal to a string when it was assigned the value ‘hello’. Operations on integers (`b=2*a`) are coded natively in Python, and so are some operations on strings such as additions and multiplications, which amount respectively to concatenation and repetition.

5.2 Basic types

5.2.1 Numerical types

Integer variables:

```
>>> 1 + 1
2
>>> a = 4
```

floats

```
>>> c = 2.1
```

complex (a native type in Python!)

```
>>> a = 1.5 + 0.5j
>>> a.real
1.5
>>> a.imag
0.5
```

and booleans:

```
>>> 3 > 4
False
>>> test = (3 > 4)
>>> test
False
>>> type(test)
<type 'bool'>
```

A Python shell can therefore replace your pocket calculator, with the basic arithmetic operations +, -, *, /, % (modulo) natively implemented:

```
>>> 7 * 3.
21.0
>>> 2**10
1024
>>> 8 % 3
2
```

Warning: Integer division

```
>>> 3 / 2
1
```

Trick: use floats:

```
>>> 3 / 2.
1.5

>>> a = 3
>>> b = 2
>>> a / b
1
>>> a / float(b)
1.5
```

- Scalar types: int, float, complex, bool:

```
>>> type(1)
<type 'int'>
>>> type(1.)
<type 'float'>
>>> type(1. + 0j )
<type 'complex'>

>>> a = 3
>>> type(a)
<type 'int'>
```

- Type conversion:

```
>>> float(1)
1.0
```

5.2.2 Containers

Python provides many efficient types of containers, in which collections of objects can be stored.

Lists

A list is an ordered collection of objects, that may have different types. For example

```
>>> l = [1, 2, 3, 4, 5]
>>> type(l)
<type 'list'>
```

- Indexing: accessing individual objects contained in the list:

```
>>> l[2]
3
```

Counting from the end with negative indices:

```
>>> l[-1]
5
>>> l[-2]
4
```

Warning: Indexing starts at 0 (as in C), not at 1 (as in Fortran or Matlab)!

- Slicing: obtaining sublists of regularly-spaced elements

```
>>> l
[1, 2, 3, 4, 5]
>>> l[2:4]
[3, 4]
```

Warning: Note that `l[start:stop]` contains the elements with indices `i` such as `start <= i < stop` (`i` ranging from `start` to `stop-1`). Therefore, `l[start:stop]` has `(stop-start)` elements.

Slicing syntax: `l[start:stop:stride]`

All slicing parameters are optional:

```
>>> l[3:]
[4, 5]
>>> l[:3]
[1, 2, 3]
>>> l[::-2]
[1, 3, 5]
```

Lists are *mutable* objects and can be modified:

```
>>> l[0] = 28
>>> l
[28, 2, 3, 4, 5]
>>> l[2:4] = [3, 8]
>>> l
[28, 2, 3, 8, 5]
```

Note: The elements of a list may have different types:

```
>>> l = [3, 2, 'hello']
>>> l
[3, 2, 'hello']
>>> l[1], l[2]
(2, 'hello')
```

For collections of numerical data that all have the same type, it is often **more efficient** to use the `array` type provided by the `numpy` module. A NumPy array is a chunk of memory containing fixed-sized items. With NumPy arrays, operations on elements can be faster because elements are regularly spaced in memory and more operations are performed through specialized C functions instead of Python loops.

Python offers a large panel of functions to modify lists, or query them. Here are a few examples; for more details, see <http://docs.python.org/tutorial/datastructures.html#more-on-lists>

Add and remove elements:

```
>>> l = [1, 2, 3, 4, 5]
>>> l.append(6)
>>> l
[1, 2, 3, 4, 5, 6]
>>> l.pop()
6
>>> l
[1, 2, 3, 4, 5]
>>> l.extend([6, 7]) # extend l, in-place
>>> l
[1, 2, 3, 4, 5, 6, 7]
>>> l = l[:-2]
>>> l
[1, 2, 3, 4, 5]
```

Reverse l:

```
>>> r = l[::-1]
>>> r
[5, 4, 3, 2, 1]
```

Concatenate and repeat lists:

```
>>> r + l
[5, 4, 3, 2, 1, 1, 2, 3, 4, 5]
>>> 2 * r
[5, 4, 3, 2, 1, 5, 4, 3, 2, 1]
```

Sort r (in-place):

```
>>> r.sort()
>>> r
[1, 2, 3, 4, 5]
```

Note: Methods and Object-Oriented Programming

The notation `r.method()` (`r.sort()`, `r.append(3)`, `l.pop()`) is our first example of object-oriented programming (OOP). Being a list, the object `r` owns the `method` function that is called using the notation `.`. No further knowledge of OOP than understanding the notation `.` is necessary for going through this tutorial.

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
```

Strings

Different string syntaxes (simple, double or triple quotes):

```
s = 'Hello, how are you?'
s = "Hi, what's up"
s = '''Hello,
how are you'''      # tripling the quotes allows the
                     # the string to span more than one line
s = """Hi,
what's up?"""
```

```
In [1]: 'Hi, what's up?'
```

```
File "<ipython console>", line 1
  'Hi, what's up?'
    ^
SyntaxError: invalid syntax
```

The newline character is \n, and the tab character is \t.

Strings are collections like lists. Hence they can be indexed and sliced, using the same syntax and rules.

Indexing:

```
>>> a = "hello"
>>> a[0]
'h'
>>> a[1]
'e'
>>> a[-1]
'o'
```

(Remember that negative indices correspond to counting from the right end.)

Slicing:

```
>>> a = "hello, world!"
>>> a[3:6] # 3rd to 6th (excluded) elements: elements 3, 4, 5
'lo,' 
>>> a[2:10:2] # Syntax: a[start:stop:step]
'lo o'
>>> a[::-3] # every three characters, from beginning to end
'hl r!'
```

Accents and special characters can also be handled in Unicode strings (see <http://docs.python.org/tutorial/introduction.html#unicode-strings>).

A string is an **immutable object** and it is not possible to modify its contents. One may however create new strings from the original one.

```
In [53]: a = "hello, world!"
In [54]: a[2] = 'z'
```

```
TypeError
last)

/home/gouillar/travail/sgr/2009/talks/dakar_python/cours/gael/essai/source/<ipython
console> in <module>()

TypeError: 'str' object does not support item assignment
In [55]: a.replace('l', 'z', 1)
Out[55]: 'hezlo, world!'
In [56]: a.replace('l', 'z')
Out[56]: 'hezzo, worzd!'
```

Strings have many useful methods, such as a.replace as seen above. Remember the a. object-oriented notation and use tab completion or help(str) to search for new methods.

Note: Python offers advanced possibilities for manipulating strings, looking for patterns or formatting. Due to lack of time this topic is not addressed here, but the interested reader is referred to <http://docs.python.org/library/stdtypes.html#string-methods> and <http://docs.python.org/library/string.html#new-string-formatting>

- String substitution:

```
>>> 'An integer: %i; a float: %f; another string: %s' % (1, 0.1, 'string')
'An integer: 1; a float: 0.100000; another string: string'

>>> i = 102
>>> filename = 'processing_of_dataset_%03d.txt'%i
>>> filename
'processing_of_dataset_102.txt'
```

Dictionaries

A dictionary is basically an efficient table that **maps keys to values**. It is an **unordered** container:

```
>>> tel = {'emmanuelle': 5752, 'sebastian': 5578}
>>> tel['francis'] = 5915
>>> tel
{'sebastian': 5578, 'francis': 5915, 'emmanuelle': 5752}
>>> tel['sebastian']
5578
>>> tel.keys()
['sebastian', 'francis', 'emmanuelle']
>>> tel.values()
[5578, 5915, 5752]
>>> 'francis' in tel
True
```

It can be used to conveniently store and retrieve values associated with a name (a string for a date, a name, etc.). See <http://docs.python.org/tutorial/datastructures.html#dictionaries> for more information.

A dictionary can have keys (resp. values) with different types:

```
>>> d = {'a':1, 'b':2, 3:'hello'}
>>> d
{'a': 1, 3: 'hello', 'b': 2}
```

More container types

- Tuples

Tuples are basically immutable lists. The elements of a tuple are written between parentheses, or just separated by commas:

```
>>> t = 12345, 54321, 'hello!'
>>> t[0]
12345
>>> t
(12345, 54321, 'hello!')
>>> u = (0, 2)
```

- Sets: unordered, unique items:

```
>>> s = set('a', 'b', 'c', 'a')
>>> s
set(['a', 'c', 'b'])
>>> s.difference('a', 'b')
set(['c'])
```

A bag of Ipython tricks

- Several Linux shell commands work in Ipython, such as ls, pwd, cd, etc.
- To get help about objects, functions, etc., type help object. Just type help() to get started.
- Use tab-completion as much as possible: while typing the beginning of an object's name (variable, function, module), press the Tab key and Ipython will complete the expression to match available names. If many names are possible, a list of names is displayed.
- History: press the up (resp. down) arrow to go through all previous (resp. next) instructions starting with the expression on the left of the cursor (put the cursor at the beginning of the line to go through all previous commands)
- You may log your session by using the Ipython "magic command" %logstart. Your instructions will be saved in a file, that you can execute as a script in a different session.

```
In [1]: %logstart commands.log
Activating auto-logging. Current session state plus future input
saved.
Filename      : commands.log
Mode          : backup
Output logging : False
Raw input log  : False
Timestamping   : False
State         : active
```

5.3 Assignment operator

Python library reference says:

Assignment statements are used to (re)bind names to values and to modify attributes or items of mutable objects.

In short, it works as follows (simple assignment):

1. an expression on the right hand side is evaluated, the corresponding object is created/obtained
2. a **name** on the left hand side is assigned, or bound, to the r.h.s. object

Things to note:

- a single object can have several names bound to it:

```
In [1]: a = [1, 2, 3]
In [2]: b = a
In [3]: a
Out[3]: [1, 2, 3]
In [4]: b
```

```
Out[4]: [1, 2, 3]
In [5]: a is b
Out[5]: True
In [6]: b[1] = 'hi!'
In [7]: a
Out[7]: [1, 'hi!', 3]
```

- to change a list *in place*, use indexing/slices:

```
In [1]: a = [1, 2, 3]
In [3]: a
Out[3]: [1, 2, 3]
In [4]: a = ['a', 'b', 'c'] # Creates another object.
In [5]: a
Out[5]: ['a', 'b', 'c']
In [6]: id(a)
Out[6]: 138641676
In [7]: a[:] = [1, 2, 3] # Modifies object in place.
In [8]: a
Out[8]: [1, 2, 3]
In [9]: id(a)
Out[9]: 138641676 # Same as in Out[6], yours will differ...
```

- the key concept here is **mutable vs. immutable**

- mutable objects can be changed in place
- immutable objects cannot be modified once created

A very good and detailed explanation of the above issues can be found in David M. Beazley's article [Types and Objects in Python](#).

5.4 Control Flow

Controls the order in which the code is executed.

5.4.1 if/elif/else

```
In [1]: if 2**2 == 4:
...:     print 'Obvious!'
...:
Obvious!
```

Blocks are delimited by indentation

Type the following lines in your Python interpreter, and be careful to **respect the indentation depth**. The Ipython shell automatically increases the indentation depth after a column : sign; to decrease the indentation depth, go four spaces to the left with the Backspace key. Press the Enter key twice to leave the logical block.

```
In [2]: a = 10
In [3]: if a == 1:
...:     print(1)
...: elif a == 2:
...:     print(2)
...: else:
...:     print('A lot')
...:
A lot
```

Indentation is compulsory in scripts as well. As an exercise, re-type the previous lines with the same indentation in a script condition.py, and execute the script with run condition.py in Ipython.

5.4.2 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
```

5.4.3 while/break/continue

Typical C-style while loop (Mandelbrot problem):

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

In [7]: while abs(z) < 100:
...:     z = z**2 + 1
...
In [8]: z
Out[8]: (-134+352j)
```

More advanced features

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
...
...:
```

continue the next iteration of a loop.:

```
>>> a = [1, 0, 2, 4]
>>> for element in a:
...:     if element == 0:
...:         continue
...:     print 1. / element
...
1.0
0.5
0.25
```

5.4.4 Conditional Expressions

- if object

Evaluates to False:

- any number equal to zero (0, 0.0, 0+0j)
- an empty container (list, tuple, set, dictionary, ...)
- False, None

Evaluates to True:

- everything else¹

- a == b

Tests equality, with logics:

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

- a is b

Tests identity: both sides are the same object

```
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

```
>>> b = [1, 2, 3]
>>> 2 in b
True
>>> 5 in b
False
```

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

5.4.5 Advanced iteration

Iterate over any sequence

- You can iterate over any sequence (string, list, keys in a dictionary, lines in a file, ...)

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

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

```
>>> message = "Hello how are you?"
>>> message.split() # returns a list
['Hello', 'how', 'are', 'you?']
>>> for word in message.split():
```

¹ User-defined classes can customize those rules by overriding the special `__nonzero__` method.

```
...     print word
...
Hello
how
are
you?
```

Few languages (in particular, languages for scientific computing) allow to loop over anything but integers/indices. With Python it is possible to loop exactly over the objects of interest without bothering with indices you often don't care about.

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:

```
>>> words = ("cool", "powerful", 'readable')
>>> 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
```

5.4.6 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:

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

5.5 Defining functions

5.5.1 Function definition

```
In [56]: def test():
    ....:     print('in test function')
    ....:
    ....:
In [57]: test()
in test function
```

Warning: Function blocks must be indented as other control-flow blocks.

5.5.2 Return statement

Functions can *optionally* return values.

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

In [8]: disk_area(1.5)
Out[8]: 7.064999999999999
```

Note: By default, functions return `None`.

Note: Note the syntax to define a function:

- the `def` keyword;
- is followed by the function's `name`, then
- the arguments of the function are given between brackets followed by a colon.
- the function body ;
- and `return object` for optionally returning values.

5.5.3 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 # Now really big
In [128]: double_it()
Out[128]: 20
```

More involved example implementing python's slicing:

```
In [98]: def slicer(seq, start=None, stop=None, step=None):
....:     """Implement basic python slicing."""
....:     return seq[start:stop:step]
....:
In [101]: rhyme = 'one fish, two fish, red fish, blue fish'.split()
In [102]: rhyme
Out[102]: ['one', 'fish,', 'two', 'fish,', 'red', 'fish,', 'blue', 'fish']
In [103]: slicer(rhyme)
Out[103]: ['one', 'fish,', 'two', 'fish,', 'red', 'fish,', 'blue', 'fish']
In [104]: slicer(rhyme, step=2)
Out[104]: ['one', 'two', 'red', 'blue']
In [105]: slicer(rhyme, 1, step=2)
Out[105]: ['fish,', 'fish,', 'fish,', 'fish']
In [106]: slicer(rhyme, start=1, stop=4, step=2)
Out[106]: ['fish,', 'fish,']
```

The order of the keyword arguments does not matter:

```
In [107]: slicer(rhyme, step=2, start=1, stop=4)
Out[107]: ['fish,', 'fish,']
```

but it is good practice to use the same ordering as the function's definition.

Keyword arguments are a very convenient feature for defining functions with a variable number of arguments, especially when default values are to be used in most calls to the function.

5.5.4 Passed by value

Can you modify the value of a variable inside a function? Most languages (C, Java, ...) distinguish “passing by value” and “passing by reference”. In Python, such a distinction is somewhat artificial, and it is a bit subtle whether your variables are going to be modified or not. Fortunately, there exist clear rules.

Parameters to functions are references to objects, which are passed by value. When you pass a variable to a function, python passes the reference to 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 may modify the caller's variable in-place:

```
>>> def try_to_modify(x, y, z):
...     x = 23
...     y.append(42)
...     z = [99] # new reference
...     print(x)
...     print(y)
...     print(z)
...
>>> a = 77 # immutable variable
>>> b = [99] # mutable variable
>>> c = [28]
>>> try_to_modify(a, b, c)
23
[99, 42]
[99]
>>> print(a)
77
>>> print(b)
[99, 42]
>>> print(c)
[28]
```

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

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

5.5.5 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
```

5.5.6 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}
```

5.5.7 Docstrings

Documentation 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 0xeaaf0f0>
```

```
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.
```

Note: Docstring guidelines

For the sake of standardization, the [Docstring Conventions](#) webpage documents the semantics and conventions associated with Python docstrings.

Also, the Numpy and Scipy modules have defined a precised standard for documenting scientific functions, that you may want to follow for your own functions, with a `Parameters` section, an `Examples` section, etc. See <http://projects.scipy.org/numpy/wiki/CodingStyleGuidelines#docstring-standard> and <http://projects.scipy.org/numpy/browser/trunk/doc/example.py#L37>

5.5.8 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}
```

5.5.9 Methods

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

5.5.10 Exercises

Exercise: Quicksort

Implement the quicksort algorithm, as defined by wikipedia:

```
function quicksort(array)
    var list less, greater
    if length(array) < 2
        return array
    select and remove a pivot value pivot from array
    for each x in array
        if x < pivot + 1 then append x to less
        else append x to greater
    return concatenate(quicksort(less), pivot, quicksort(greater))
```

Exercise: Fibonacci sequence

Write a function that displays the n first terms of the Fibonacci sequence, defined by:

- $u_0 = 1; u_1 = 1$
- $u_{(n+2)} = u_{(n+1)} + u_n$

5.6 Reusing code: scripts and modules

For now, we have typed all instructions in the interpreter. For longer sets of instructions we need to change tack and write the code in text files (using a text editor), that we will call either **scripts** or **modules**. Use your favorite text editor (provided it offers syntax highlighting for Python), or the editor that comes with the Scientific Python Suite you may be using (e.g., Scite with Python(x,y)).

5.6.1 Scripts

Let us first write a **script**, that is a file with a sequence of instructions that are executed each time the script is called.

Instructions may be e.g. copied-and-pasted from the interpreter (but take care to respect indentation rules!). The extension for Python files is **.py**. Write or copy-and-paste the following lines in a file called **test.py**

```
message = "Hello how are you?"
for word in message.split():
    print word
```

Let us now execute the script interactively, that is inside the Ipython interpreter. This is maybe the most common use of scripts in scientific computing.

- in Ipython, the syntax to execute a script is `%run script.py`. For example,

```
In [1]: %run test.py
Hello
how
are
you?

In [2]: message
Out[2]: 'Hello how are you?'
```

The script has been executed. Moreover the variables defined in the script (such as `message`) are now available inside the interpreter's namespace.

Other interpreters also offer the possibility to execute scripts (e.g., `execfile` in the plain Python interpreter, etc.).

It is also possible In order to execute this script as a **standalone program**, by executing the script inside a shell terminal (Linux/Mac console or cmd Windows console). For example, if we are in the same directory as the `test.py` file, we can execute this in a console:

```
epsilon:~/sandbox$ python test.py
Hello
how
are
you?
```

Standalone scripts may also take command-line arguments

In `file.py`:

```
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`.

5.6.2 Importing objects from modules

```
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 vice-versa.
- Creates possible name clashes between modules.
- Makes the code impossible to statically check for undefined symbols.

Modules are thus a good way to organize code in a hierarchical way. Actually, all the scientific computing tools we are going to use are modules:

```
>>> import numpy as np # data arrays
>>> np.linspace(0, 10, 6)
array([ 0.,  2.,  4.,  6.,  8., 10.])
>>> import scipy # scientific computing
```

In Python(x,y) software, Ipython(x,y) execute the following imports at startup:

```
>>> import numpy
>>> import numpy as np
```

```
>>> from pylab import *
>>> import scipy
```

and it is not necessary to re-import these modules.

5.6.3 Creating modules

If we want to write larger and better organized programs (compared to simple scripts), where some objects are defined, (variables, functions, classes) and that we want to reuse several times, we have to create our own **modules**.

Let us create a module `demo` contained in the file `demo.py`:

```
"A demo module."
def print_b():
    "Prints b."
    print 'b'

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

c = 2
d = 2
```

In this file, we defined two functions `print_a` and `print_b`. Suppose we want to call the `print_a` function from the interpreter. We could execute the file as a script, but since we just want to have access to the function `print_a`, we are rather going to **import it as a module**. The syntax is as follows.

```
In [1]: import demo

In [2]: demo.print_a()
a

In [3]: demo.print_b()
b
```

Importing the module gives access to its objects, using the `module.object` syntax. Don't forget to put the module's name before the object's name, otherwise Python won't recognize the instruction.

Introspection

```
In [4]: 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 [5]: who
demo

In [6]: whos
Variable      Type      Data/Info
-----
demo        module    <module 'demo' from 'demo.py'>

In [7]: dir(demo)
```

```
Out[7]:
['__builtins__',
 '__doc__',
 '__file__',
 '__name__',
 '__package__',
 'c',
 'd',
 'print_a',
 'print_b']
```

```
In [8]: demo.
demo.__builtins__      demo.__init__      demo.__str__
demo.__class__         demo.__name__      demo.__subclasshook__
demo.__delattr__       demo.__new__       demo.c
demo.__dict__          demo.__package__  demo.d
demo.__doc__           demo.__reduce__   demo.print_a
demo.__file__          demo.__reduce_ex__ demo.print_b
demo.__format__        demo.__repr__    demo.py
demo.__getattribute__  demo.__setattr__ demo.pyc
demo.__hash__          demo.__sizeof__
```

Importing objects from modules into the main namespace

```
In [9]: from demo import print_a, print_b
```

```
In [10]: whos
Variable      Type      Data/Info
-----
demo        module    <module 'demo' from 'demo.py'>
print_a     function   <function print_a at 0xb7421534>
print_b     function   <function print_b at 0xb74214c4>
```

```
In [11]: print_a()
a
```

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)
```

5.6.4 '`__main__`' and module loading

File `demo2.py`:

```
import sys

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

print sys.argv

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

Importing it:

```
In [11]: import demo2
b

In [12]: import demo2
```

Running it:

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

5.6.5 Scripts or modules? How to organize your code

Note: Rule of thumb

- Sets of instructions that are called several times should be written inside **functions** for better code reusability.
- Functions (or other bits of code) that are called from several scripts should be written inside a **module**, so that only the module is imported in the different scripts (do not copy-and-paste your functions in the different scripts!).

Note: How to import a module from a remote directory?

Many solutions exist, depending mainly on your operating system. When the `import mymodule` statement is executed, the module `mymodule` is searched in a given list of directories. This list includes a list of installation-dependent default path (e.g., `/usr/lib/python`) as well as the list of directories specified by the environment variable `PYTHONPATH`.

The list of directories searched by Python is given by the `sys.path` variable

```
In [1]: import sys
In [2]: sys.path
Out[2]:
['',
 '/usr/bin',
 '/usr/local/include/enthought.traits-1.1.0',
 '/usr/lib/python2.6',
 '/usr/lib/python2.6/plat-linux2',
 '/usr/lib/python2.6/lib-tk',
 '/usr/lib/python2.6/lib-old',
 '/usr/lib/python2.6/lib-dynload',
 '/usr/lib/python2.6/dist-packages',
 '/usr/lib/pymodules/python2.6',
 '/usr/lib/pymodules/python2.6/gtk-2.0',
 '/usr/lib/python2.6/dist-packages/wx-2.8-gtk2-unicode',
 '/usr/local/lib/python2.6/dist-packages',
 '/usr/lib/pymodules/python2.6/IPython/Extensions',
 u'/home/gouillar/.ipython']
```

Modules must be located in the search path, therefore you can:

- write your own modules within directories already defined in the search path (e.g. `/usr/local/lib/python2.6/dist-packages`). You may use symbolic links (on Linux) to keep the code somewhere else.
- modify the environment variable **PYTHONPATH** to include the directories containing the user-defined modules. On Linux/Unix, add the following line to a file read by the shell at startup (e.g. `/etc/profile`, `.profile`)

```
export PYTHONPATH=$PYTHONPATH:/home/emma/user_defined_modules
```

On Windows, <http://support.microsoft.com/kb/310519> explains how to handle environment variables.

- or modify the `sys.path` variable itself within a Python script.

```
import sys
new_path = '/home/emma/user_defined_modules'
if new_path not in sys.path:
    sys.path.append(new_path)
```

This method is not very robust, however, because it makes the code less portable (user-dependent path) and because you have to add the directory to your `sys.path` each time you want to import from a module in this directory.

See <http://docs.python.org/tutorial/modules.html> for more information about modules.

5.6.6 Packages

A directory that contains many modules is called a **package**. A package is a module with submodules (which can have submodules themselves, etc.). A special file called `__init__.py` (which may be empty) tells Python that the directory is a Python package, from which modules can be imported.

```
sd-2116 /usr/lib/python2.6/dist-packages/scipy $ ls
[17:07]
cluster/      io/        README.txt@  stsci/
__config__.py@ LATEST.txt@  setup.py@   __svn_version__.py@
__config__.pyc lib/        setup.pyc   __svn_version__.pyc
constants/    linalg/    setupscs.py@ THANKS.txt@
fftpack/      linsolve/  setupscs.pyc TOCHANGE.txt@
__init__.py@  maxentropy/ signal/    version.py@
__init__.pyc  misc/      sparse/   version.pyc
INSTALL.txt@ ndimage/   spatial/  weave/
integrate/   odr/       special/
interpolate/ optimize/  stats/
sd-2116 /usr/lib/python2.6/dist-packages/scipy $ cd ndimage
[17:07]

sd-2116 /usr/lib/python2.6/dist-packages/scipy/ndimage $ ls
[17:07]
doccer.py@  fourier.pyc  interpolation.py@ morphology.pyc  setup.pyc
doccer.pyc  info.py@    interpolation.pyc _nd_image.so
setupscs.py@ info.pyc   measurements.py@ _ni_support.py@
filters.py@ info.pyc   measurements.pyc _ni_support.pyc tests/
setupscs.pyc
filters.pyc __init__.py@ measurements.pyc _ni_support.pyc
fourier.py@ __init__.pyc morphology.py@ setup.py@
```

From Ipython:

```
In [1]: import scipy
In [2]: scipy.__file__
Out[2]: '/usr/lib/python2.6/dist-packages/scipy/__init__.pyc'

In [3]: import scipy.version
In [4]: scipy.version.version
Out[4]: '0.7.0'

In [5]: import scipy.ndimage.morphology
In [6]: from scipy.ndimage import morphology
In [17]: morphology.binary_dilation?
Type:           function
Base Class: <type 'function'>
String Form:   <function binary_dilation at 0x9bedd84>
```

```

Namespace: Interactive
File:      /usr/lib/python2.6/dist-packages/scipy/ndimage/morphology.py
Definition: morphology.binary_dilation(input, structure=None,
iterations=1, mask=None, output=None, border_value=0, origin=0,
brute_force=False)
Docstring:
    Multi-dimensional binary dilation with the given structure.

    An output array can optionally be provided. The origin parameter
    controls the placement of the filter. If no structuring element is
    provided an element is generated with a squared connectivity equal
    to one. The dilation operation is repeated iterations times. If
    iterations is less than 1, the dilation is repeated until the
    result does not change anymore. If a mask is given, only those
    elements with a true value at the corresponding mask element are
    modified at each iteration.

```

5.6.7 Good practices

Note: Good practices

- Indentation: no choice!

Indenting is compulsory in Python. Every command block following a colon bears an additional indentation level with respect to the previous line with a colon. One must therefore indent after `def f():` or `while::`. At the end of such logical blocks, one decreases the indentation depth (and re-increases it if a new block is entered, etc.)

Strict respect of indentation is the price to pay for getting rid of { or ; characters that delineate logical blocks in other languages. Improper indentation leads to errors such as

```
IndentationError: unexpected indent (test.py, line 2)
```

All this indentation business can be a bit confusing in the beginning. However, with the clear indentation, and in the absence of extra characters, the resulting code is very nice to read compared to other languages.

- Indentation depth:

Inside your text editor, you may choose to indent with any positive number of spaces (1, 2, 3, 4, ...). However, it is considered good practice to **indent with 4 spaces**. You may configure your editor to map the Tab key to a 4-space indentation. In Python(x,y), the editor Scite is already configured this way.

- Style guidelines

Long lines: you should not write very long lines that span over more than (e.g.) 80 characters. Long lines can be broken with the \ character

```
>>> long_line = "Here is a very very long line \
... that we break in two parts."
```

Spaces

Write well-spaced code: put whitespaces after commas, around arithmetic operators, etc.:

```
>>> a = 1 # yes
>>> a=1 # too cramped
```

A certain number of rules for writing “beautiful” code (and more importantly using the same conventions as anybody else!) are given in the [Style Guide for Python Code](#).

- Use **meaningful object names**

5.7 Input and Output

To be exhaustive, here are some information about input and output in Python. Since we will use the Numpy methods to read and write files, you may skip this chapter at first reading.

We write or read **strings** to/from files (other types must be converted to strings). To write in a file:

```
>>> f = open('workfile', 'w') # opens the workfile file
>>> type(f)
<type 'file'>
>>> f.write('This is a test \nand another test')
>>> f.close()
```

To read from a file

```
In [1]: f = open('workfile', 'r')
In [2]: s = f.read()
In [3]: print(s)
This is a test
and another test
In [4]: f.close()
```

For more details: <http://docs.python.org/tutorial/inputoutput.html>

5.7.1 Iterating over a file

```
In [6]: f = open('workfile', 'r')
In [7]: for line in f:
...:     print line
...:
...:
This is a test
and another test
In [8]: f.close()
```

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.

5.8 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

5.8.1 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.swp',
 '.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.swp
/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',
 'FSLREMOTECELL',
 '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'
```

5.8.2 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.

5.8.3 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']
```

5.8.4 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',
 ...]
```

5.8.5 pickle: easy persistence

Useful to store arbitrary 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`.

`path_site`

5.9 Exceptions handling in Python

It is highly unlikely that you haven't yet raised Exceptions if you have typed all the previous commands of the tutorial. For example, you may have raised an exception if you entered a command with a typo.

Exceptions are raised by different kinds of errors arising when executing Python code. In your own code, you may also catch errors, or define custom error types.

5.9.1 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.

5.9.2 Catching exceptions

`try/except`

```
In [8]: while True:
....:     try:
....:         x = int(raw_input('Please enter a number: '))
....:     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

```
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
```

5.9.3 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\xabel'

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

- 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)

5.10 Object-oriented programming (OOP)

Python supports object-oriented programming (OOP). The goals of OOP are:

- to organize the code, and
- to re-use code in similar contexts.

Here is a small example: we create a `Student` class, which is an object gathering several custom functions (**methods**) and variables (**attributes**), we will be able to use:

```
>>> class Student(object):
...     def __init__(self, name):
...         self.name = name
...     def set_age(self, age):
...         self.age = age
...     def set_major(self, major):
...         self.major = major
...
...
>>> anna = Student('anna')
>>> anna.set_age(21)
>>> anna.set_major('physics')
```

In the previous example, the `Student` class has `__init__`, `set_age` and `set_major` methods. Its attributes are `name`, `age` and `major`. We can call these methods and attributes with the following notation: `classinstance.method` or `classinstance.attribute`. The `__init__` constructor is a special method we call with: `MyClass(init parameters if any)`.

Now, suppose we want to create a new class `MasterStudent` with the same methods and attributes as the previous one, but with an additional `internship` attribute. We won't copy the previous class, but **inherit** from it:

```
>>> class MasterStudent(Student):
...     internship = 'mandatory, from March to June'
...
...
>>> james = MasterStudent('james')
>>> james.internship
'mandatory, from March to June'
>>> james.set_age(23)
>>> james.age
23
```

The `MasterStudent` class inherited from the `Student` attributes and methods.

Thanks to classes and object-oriented programming, we can organize code with different classes corresponding to different objects we encounter (an `Experiment` class, an `Image` class, a `Flow` class, etc.), with their own methods and attributes. Then we can use inheritance to consider variations around a base class and **re-use** code. Ex : from a `Flow` base class, we can create derived `StokesFlow`, `TurbulentFlow`, `PotentialFlow`, etc.

NumPy: creating and manipulating numerical data

authors Emmanuelle Gouillart, Didrik Pinte, Gaël Varoquaux, and Pauli Virtanen

6.1 Intro

6.1.1 What is Numpy

Python has:

- built-in: lists, integers, floating point
- for numerics — more is needed (efficiency, convenience)

Numpy is:

- extension package to Python for multidimensional arrays
- closer to hardware (efficiency)
- designed for scientific computation (convenience)

For example:

An array containing —

- discretized time of an experiment/simulation
- signal recorded by a measurement device
- pixels of an image
- ...

6.2 1. Basics I

6.2.1 Getting started

```
>>> import numpy as np
>>> a = np.array([0, 1, 2, 3])
>>> a
array([0, 1, 2, 3])
```

6.2.2 Reference documentation

- On the web: <http://docs.scipy.org/>
- Interactive help:

```
>>> help(np.array)
array(object, dtype=None, copy=True, order=None, subok=False, ndmin=0)

Create an array.

Parameters
-----
object : array_like
...
Examples
-----
>>> np.array([1, 2, 3])
array([1, 2, 3])
...</pre>
```

- Looking for something:

```
>>> np.lookfor('create array')
Search results for 'create array'
-----
numpy.array
    Create an array.
numpy.memmap
    Create a memory-map to an array stored in a *binary* file on disk.
...
>>> help(np.lookfor)
...</pre>
```

6.2.3 Creating arrays

1-D

```
>>> a = np.array([0, 1, 2, 3])
>>> a
array([0, 1, 2, 3])
>>> a.ndim
1
>>> a.shape
(4,)
>>> len(a)
4</pre>
```

2-D, 3-D, ...

```
>>> b = np.array([[0, 1, 2], [3, 4, 5]])      # 2 x 3 array
>>> b
array([[ 0,  1,  2],
       [ 3,  4,  5]])
>>> b.ndim
2
>>> b.shape
(2, 3)
>>> len(b)      # returns the size of the first dimension
2</pre>
```

```
>>> c = np.array([[[1], [2]], [[3], [4]]])
>>> c
array([[[1],
         [2]],
        [[3],
         [4]]])
>>> c.shape
(2, 2, 1)</pre>
```

In practice, we rarely enter items one by one...

- Evenly spaced:

```
>>> import numpy as np
>>> a = np.arange(10) # 0 .. n-1 (!)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> b = np.arange(1, 9, 2) # start, end (exclusive), step
>>> b
array([1, 3, 5, 7])</pre>
```

or by number of points:

```
>>> c = np.linspace(0, 1, 6) # start, end, num-points
>>> c
array([ 0.,  0.2,  0.4,  0.6,  0.8,  1. ])
>>> d = np.linspace(0, 1, 5, endpoint=False)
>>> d
array([ 0.,  0.2,  0.4,  0.6,  0.8])</pre>
```

- Common arrays:

```
>>> a = np.ones((3, 3)) # reminder: (3, 3) is a tuple
>>> a
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
>>> b = np.zeros((2, 2))
>>> b
array([[ 0.,  0.],
       [ 0.,  0.]])
>>> c = np.eye(3)
>>> c
array([[ 1.,  0.,  0.],
       [ 0.,  1.,  0.],
       [ 0.,  0.,  1.]])
>>> d = np.diag(np.array([1, 2, 3, 4, 5]))
>>> d
array([[1, 0, 0, 0, 0],
       [0, 2, 0, 0, 0],
       [0, 0, 3, 0, 0],
       [0, 0, 0, 4, 0],
       [0, 0, 0, 0, 5]])</pre>
```

- Random numbers (Mersenne Twister PRNG):

```
>>> a = np.random.rand(4)          # uniform in [0, 1]
>>> a
array([ 0.58597729,  0.86110455,  0.9401114 ,  0.54264348])
>>> b = np.random.randn(4)         # gaussian
>>> b
array([-2.56844807,  0.06798064, -0.36823781,  0.86966886])</pre>
```

```
>>> c = np.random.rand(3, 3)
>>> c
array([[ 0.31976645,  0.64807526,  0.74770801],
       [ 0.8280203 ,  0.8669403 ,  0.07663683],
       [ 0.11527489,  0.11494884,  0.13503285]])

>>> d = np.random.zipf(1.5, size=(2, 8)) # Zipf distribution (s=1.5)
>>> d
array([[5290,    1,    6,    9,    1,    1,    1,    2],
       [ 1,    5,    1,   13,    1,    1,    2,    1]])

>>> np.random.seed(1234)           # Setting the random seed
>>> np.random.rand(3)
array([ 0.19151945,  0.62210877,  0.43772774])
>>> np.random.seed(1234)
>>> np.random.rand(5)
array([ 0.19151945,  0.62210877,  0.43772774,  0.78535858,  0.77997581])
```

6.2.4 Basic data types

You probably noted the 1 and 1. above. These are different data types:

```
>>> a = np.array([1, 2, 3])
>>> a.dtype
dtype('int64')
```

```
>>> b = np.array([1., 2., 3.])
>>> b.dtype
dtype('float64')
```

Much of the time you don't necessarily need to care, but remember they are there.

You can also choose which one you want:

```
>>> c = np.array([1, 2, 3], dtype=float)
>>> c.dtype
dtype('float64')
```

The **default** data type is floating point:

```
>>> a = np.ones((3, 3))
>>> a.dtype
dtype('float64')
>>> b = np.linspace(0, 1, 6)
>>> b.dtype
dtype('float64')
```

There are also other types:

```
>>> d = np.array([1+2j, 3+4j, 5+6j])
>>> d.dtype
dtype('complex128')
```

```
>>> e = np.array([True, False, False, True])
>>> e.dtype
dtype('bool')
```

```
>>> f = np.array(['Bonjour', 'Hello', 'Hallo', 'Terve', 'Hej'])
>>> f.dtype
dtype('S7')      # <-- strings containing max. 7 letters
```

6.2.5 Basic visualization

Now that we have our first data arrays, we are going to visualize them.

Matplotlib is a 2D plotting package. We can import its functions as below:

```
>>> import matplotlib.pyplot as plt # the tidy way
>>> # ... or ...
>>> from matplotlib.pyplot import * # imports everything in the namespace
```

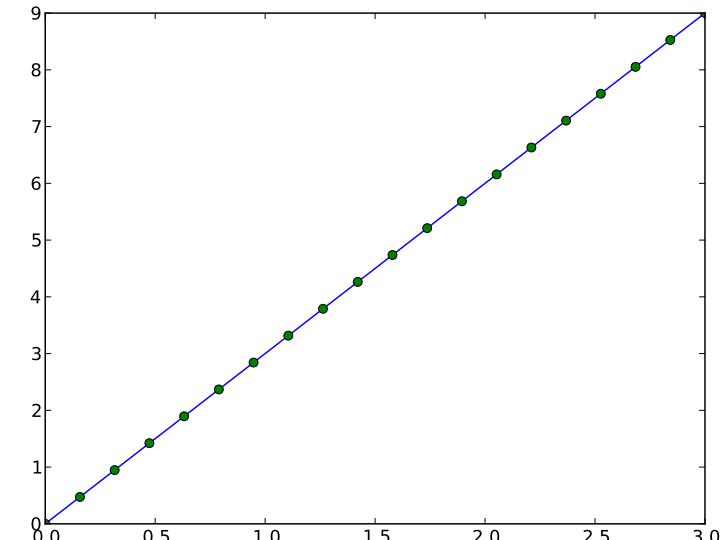
If you launched Ipython with python(x,y), or with ipython -pylab (under Linux), both of the above commands have been run. In the remainder of this tutorial, we assume you have run

```
>>> import matplotlib.pyplot as plt
```

or are using ipython -pylab which does it automatically.

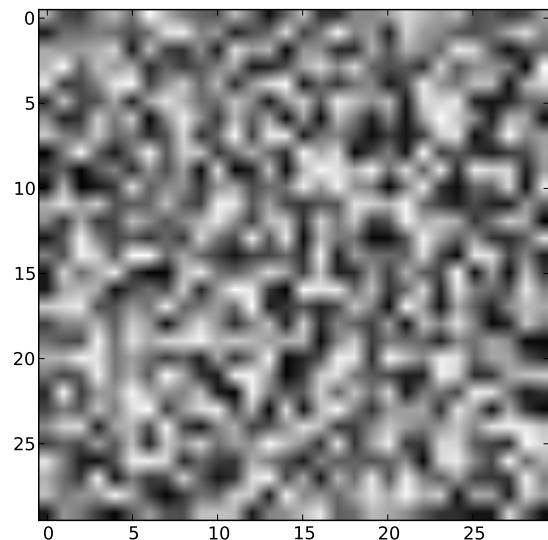
1D plotting

```
>>> x = np.linspace(0, 3, 20)
>>> y = np.linspace(0, 9, 20)
>>> plt.plot(x, y)      # line plot
>>> plt.plot(x, y, 'o') # dot plot
>>> plt.show()          # <-- shows the plot (not needed with Ipython)
```

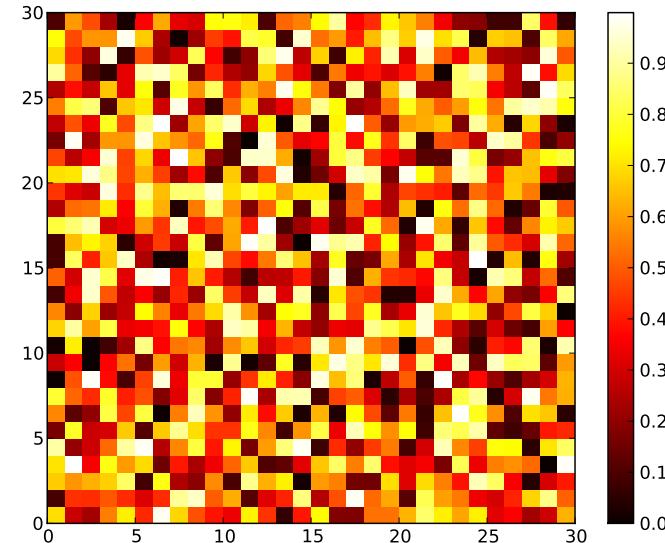


2D arrays (such as images)

```
>>> image = np.random.rand(30, 30)
>>> plt.imshow(image)
>>> plt.gray()
>>> plt.show()
```



```
>>> plt.pcolor(image)
>>> plt.hot()
>>> plt.colorbar()
>>> plt.show()
```



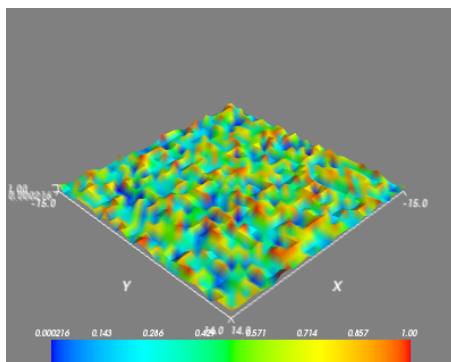
See Also:

More on matplotlib in the tutorial by Mike Müller tomorrow!

3D plotting

For 3D visualization, we can use another package: **Mayavi**. A quick example: start with **relaunching iPython** with these options: **ipython -pylab -wthread** (or **ipython -pylab=wx** in IPython >= 0.10).

```
In [59]: from enthought.mayavi import mlab
In [60]: mlab.figure()
get fences failed: -1
param: 6, val: 0
Out[60]: <enthought.mayavi.core.scene.Scene object at 0xcb2677c>
In [61]: mlab.surf(image)
Out[61]: <enthought.mayavi.modules.surface.Surface object at 0xd0862fc>
In [62]: mlab.axes()
Out[62]: <enthought.mayavi.modules.axes.Axes object at 0xd07892c>
```



The mayavi/mlab window that opens is interactive : by clicking on the left mouse button you can rotate the image, zoom with the mouse wheel, etc.

For more information on Mayavi : <http://code.enthought.com/projects/mayavi/docs/development/html/mayavi/index.html>

6.2.6 Indexing and slicing

The items of an array can be accessed and assigned to the same way as other Python sequences (list, tuple)

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

Warning: Indices begin at 0, like other Python sequences (and C/C++). In contrast, in Fortran or Matlab, indices begin at 1.

For multidimensional arrays, indexes are tuples of integers:

```
>>> a = np.diag(np.arange(5))
>>> a
array([[0, 0, 0, 0, 0],
       [0, 1, 0, 0, 0],
       [0, 0, 2, 0, 0],
       [0, 0, 0, 3, 0],
       [0, 0, 0, 0, 4]])
>>> a[1,1]
1
>>> a[2,1] = 10 # third line, second column
>>> a
array([[ 0,   0,   0,   0,   0],
       [ 0,   1,   0,   0,   0],
       [ 0,  10,   2,   0,   0],
       [ 0,   0,   0,   3,   0],
       [ 0,   0,   0,   0,   4]])
>>> a[1]
array([0, 1, 0, 0, 0])
```

Note that:

- In 2D, the first dimension corresponds to rows, the second to columns.
- for multidimensional a, 'a[0]' is interpreted by taking all elements in the unspecified dimensions.

Slicing

Arrays, like other Python sequences can also be sliced:

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

Note that the last index is not included!:

```
>>> a[:4]
array([0, 1, 2, 3])
```

start:end:step is a slice object which represents the set of indexes range(start, end, step). A slice can be explicitly created:

```
>>> sl = slice(1, 9, 2)
>>> a = np.arange(10)
>>> b = np.arange(1, 20, 2)
>>> a, b
(array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9]), array([ 1,  3,  5,  7,  9, 11, 13, 15, 17, 19]))
>>> a[sl], b[sl]
(array([1, 3, 5, 7]), array([ 3,  7, 11, 15]))
```

All three slice components are not required: by default, start is 0, end is the last and step is 1:

```
>>> a[1:3]
array([1, 2])
>>> a[::-2]
array([0, 2, 4, 6, 8])
>>> a[3:]
array([3, 4, 5, 6, 7, 8, 9])
```

Of course, it works with multidimensional arrays:

```
>>> a = np.eye(5)
>>> a
array([[ 1.,  0.,  0.,  0.,  0.],
       [ 0.,  1.,  0.,  0.,  0.],
       [ 0.,  0.,  1.,  0.,  0.],
       [ 0.,  0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  0.,  1.]])
>>> a[2:4,:3] # 3rd and 4th rows, 3 first columns
array([[ 0.,  0.,  1.],
       [ 0.,  0.,  0.]])
```

All elements specified by a slice can be easily modified:

```
>>> a[:,3,:] = 4
>>> a
array([[ 4.,  4.,  4.,  0.,  0.],
       [ 4.,  4.,  4.,  0.,  0.],
       [ 4.,  4.,  4.,  0.,  0.],
       [ 0.,  0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  0.,  1.]])
```

A small illustrated summary of Numpy indexing and slicing...

```
>>> a[0,3:5]
array([3,4])
```

```
>>> a[4:,4:]
array([[44, 45],
       [54, 55]])
```

```
>>> a[:,2]
array([2,22,52])
```

```
>>> a[2::2,:,:2]
array([[20,22,24],
       [40,42,44]])
```

0	1	2	3	4	5
10	11	12	13	14	15
20	21	22	23	24	25
30	31	32	33	34	35
40	41	42	43	44	45
50	51	52	53	54	55

6.2.7 Copies and views

A slicing operation creates a **view** on the original array, which is just a way of accessing array data. Thus the original array is not copied in memory.

When modifying the view, the original array is modified as well:

```
>>> a = np.arange(10)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> b = a[::2]; b
array([0, 2, 4, 6, 8])
>>> b[0] = 12
>>> b
array([12, 2, 4, 6, 8])
>>> a # (!)
array([12, 1, 2, 3, 4, 5, 6, 7, 8, 9])

>>> a = np.arange(10)
>>> b = a[::2].copy() # force a copy
>>> b[0] = 12
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

This behavior can be surprising at first sight... but it allows to save both memory and time.

6.2.8 Data files

Text files

Example: populations.txt:

```
1900      30e3    4e3     51300
1901      47.2e3   6.1e3   48200
1902      70.2e3   9.8e3   41500
...
```

```
>>> data = np.loadtxt('populations.txt') # if in current directory
>>> data
array([[ 1900., 30000., 4000., 51300.],
       [ 1901., 47200., 6100., 48200.],
       [ 1902., 70200., 9800., 41500.],
       ...])
```

```
>>> np.savetxt('pop2.txt', data)
>>> data2 = np.loadtxt('pop2.txt')
```

Note: If you have a complicated text file, what you can try are:

- np.genfromtxt
- Using Python's I/O functions and e.g. regexps for parsing (Python is quite well suited for this)

Navigating the filesystem in Python shells

Ipython

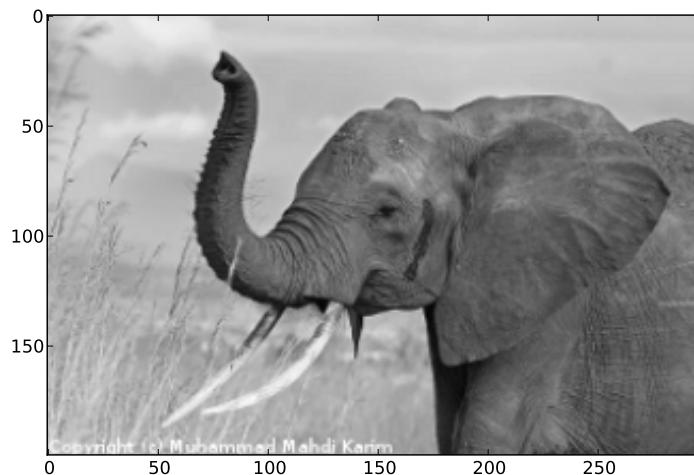
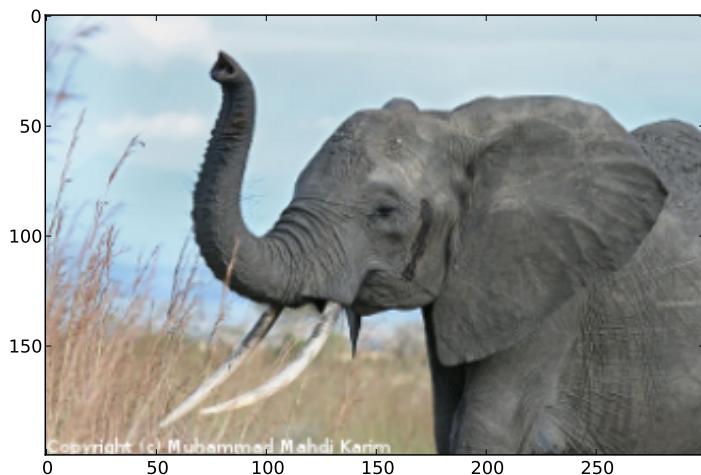
```
In [1]: pwd      # show current directory
'/home/user/stuff/2011-numpy-tutorial'
In [2]: cd ex
'/home/user/stuff/2011-numpy-tutorial/ex'
In [3]: ls
populations.txt  species.txt
```

Python (here's yet one reason to use Ipython for interactive use :)

```
>>> import os
>>> os.getcwd()
'/home/user/stuff/2011-numpy-tutorial'
>>> os.chdir('ex')
>>> os.getcwd()
'/home/user/stuff/2011-numpy-tutorial/ex'
>>> os.listdir('.')
['populations.txt',
 'species.txt',
 ...]
```

Images

```
>>> img = plt.imread('.../data/elephant.png')
>>> img.shape, img.dtype
((200, 300, 3), dtype('float32'))
>>> plt.imshow(img)
>>> plt.savefig('plot.png')
>>> plt.show()
```



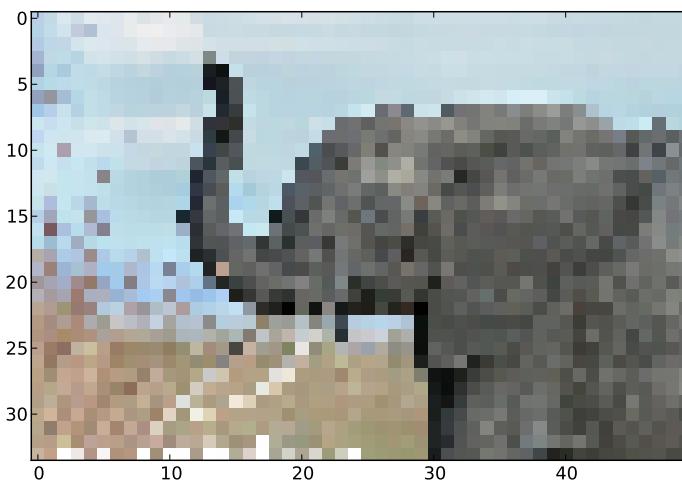
```
>>> plt.imsave('red_elephant', img[:, :, 0], cmap=plt.cm.gray)
```

This saved only one channel (of RGB)

```
>>> plt.imshow(plt.imread('red_elephant.png'))
>>> plt.show()
```

Other libraries:

```
>>> from scipy.misc import imsave
>>> imsave('tiny_elephant.png', img[:6, :6])
>>> plt.imshow(plt.imread('tiny_elephant.png'), interpolation='nearest')
>>> plt.show()
```



Numpy's own format

```
>>> np.save('pop.npy', data)
>>> data3 = np.load('pop.npy')
```

Well-known (& more obscure) file formats

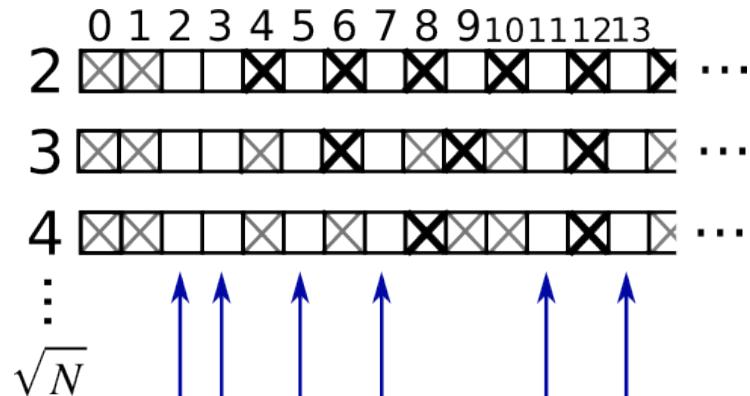
- HDF5: h5py, PyTables
- NetCDF: scipy.io.netcdf_file, netcdf4-python, ...
- Matlab: scipy.io.loadmat, scipy.io.savemat
- MatrixMarket: scipy.io.mmread, scipy.io.mmread

... if somebody uses it, there's probably also a Python library for it.

6.2.9 Summary & Exercises

- Creating arrays: array, linspace, arange, zeros, ones, rand
- Data types: integers, floats, complex floats, and strings
- Simple plotting with Matplotlib: plot(x, y)
- Indexing, slicing, and assignment into arrays — slicing creates views
- Reading data from files: loadtxt, savetxt, et al.

Worked example: Prime number sieve



Compute prime numbers in 0–99, with a sieve

- Construct a shape (100,) boolean array is_prime, filled with True in the beginning:

```
>>> is_prime = np.ones((100,), dtype=bool)
```

- Cross out 0 and 1 which are not primes

```
>>> is_prime[:2] = 0
```

- For each integer j starting from 2, cross out its higher multiples

```
>>> N_max = int(np.sqrt(len(is_prime)))
>>> for j in range(2, N_max):
...     is_prime[2*j::j] = False
```

- Skim through help(np.nonzero), and print the prime numbers

- Follow-up:

- Move the above code into a script file named prime_sieve.py
- Run it to check it works
- Convert the simple sieve to the sieve of Eratosthenes:
 1. Skip j which are already known to not be primes
 2. The first number to cross out is j^2

Reminder – Python scripts:

A very basic script file contains:

```
import numpy as np
import matplotlib.pyplot as plt # <- if you use it

# any numpy-using commands follow

a = np.array([1, 2, 3, 4])
print a
```

Run on command line:

```
python my_script_1_2.py
```

Or, in Python shell:

```
In [10]: %run my_script_1_2.py
>>> execfile('2_2_data_statistics.py')
```

Exercise 1.1: Certain arrays

Create the following arrays (with correct data types):

```
[[ 1  1  1  1]
 [ 1  1  1  1]
 [ 1  1  1  2]
 [ 1  6  1  1]]

[[0. 0. 0. 0. 0.]
 [2. 0. 0. 0. 0.]
 [0. 3. 0. 0. 0.]
 [0. 0. 4. 0. 0.]
 [0. 0. 0. 5. 0.]
 [0. 0. 0. 0. 6.]]
```

Par on course: 3 statements for each (53 & 54 characters)

Exercise 1.2: Text data files

Write a Python script that loads data from `populations.txt` and drop the last column and the first 5 rows. Save the smaller dataset to `pop2.txt`.

Exercise 1.3: Tiling

Skim through the documentation for `np.tile`, and use this function to construct the array:

```
[[4 3 4 3 4 3]
 [2 1 2 1 2 1]
 [4 3 4 3 4 3]
 [2 1 2 1 2 1]]
```

6.3 2. Basics II**6.3.1 Elementwise operations**

With scalars:

```
>>> a = np.array([1, 2, 3, 4])
>>> a + 1
array([2, 3, 4, 5])
>>> 2**a
array([ 2,  4,  8, 16])
```

All arithmetic operates elementwise:

```
>>> b = np.ones(4) + 1
>>> a - b
array([-1.,  0.,  1.,  2.])
>>> a * b
array([ 2.,  4.,  6.,  8.])
```

```
>>> j = np.arange(5)
>>> 2**j - j
array([ 2,  3,  6, 13, 28])
```

Warning: ... including multiplication

```
>>> c = np.ones((3, 3)) # NOT matrix multiplication!
>>> c * c
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
```

Note: Matrix multiplication:

```
>>> c.dot(c)
array([[ 3.,  3.,  3.],
       [ 3.,  3.,  3.],
       [ 3.,  3.,  3.]])
```

Comparisons:

```
>>> a = np.array([1, 2, 3, 4])
>>> b = np.array([4, 2, 2, 4])
>>> a == b
array([False,  True, False,  True], dtype=bool)
>>> a > b
array([False, False,  True, False], dtype=bool)
```

Logical operations:

```
>>> a = np.array([1, 1, 0, 0], dtype=bool)
>>> b = np.array([1, 0, 1, 0], dtype=bool)
>>> a | b
array([ True,  True,  True, False], dtype=bool)
>>> a & b
array([ True, False, False, False], dtype=bool)
```

Note: For arrays: “`&`” and “`|`” for logical operations, not “`and`” and “`or`“.

Shape mismatches:

```
>>> a
array([1, 2, 3, 4])
>>> a + np.array([1, 2])
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: shape mismatch: objects cannot be broadcast to a single shape
```

'Broadcast'? We'll return to that later.

6.3.2 Basic linear algebra

Matrix multiplication:

```
>>> a = np.triu(np.ones((3, 3)), 1) # see help(np.triu)
>>> a
array([[ 0.,  1.,  1.],
       [ 0.,  0.,  1.],
       [ 0.,  0.,  0.]])
>>> b = np.diag([1, 2, 3])
>>> a.dot(b)
array([[ 0.,  2.,  3.],
       [ 0.,  0.,  3.],
       [ 0.,  0.,  0.]])
>>> np.dot(a, a)
array([[ 0.,  0.,  1.],
       [ 0.,  0.,  0.],
       [ 0.,  0.,  0.]])
```

Transpose:

```
>>> a.T
array([[ 0.,  0.,  0.],
       [ 1.,  0.,  0.],
       [ 1.,  1.,  0.]])
```

Inverses and linear equation systems:

```
>>> A = a + b
>>> A
array([[ 1.,  1.,  1.],
       [ 0.,  2.,  1.],
       [ 0.,  0.,  3.]])
>>> B = np.linalg.inv(A)
>>> B.dot(A)
array([[ 1.,  0.,  0.],
       [ 0.,  1.,  0.],
       [ 0.,  0.,  1.]])
```



```
>>> x = np.linalg.solve(A, [1, 2, 3])
>>> x
array([-0.5,  0.5,  1. ])
```

Eigenvalues:

```
>>> np.linalg.eigvals(A)
array([ 1.,  2.,  3.])
```

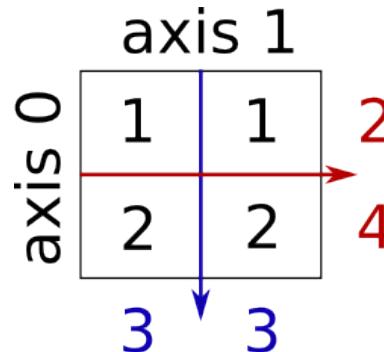
... and so on, see `help(np.linalg)`

6.3.3 Basic reductions

Computing sums:

```
>>> x = np.array([1, 2, 3, 4])
>>> np.sum(x)
10
>>> x.sum()
10
```

Sum by rows and by columns:



```
>>> x = np.array([[1, 1], [2, 2]])
>>> x
array([[1, 1],
       [2, 2]])
>>> x.sum(axis=0) # columns (first dimension)
array([3, 3])
>>> x[:,0].sum(), x[:,1].sum()
(3, 3)
>>> x.sum(axis=1) # rows (second dimension)
array([2, 4])
>>> x[0,:].sum(), x[1,:].sum()
(2, 4)
```

Same idea in higher dimensions:

```
>>> x = np.random.rand(2, 2, 2)
>>> x.sum(axis=2)[0,1]
1.1600112273698793
>>> x[0,1,:,:].sum()
1.1600112273698793
```

Other reductions — works the same way (and take `axis=`)

- Statistics:

```
>>> x = np.array([1, 2, 3, 1])
>>> y = np.array([[1, 2, 3], [5, 6, 1]])
>>> x.mean()
1.75
>>> np.median(x)
1.5
>>> np.median(y, axis=-1) # last axis
array([ 2.,  5.])
```

```
>>> x.std()          # full population standard dev.  
0.82915619758884995  
>>> x.std(ddof=1)   # sample std (with N-1 in divisor)  
0.9574271077563381
```

- Extrema:

```
>>> x = np.array([1, 3, 2])  
>>> x.min()  
1  
>>> x.max()  
3
```

```
>>> x.argmin()      # index of minimum  
0  
>>> x.argmax()    # index of maximum  
1
```

- Logical operations:

```
>>> np.all([True, True, False])  
False  
>>> np.any([True, True, False])  
True
```

Note: Can be used for array comparisons:

```
>>> a = np.zeros((100, 100))  
>>> np.any(a != 0)  
False  
>>> np.all(a == a)  
True
```

```
>>> a = np.array([1, 2, 3, 2])  
>>> b = np.array([2, 2, 3, 2])  
>>> c = np.array([6, 4, 4, 5])  
>>> ((a <= b) & (b <= c)).all()  
True
```

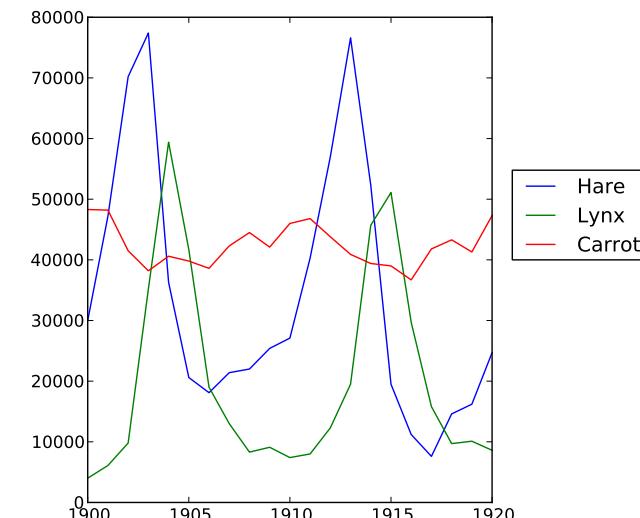
- ... and many more (best to learn as you go).

Example: data statistics

Data in `populations.txt` describes the populations of hares and lynxes (and carrots) in northern Canada during 20 years.

We can first plot the data:

```
>>> data = np.loadtxt('..../data/populations.txt')  
>>> year, hares, lynxes, carrots = data.T # trick: columns to variables  
  
>>> plt.axes([0.2, 0.1, 0.5, 0.8])  
>>> plt.plot(year, hares, year, lynxes, year, carrots)  
>>> plt.legend(['Hare', 'Lynx', 'Carrot'], loc=(1.05, 0.5))  
>>> plt.show()
```



The mean populations over time:

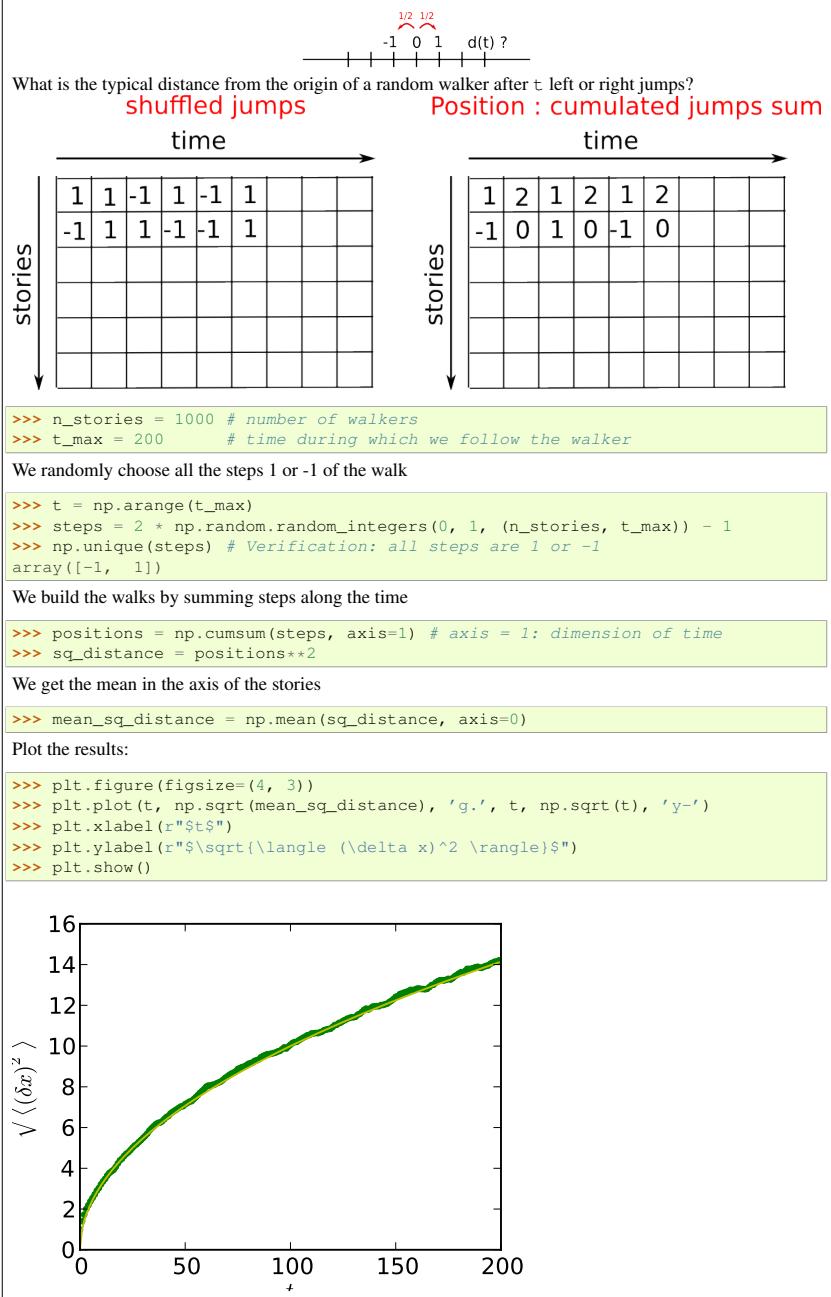
```
>>> populations = data[:,1:]  
>>> populations.mean(axis=0)  
array([ 34080.95238095,  20166.66666667,  42400.         ])
```

The sample standard deviations:

```
>>> populations.std(axis=0, ddof=1)  
array([ 21413.98185877,  16655.99991995,  3404.55577132])
```

Which species has the highest population each year?

```
>>> np.argmax(populations, axis=1)  
array([2, 2, 0, 0, 1, 1, 2, 2, 2, 2, 0, 0, 0, 1, 2, 2, 2, 2, 2])
```

Example: diffusion simulation using a random walk algorithm

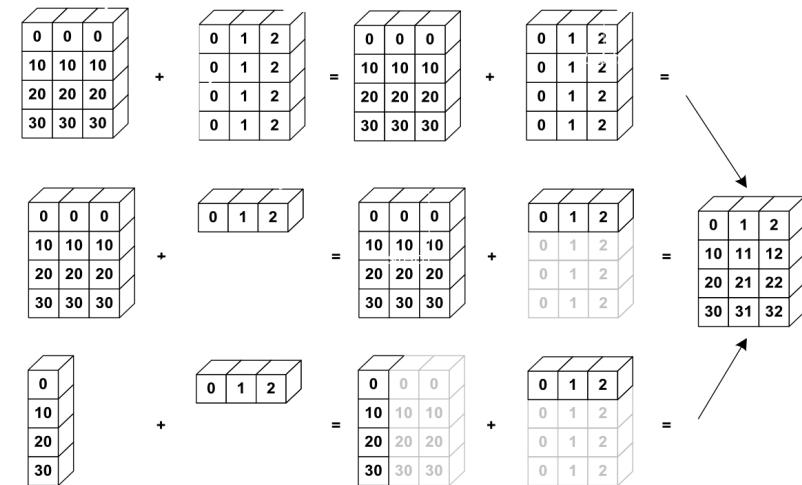
The RMS distance grows as the square root of the time!

6.3.4 Broadcasting

- Basic operations on numpy arrays (addition, etc.) are elementwise
- This works on arrays of the same size.

Nevertheless, It's also possible to do operations on arrays of different sizes if Numpy can transform these arrays so that they all have the same size: this conversion is called **broadcasting**.

The image below gives an example of broadcasting:



Let's verify:

```

>>> a = np.tile(np.arange(0, 40, 10), (3, 1)).T
>>> a
array([[ 0,  0,  0],
       [10, 10, 10],
       [20, 20, 20],
       [30, 30, 30]])
>>> b = np.array([0, 1, 2])
>>> a + b
array([[ 0,  1,  2],
       [10, 11, 12],
       [20, 21, 22],
       [30, 31, 32]])

```

An useful trick:

```

>>> a = np.arange(0, 40, 10)
>>> a.shape

```

```
(4, )
>>> a = a[:, np.newaxis]           # adds a new axis -> 2D array
>>> a.shape
(4, 1)
>>> a
array([[ 0,
       10,
      20,
      30]])
>>> a + b
array([[ 0,  1,  2],
       [10, 11, 12],
      [20, 21, 22],
      [30, 31, 32]])
```

We have already used broadcasting without knowing it!:

```
>>> a = np.ones((4, 5))
>>> a[0] = 2 # we assign an array of dimension 0 to an array of dimension 1
array([[ 2.,  2.,  2.,  2.,  2.],
       [ 1.,  1.,  1.,  1.,  1.],
      [ 1.,  1.,  1.,  1.,  1.],
      [ 1.,  1.,  1.,  1.,  1.]])
```

Broadcasting seems a bit magical, but it is actually quite natural to use it when we want to solve a problem whose output data is an array with more dimensions than input data.

Example

Let's construct an array of distances (in miles) between cities of Route 66: Chicago, Springfield, Saint-Louis, Tulsa, Oklahoma City, Amarillo, Santa Fe, Albuquerque, Flagstaff and Los Angeles.

```
>>> mileposts = np.array([0, 198, 303, 736, 871, 1175, 1475, 1544,
...                      1913, 2448])
>>> distance_array = np.abs(mileposts - mileposts[:, np.newaxis])
>>> distance_array
array([[ 0,  198,  303,  736,  871,  1175,  1475,  1544,  1913,  2448],
       [198,  0,  105,  538,  673,  977,  1277,  1346,  1715,  2250],
      [303,  105,  0,  433,  568,  872,  1172,  1241,  1610,  2145],
      [736,  538,  433,  0,  135,  439,  739,  808,  1177,  1712],
      [871,  673,  568,  135,  0,  304,  604,  673,  1042,  1577],
     [1175,  977,  872,  439,  304,  0,  300,  369,  738,  1273],
     [1475,  1277,  1172,  739,  604,  300,  0,  69,  438,  973],
     [1544,  1346,  1241,  808,  673,  369,  69,  0,  369,  904],
     [1913,  1715,  1610,  1177,  1042,  738,  438,  369,  0,  535],
    [2448,  2250,  2145,  1712,  1577,  1273,  973,  904,  535,  0]])
```



Good practices

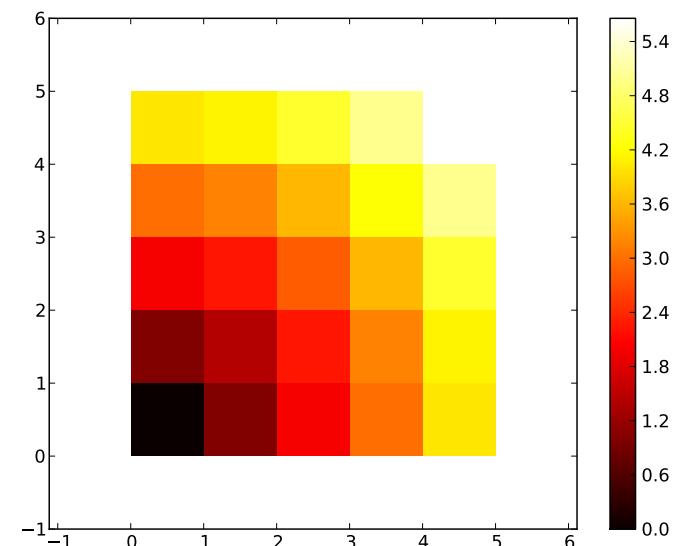
- Explicit variable names (no need of a comment to explain what is in the variable)
- Style: spaces after commas, around =, etc.
- A certain number of rules for writing “beautiful” code (and, more importantly, using the same conventions as everybody else!) are given in the [Style Guide for Python Code](#) and the [Docstring Conventions](#) page (to manage help strings).
- Except some rare cases, variable names and comments in English.

A lot of grid-based or network-based problems can also use broadcasting. For instance, if we want to compute the distance from the origin points on a 10x10 grid, we can do:

```
>>> x, y = np.arange(5), np.arange(5)
>>> distance = np.sqrt(x**2 + y[:, np.newaxis]**2)
>>> distance
array([[ 0.          ,  1.        ,  2.        ,  3.        ,  4.        ],
       [ 1.          ,  1.41421356,  2.23606798,  3.16227766,  4.12310563],
       [ 2.          ,  2.23606798,  2.82842712,  3.60555128,  4.47213595],
       [ 3.          ,  3.16227766,  3.60555128,  4.24264069,  5.          ],
       [ 4.          ,  4.12310563,  4.47213595,  5.          ,  5.65685425]])
```

Or in color:

```
>>> plt.pcolor(distance)
>>> plt.colorbar()
>>> plt.axis('equal')
>>> plt.show()           # <-- again, not needed in interactive Python
```



Remark : the `numpy.ogrid` function allows to directly create vectors `x` and `y` of the previous example, with two “significant dimensions”:

```
>>> x, y = np.ogrid[0:5, 0:5]
>>> x, y
(array([[0],
       [1],
       [2],
       [3],
       [4]]), array([[0, 1, 2, 3, 4]]))
>>> x.shape, y.shape
((5, 1), (1, 5))
>>> distance = np.sqrt(x**2 + y**2)
```

So, `np.ogrid` is very useful as soon as we have to handle computations on a grid. On the other hand, `np.mgrid` directly provides matrices full of indices for cases where we can't (or don't want to) benefit from broadcasting:

```
>>> x, y = np.mgrid[0:4, 0:4]
>>> x
array([[0, 0, 0, 0],
       [1, 1, 1, 1],
       [2, 2, 2, 2],
       [3, 3, 3, 3]])
>>> y
array([[0, 1, 2, 3],
       [0, 1, 2, 3],
       [0, 1, 2, 3],
       [0, 1, 2, 3]])
```

However, in practice, this is rarely needed!

6.3.5 Array shape manipulation

Flattening

```
>>> a = np.array([[1, 2, 3], [4, 5, 6]])
>>> a.ravel()
array([1, 2, 3, 4, 5, 6])
>>> a.T
array([[1, 4],
       [2, 5],
       [3, 6]])
>>> a.T.ravel()
array([1, 4, 2, 5, 3, 6])
```

Higher dimensions: last dimensions ravel out “first”.

Reshaping

The inverse operation to flattening:

```
>>> a.shape
(2, 3)
>>> b = a.ravel()
>>> b.reshape((2, 3))
array([[1, 2, 3],
       [4, 5, 6]])
```

Creating an array with a different shape, from another array:

```
>>> a = np.arange(36)
>>> b = a.reshape((6, 6))
>>> b
```

```
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],
       [30, 31, 32, 33, 34, 35]])
```

Or,

```
>>> b = a.reshape((6, -1))      # unspecified (-1) value is inferred
```

Copies or views

`ndarray.reshape` may return a view (cf `help(np.reshape)`), not a copy:

```
>>> b[0,0] = 99
>>> a
array([99,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16,
       17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33,
       34, 35])
```

Beware!

```
>>> a = np.zeros((3,2))
>>> b = a.T.reshape(3*2)
>>> b[0] = 9
>>> a
array([[ 0.,  0.],
       [ 0.,  0.],
       [ 0.,  0.]])
```

To understand, see “Under the hood” below.

Dimension shuffling

```
>>> a = np.arange(4*3*2).reshape(4, 3, 2)
>>> a.shape
(4, 3, 2)
>>> a[0,2,1]
5
>>> b = a.transpose(1, 2, 0)
>>> b.shape
(3, 2, 4)
>>> b[2,1,0]
5
```

Also creates a view:

```
>>> b[2,1,0] = -1
>>> a[0,2,1]
-1
```

Resizing

Size of an array can be changed with `ndarray.resize`:

```
>>> a = np.arange(4)
>>> a.resize((8,))
```

```
>>> a
array([0, 1, 2, 3, 0, 0, 0, 0])
```

However, it must not be referred to somewhere else:

```
>>> b = a
>>> a.resize((4,))
...
ValueError: cannot resize an array references or is referenced
by another array in this way. Use the resize function
```

Some examples of real-world use cases

Case 2.a: Calling (legacy) Fortran code

Shape-preserving functions with elementwise non-Python routines. For instance, Fortran

```
! 2_a_fortran_module.f90
subroutine some_function(n, a, b)
    integer :: n
    double precision, dimension(n), intent(in) :: a
    double precision, dimension(n), intent(out) :: b
    b = a + 1
end subroutine some_function

f2py -c -m fortran_module 2_a_fortran_module.f90

import numpy as np
import fortran_module

def some_function(input):
    """
    Call a Fortran routine, and preserve input shape
    """
    input = np.asarray(input)
    # fortran_module.some_function() takes 1-D arrays!
    output = fortran_module.some_function(input.ravel())
    return output.reshape(input.shape)

print some_function(np.array([1, 2, 3]))
print some_function(np.array([[1, 2], [3, 4]]))

# -
# [ 2.  3.  4.]
# [[ 2.  3.]
# [ 4.  5.]])
```

Case 2.b: Block matrices and vectors (and tensors)

Vector space: quantum level \otimes spin

$$\check{\psi} = \begin{pmatrix} \hat{\psi}_1 \\ \hat{\psi}_2 \end{pmatrix}, \quad \hat{\psi}_1 = \begin{pmatrix} \psi_{1\uparrow} \\ \psi_{1\downarrow} \end{pmatrix} \quad \hat{\psi}_2 = \begin{pmatrix} \psi_{2\uparrow} \\ \psi_{2\downarrow} \end{pmatrix}$$

In short: for **block matrices and vectors**, it can be useful to preserve the **block structure**.

In Numpy:

```
>>> psi = np.zeros((2, 2)) # dimensions: level, spin
>>> psi[0,1] # --> psi_{1,downarrow}
```

Linear operators on such block vectors have similar block structure:

$$\check{H} = \begin{pmatrix} \hat{h}_{11} & \hat{V} \\ \hat{V}^\dagger & \hat{h}_{22} \end{pmatrix}, \quad \hat{h}_{11} = \begin{pmatrix} \epsilon_{1,\uparrow} & 0 \\ 0 & \epsilon_{1,\downarrow} \end{pmatrix}, \quad \dots$$

```
>>> H = np.zeros((2, 2, 2, 2)) # dimensions: level1, level2, spin1, spin2
>>> h_11 = H[0, 0, :, :]
>>> V = H[0, 1]
```

Doing the matrix product: get rid of the block structure, do the 4×4 matrix product, then put it back

$$\check{H}\check{\psi}$$

```
>>> def mdot(operator, psi):
...     return operator.transpose(0, 2, 1, 3).reshape(4, 4).dot(
...         psi.reshape(4)).reshape(2, 2)
```

I.e., reorder dimensions first to level1, spin1, level2, spin2 and then reshape => correct matrix product.

6.3.6 Fancy indexing

Numpy arrays can be indexed with slices, but also with boolean or integer arrays (**masks**). This method is called *fancy indexing*.

Masks

```
>>> np.random.seed(3)
>>> a = np.random.randint(0, 20, 15)
>>> a
array([10,  3,  8,  0, 19, 10, 11,  9, 10,  6,  0, 20, 12,  7, 14])
>>> (a % 3 == 0)
array([False,  True, False,  True, False, False,  True, False,
       True,  True, False,  True, False, False], dtype=bool)
>>> mask = (a % 3 == 0)
>>> extract_from_a = a[mask] # or, a[a%3==0]
>>> extract_from_a          # extract a sub-array with the mask
array([ 3,  0,  9,  6,  0, 12])
```

Extracting a sub-array using a mask produces a copy of this sub-array, not a view like slicing:

```
>>> extract_from_a[0] = -1
>>> a
array([10,  3,  8,  0, 19, 10, 11,  9, 10,  6,  0, 20, 12,  7, 14])
```

Indexing with a mask can be very useful to assign a new value to a sub-array:

```
>>> a[a % 3 == 0] = -1
>>> a
array([10, -1,  8, -1, 19, 10, 11, -1, 10, -1, -1, 20, -1,  7, 14])
```

Indexing with an array of integers

```
>>> a = np.arange(10)
>>> a[::2] += 3 # to avoid having always the same np.arange(10)...
>>> a
array([ 3,  1,  5,  3,  7,  5,  9,  7, 11,  9])
>>> a[[2, 5, 1, 8]] # or, a[np.array([2, 5, 1, 8])]
array([ 5,  5,  1, 11])
```

Indexing can be done with an array of integers, where the same index is repeated several time:

```
>>> a[[2, 3, 2, 4, 2]] # note: [2, 3, 2, 4, 2] is a Python list
array([5, 3, 5, 7, 5])
```

New values can be assigned with this kind of indexing:

```
>>> a[[9, 7]] = -10
>>> a
array([ 3,  1,  5,  3,  7,  5,  9, -10, 11, -10])
>>> a[[2, 3, 2, 4, 2]] += 1
>>> a
array([ 3,  1,  6,  4,  8,  5,  9, -10, 11, -10])
```

When a new array is created by indexing with an array of integers, the new array has the same shape than the array of integers:

```
>>> a = np.arange(10)
>>> idx = np.array([[3, 4], [9, 7]])
>>> a[idx]
array([[3, 4],
       [9, 7]])
>>> b = np.arange(10)

>>> a = np.arange(12).reshape(3, 4)
>>> a
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
>>> i = np.array([0, 1, 1, 2])
>>> j = np.array([2, 1, 3, 3])
>>> a[i, j]
array([ 2,  5,  7, 11])

>>> i = np.array([[0, 1], [1, 2]])
>>> j = np.array([[2, 1], [3, 3]])
>>> i
array([[0, 1],
       [1, 2]])
>>> j
array([[2, 1],
       [3, 3]])
>>> a[i, j]
array([[ 2,  5],
       [ 7, 11]])
```

```
>>> a[(0,1,2,3,4),(1,2,3,4,5)]
array([ 1, 12, 23, 34, 45])
```

```
>>> a[3:,[0, 2, 5]]
array([[30, 32, 35],
       [40, 42, 45],
       [50, 52, 55]])
```

```
>>> mask = array([1,0,1,0,0,1], dtype=bool)
>>> a[mask,2]
array([2,22,52])
```

We can even use fancy indexing and broadcasting at the same time:

```
>>> a = np.arange(12).reshape(3,4)
>>> a
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
>>> i = np.array([[0, 1], [1, 2]])
>>> a[i, 2] # same as a[i, 2]*np.ones((2,2), dtype=int)
array([[ 2,  6],
       [ 6, 10]])
```

6.3.7 Sorting data

Sorting along an axis:

```
>>> a = np.array([[4, 3, 5], [1, 2, 1]])
>>> b = np.sort(a, axis=1)
>>> b
array([[3, 4, 5],
       [1, 1, 2]])
```

Note: Sorts each row separately!

In-place sort:

```
>>> a.sort(axis=1)
>>> a
array([[3, 4, 5],
       [1, 1, 2]])
```

Sorting with fancy indexing:

```
>>> a = np.array([4, 3, 1, 2])
>>> j = np.argsort(a)
array([2, 3, 1, 0])
>>> a[j]
array([1, 2, 3, 4])
```

Finding minima and maxima:

```
>>> a = np.array([4, 3, 1, 2])
>>> j_max = np.argmax(a)
>>> j_min = np.argmin(a)
>>> j_max, j_min
(0, 2)
```

6.3.8 Summary & Exercises

- Arithmetic etc. are elementwise operations
- Basic linear algebra, `.dot()`
- Reductions: `sum(axis=1)`, `std()`, `all()`, `any()`
- Broadcasting: `a = np.arange(4); a[:,np.newaxis] + a[np.newaxis,:]`
- Shape manipulation: `a.ravel()`, `a.reshape(2, 2)`
- Fancy indexing: `a[a > 3], a[[2, 3]]`
- Sorting data: `.sort()`, `np.sort`, `np.argsort`, `np.argmax`

Worked example: Framing Lena

Let's do some manipulations on numpy arrays by starting with the famous image of Lena (<http://www.cs.cmu.edu/~chuck/lennapg/>). `scipy` provides a 2D array of this image with the `scipy.lena` function:

```
>>> import scipy
>>> lena = scipy.lena()
```

Here are a few images we will be able to obtain with our manipulations: use different colormaps, crop the image, change some parts of the image.



- Let's use the `imshow` function of `pylab` to display the image.

```
In [3]: import pylab as plt
In [4]: lena = scipy.lena()
In [5]: plt.imshow(lena)
```

- Lena is then displayed in false colors. A colormap must be specified for her to be displayed in grey.

```
In [6]: plt.imshow(lena, plt.cm.gray)
In [7]: # or,
In [7]: plt.gray()
```

- Create an array of the image with a narrower centering : for example, remove 30 pixels from all the borders of the image. To check the result, display this new array with `imshow`.

```
In [9]: crop_lena = lena[30:-30, 30:-30]
```

- We will now frame Lena's face with a black locket. For this, we need to

- create a mask corresponding to the pixels we want to be black. The mask is defined by this condition $(y-256)^2 + (x-256)^2 > 230^2$

```
In [15]: y, x = np.ogrid[0:512,0:512] # x and y indices of pixels
In [16]: y.shape, x.shape
Out[16]: ((512, 1), (1, 512))
In [17]: centerx, centery = (256, 256) # center of the image
In [18]: mask = ((y - centery)**2 + (x - centerx)**2) > 230**2 # circle
```

then

- assign the value 0 to the pixels of the image corresponding to the mask. The syntax is extremely simple and intuitive:

```
In [19]: lena[mask] = 0
In [20]: plt.imshow(lena)
Out[20]: <matplotlib.image.AxesImage object at 0xa36534c>
```

- Follow-up: copy all instructions of this exercise in a script called `lena_locket.py` then execute this script in IPython with `%run lena_locket.py`.

Change the circle to an ellipsoid.

Exercise 2.1: Matrix manipulations

1. Form the 2-D array (without typing it in explicitly):

```
1  6 11
2  7 12
3  8 13
4  9 14
5 10 15
```

and generate a new array containing its 2nd and 4th rows.

2. Divide each column of the array

```
>>> a = np.arange(25).reshape(5, 5)
```

elementwise with the array `b = np.array([1., 5, 10, 15, 20])`. (Hint: `np.newaxis`).

3. Harder one: Generate a 10 x 3 array of random numbers (in range [0,1]). For each row, pick the number closest to 0.5.

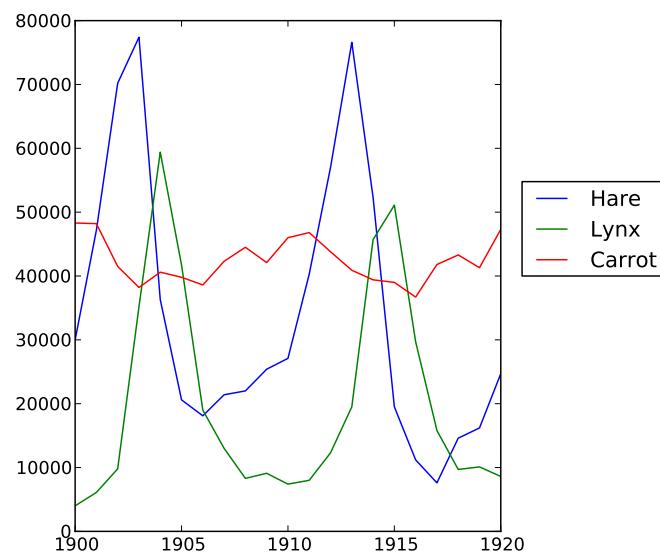
- Use `abs` and `argsort` to find the column `j` closest for each row.
- Use fancy indexing to extract the numbers. (Hint: `a[i, j]` – the array `i` must contain the row numbers corresponding to stuff in `j`.)

Exercise 2.2: Data statistics

The data in `populations.txt` describes the populations of hares and lynxes (and carrots) in northern Canada during 20 years:

```
>>> data = np.loadtxt('..../data/populations.txt')
>>> year, hares, lynxes, carrots = data.T # trick: columns to variables
```

```
>>> plt.axes([0.2, 0.1, 0.5, 0.8])
>>> plt.plot(year, hares, year, lynxes, year, carrots)
>>> plt.legend(['Hare', 'Lynx', 'Carrot'], loc=(1.05, 0.5))
>>> plt.show()
```



Computes and prints, based on the data in `populations.txt`...

1. The mean and std of the populations of each species for the years in the period.
2. Which year each species had the largest population.
3. Which species has the largest population for each year. (Hint: `argsort` & fancy indexing of `np.array(['H', 'L', 'C'])`)
4. Which years any of the populations is above 50000. (Hint: comparisons and `np.any`)
5. The top 2 years for each species when they had the lowest populations. (Hint: `argsort`, fancy indexing)
6. Compare (plot) the change in hare population (see `help(np.gradient)`) and the number of lynxes. Check correlation (see `help(np.corrcoef)`).

... all without for-loops.

Exercise 2.3: Crude integral approximations

Write a function `f(a, b, c)` that returns $a^b - c$. Form a $24 \times 12 \times 6$ array containing its values in parameter ranges $[0, 1] \times [0, 1] \times [0, 1]$.

Approximate the 3-d integral

$$\int_0^1 \int_0^1 \int_0^1 (a^b - c) da db dc$$

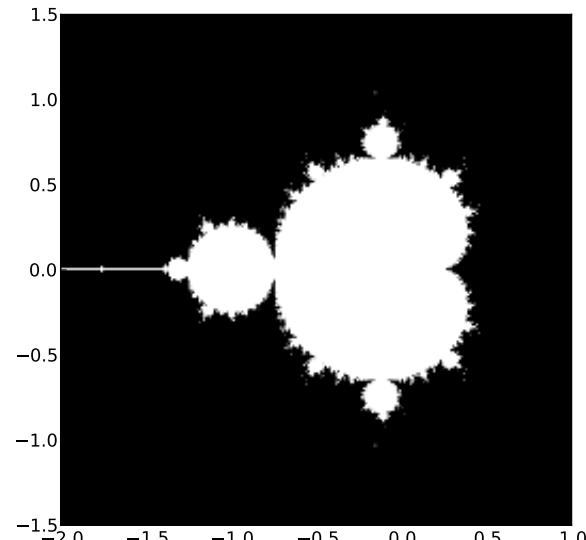
over this volume with the mean. The exact result is: $\ln 2 - \frac{1}{2} \approx 0.1931 \dots$ — what is your relative error?

(Hints: use elementwise operations and broadcasting. You can make `np.ogrid` give a number of points in given range with `np.ogrid[0:1:20j]`.)

Reminder – Python functions

```
def f(a, b, c):
    return some_result
```

Exercise 2.4: Mandelbrot set



Write a script that computes the Mandelbrot fractal. The Mandelbrot iteration:

```
N_max = 50
some_threshold = 50

c = x + 1j*y

for j in xrange(N_max):
    z = z**2 + c
```

Point (x, y) belongs to the Mandelbrot set if $|c| < \text{some_threshold}$.

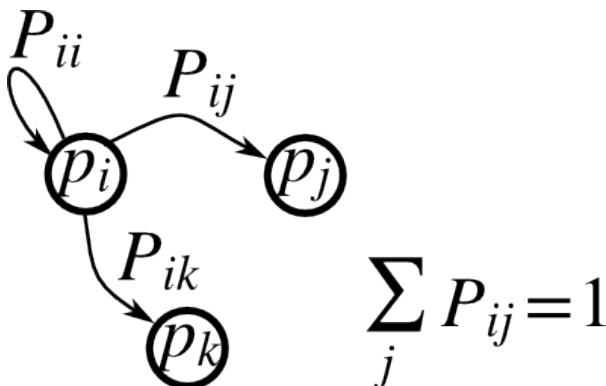
Do this computation by:

1. Construct a grid of $c = x + 1j*y$ values in range $[-2, 1] \times [-1.5, 1.5]$
2. Do the iteration

3. Form the 2-d boolean mask indicating which points are in the set
4. Save the result to an image with:

```
>>> import matplotlib.pyplot as plt
>>> plt.imshow(mask.T, extent=[-2, 1, -1.5, 1.5])
>>> plt.gray()
>>> plt.savefig('mandelbrot.png')
```

Exercise 2.5: Markov chain



Markov chain transition matrix P , and probability distribution on the states p :

1. $0 \leq P[i, j] \leq 1$: probability to go from state i to state j
2. Transition rule: $p_{new} = P^T p_{old}$
3. $\text{all}(\text{sum}(P, \text{axis}=1) == 1), p.\text{sum}() == 1$: normalization

Write a script that works with 5 states, and:

- Constructs a random matrix, and normalizes each row so that it is a transition matrix.
 - Starts from a random (normalized) probability distribution p and takes 50 steps => p_{50}
 - Computes the stationary distribution: the eigenvector of $P.T$ with eigenvalue 1 (numerically: closest to 1) => $p_{\text{stationary}}$
- Remember to normalize the eigenvector — I didn't...
- Checks if p_{50} and $p_{\text{stationary}}$ are equal to tolerance $1e-5$

Toolbox: `np.random.rand`, `.dot()`, `np.linalg.eig`, `reductions`, `abs()`, `argmin`, `comparisons`, `all`, `np.linalg.norm`, etc.

6.3.9 Conclusions

What do you need to know to get started?

- Know how to create arrays: `array`, `arange`, `ones`, `zeros`.
- Know the shape of the array with `array.shape`, then use slicing to obtain different views of the array: `array[:, ::2]`, etc. Adjust the shape of the array using `reshape` or flatten it with `ravel`.

- Obtain a subset of the elements of an array and/or modify their values with masks:

```
>>> a[a < 0] = 0
```

- Know miscellaneous operations on arrays, such as finding the mean or max (`array.max()`, `array.mean()`). No need to retain everything, but have the reflex to search in the documentation (online docs, `help()`, `lookfor()`)!!
- For advanced use: master the indexing with arrays of integers, as well as broadcasting. Know more Numpy functions to handle various array operations.

6.4 3. Moving on

6.4.1 More data types

Casting

“Bigger” type wins in mixed-type operations:

```
>>> np.array([1, 2, 3]) + 1.5
array([ 2.5,  3.5,  4.5])
```

Assignment never changes the type!

```
>>> a = np.array([1, 2, 3])
>>> a.dtype
dtype('int64')
>>> a[0] = 1.9      # <-- float is truncated to integer
>>> a
array([1, 2, 3])
```

Forced casts:

```
>>> a = np.array([1.7, 1.2, 1.6])
>>> b = a.astype(int)    # <-- truncates to integer
>>> b
array([1, 1, 1])
```

Rounding:

```
>>> a = np.array([1.7, 1.2, 1.6])
>>> b = np.around(a)
>>> b
array([ 2.,  1.,  2.])    # still floating-point
>>> c = np.around(a).astype(int)
>>> c
array([2, 1, 2])
```

Different data type sizes

Integers (signed):

int8	8 bits
int16	16 bits
int32	32 bits (same as int on 32-bit platform)
int64	64 bits (same as int on 64-bit platform)

```
>>> np.array([1], dtype=int).dtype
dtype('int64')
>>> np.iinfo(np.int32).max, 2**31 - 1
```

```
(2147483647, 2147483647)
>>> np.iinfo(np.int64).max, 2**63 - 1
(9223372036854775807, 9223372036854775807L)
```

Unsigned integers:

uint8	8 bits
uint16	16 bits
uint32	32 bits
uint64	64 bits

```
>>> np.iinfo(np.uint32).max, 2**32 - 1
(2147483647, 2147483647)
>>> np.iinfo(np.uint64).max, 2**64 - 1
(9223372036854775807, 9223372036854775807L)
```

Floating-point numbers:

float16	16 bits
float32	32 bits
float64	64 bits (same as float)
float96	96 bits, platform-dependent (same as np.longdouble)
float128	128 bits, platform-dependent (same as np.longdouble)

```
>>> np.finfo(np.float32).eps
1.1920929e-07
>>> np.finfo(np.float64).eps
2.2204460492503131e-16
```

```
>>> np.float32(1e-8) + np.float32(1) == 1
True
>>> np.float64(1e-8) + np.float64(1) == 1
False
```

Complex floating-point numbers:

complex64	two 32-bit floats
complex128	two 64-bit floats
complex192	two 96-bit floats, platform-dependent
complex256	two 128-bit floats, platform-dependent

Smaller data types

If you don't know you need special data types, then you probably don't.

Comparison on using float32 instead of float64:

- Half the size in memory and on disk
- Half the memory bandwidth required (may be a bit faster in some operations)

```
In [1]: a = np.zeros((1e6), dtype=np.float64)

In [2]: b = np.zeros((1e6), dtype=np.float32)

In [3]: %timeit a*a
1000 loops, best of 3: 1.78 ms per loop

In [4]: %timeit b*b
1000 loops, best of 3: 1.07 ms per loop
```

- But: bigger rounding errors — sometimes in surprising places (i.e., don't use them unless you really need them)

6.4.2 Structured data types

Composite data types

sensor_code (4-character string)	
position (float)	
value (float)	

```
>>> samples = np.zeros((6,), dtype=[('sensor_code', 'S4'),
...                                         ('position', float), ('value', float)])
>>> samples.ndim
1
>>> samples.shape
(6,)
>>> samples.dtype.names
('sensor_code', 'position', 'value')
```

```
>>> samples[:] = [('ALFA', 1, 0.35), ('BETA', 1, 0.11), ('TAU', 1, 0.39),
...                  ('ALFA', 1.5, 0.35), ('ALFA', 2.1, 0.11), ('TAU', 1.2, 0.39)]
>>> samples
array([('ALFA', 1.0, 0.35), ('BETA', 1.0, 0.11), ('TAU', 1.0, 0.39),
       ('ALFA', 1.5, 0.35), ('ALFA', 2.1, 0.11), ('TAU', 1.2, 0.39)],
      dtype=[('sensor_code', '|S4'), ('position', '<f8'), ('value', '<f8')])
```

Field access works by indexing with field names:

```
>>> samples['sensor_code']
array(['ALFA', 'BETA', 'TAU', 'ALFA', 'ALFA', 'TAU'],
      dtype='|S4')
>>> samples['value']
array([ 0.35,  0.11,  0.39,  0.35,  0.11,  0.39])
>>> samples[0]
('ALFA', 1.0, 0.35)
```

```
>>> samples[0]['sensor_code'] = 'TAU'
>>> samples[0]
('TAU', 1.0, 0.35)
```

Multiple fields at once:

```
>>> samples[['position', 'value']]
array([(1.0, 0.35), (1.0, 0.11), (1.0, 0.39), (1.5, 0.35), (2.1, 0.11),
       (1.2, 0.39)],
      dtype=[('position', '<f8'), ('value', '<f8')])
```

Fancy indexing works, as usually:

```
>>> samples[samples['sensor_code'] == 'ALFA']
array([('ALFA', 1.0, 0.35), ('ALFA', 1.5, 0.35), ('ALFA', 2.1, 0.11)],
      dtype=[('sensor_code', '|S4'), ('position', '<f8'), ('value', '<f8')])
```

Note: There are a bunch of other syntaxes for constructing structured arrays, see [here](#) and [here](#).

6.4.3 Fourier transforms

Numpy contains 1-D, 2-D, and N-D fast discrete Fourier transform routines, which compute:

$$A_k = \sum_{m=0}^{n-1} a_m \exp \left\{ -2\pi i \frac{mk}{n} \right\} \quad k = 0, \dots, n-1.$$

Full details of what you can use such standard routines is beyond this tutorial. Nevertheless, there they are, if you need them:

```
>>> a = np.exp(2j*np.pi*np.arange(10))
>>> fa = np.fft.fft(a)
>>> np.set_printoptions(suppress=True) # print small number as 0
>>> fa
array([ 10.-0.j,   0.+0.j,   0.+0.j,   0.+0.j,   0.+0.j,   0.+0.j,
       -0.+0.j,  -0.+0.j,  -0.+0.j,  -0.+0.j])
```

```
>>> a = np.exp(2j*np.pi*np.arange(3))
>>> b = a[:,np.newaxis] + a[np.newaxis,:]
>>> np.fft.fftn(b)
array([[ 18.-0.j,   0.+0.j,  -0.+0.j],
       [  0.+0.j,   0.+0.j,   0.+0.j],
       [ -0.+0.j,   0.+0.j,   0.+0.j]])
```

See `help(np.fft)` and `help(np.fft.freq)` for more. These functions in general take the `axes` argument, and you can additionally specify padding etc.

Worked example: Crude periodicity finding

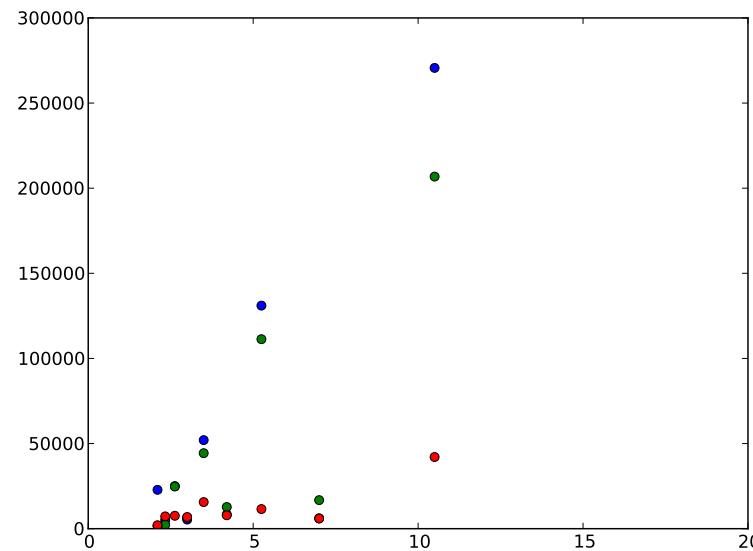
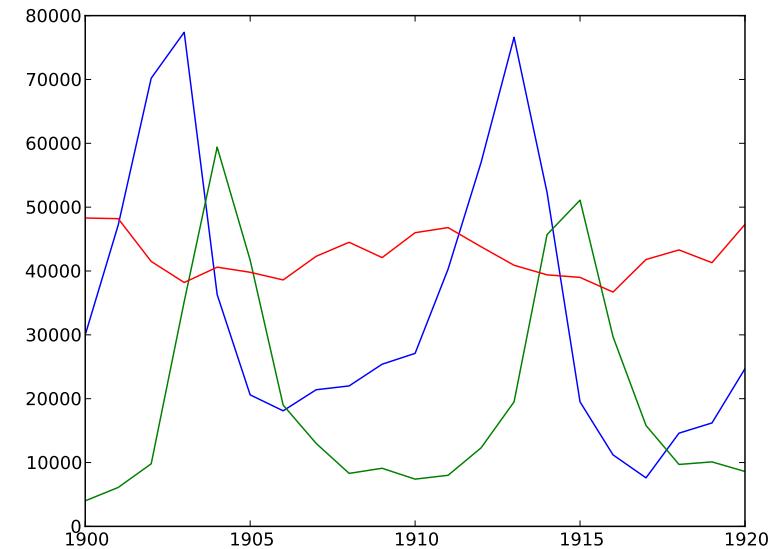
```
"""
Discover the periods in ../../data/populations.txt
"""

import numpy as np
import matplotlib.pyplot as plt

data = np.loadtxt('../../data/populations.txt')
years = data[:,0]
populations = data[:,1:]

ft_populations = np.fft.fft(populations, axis=0)
frequencies = np.fft.fftfreq(populations.shape[0], years[1] - years[0])

plt.figure()
plt.plot(years, populations)
plt.figure()
plt.plot(1/frequencies, abs(ft_populations), 'o')
plt.xlim(0, 20)
plt.show()
```



```
# There's probably a period of around 10 years (obvious from the
# plot), but for this crude a method, there's not enough data to say
# much more.
```

Worked example: Gaussian image blur

Convolution:

$$f_1(t) = \int dt' K(t - t') f_0(t')$$

$$\tilde{f}_1(\omega) = \tilde{K}(\omega) \tilde{f}_0(\omega)$$

```
"""
Simple image blur by convolution with a Gaussian kernel
"""

import numpy as np
from numpy import newaxis
import matplotlib.pyplot as plt

# read image
img = plt.imread('...../data/elephant.png')

# prepare an 1-D Gaussian convolution kernel
t = np.linspace(-10, 10, 30)
bump = np.exp(-0.1*t**2)
bump /= np.trapz(bump) # normalize the integral to 1

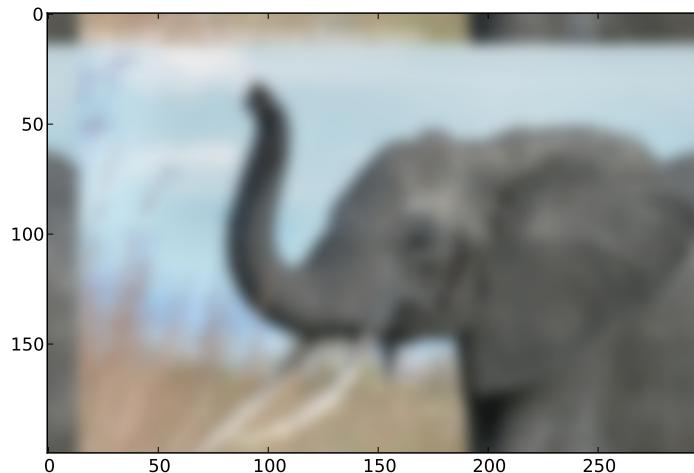
# make a 2-D kernel out of it
kernel = bump[:,newaxis] * bump[newaxis,:]

# padded fourier transform, with the same shape as the image
kernel_ft = np.fft.fft2(kernel, s=img.shape[:2], axes=(0, 1))

# convolve
img_ft = np.fft.fft2(img, axes=(0, 1))
img2_ft = kernel_ft[:, :, newaxis] * img_ft
img2 = np.fft.ifft2(img2_ft, axes=(0, 1)).real

# clip values to range
img2 = np.clip(img2, 0, 1)

# plot output
plt.imshow(img2)
plt.show()
```



```
# Further exercise (only if you are familiar with this stuff):
#
# A "wrapped border" appears in the upper left and top edges of the
# image. This is because the padding is not done correctly, and does
# not take the kernel size into account (so the convolution "flows out
# of bounds of the image"). Try to remove this artifact.
```

6.4.4 Masked arrays

Masked arrays are arrays that may have missing or invalid entries.

For example, suppose we have an array where the fourth entry is invalid:

```
>>> x = np.array([1, 2, 3, -99, 5])
```

One way to describe this is to create a masked array:

```
>>> mx = ma.masked_array(x, mask=[0, 0, 0, 1, 0])
>>> mx
masked_array(data = [1 2 3 -- 5],
              mask = [False False False  True False],
              fill_value = 999999)
```

Masked mean ignores masked data:

```
>>> mx.mean()
2.75
>>> np.mean(mx)
2.75
```

Warning: Not all Numpy functions respect masks, for instance `np.dot`, so check the return types.

The `masked_array` returns a `view` to the original array:

```
>>> mx[1] = 9
>>> x
array([ 1,  9,  3, -99,  5])
```

The mask

You can modify the mask by assigning:

```
>>> mx[1] = np.ma.masked
>>> mx
masked_array(data = [1 -- 3 -- 5],
              mask = [False True False True False],
              fill_value = 999999)
```

The mask is cleared on assignment:

```
>>> mx[1] = 9
>>> mx
masked_array(data = [1 9 3 -- 5],
              mask = [False False False True False],
              fill_value = 999999)
```

The mask is also available directly:

```
>>> mx.mask
array([False, False, False, True, False], dtype=bool)
```

The masked entries can be filled with a given value to get an usual array back:

```
>>> x2 = mx.filled(-1)
>>> x2
array([ 1,  9,  3, -1,  5])
```

The mask can also be cleared:

```
>>> mx.mask = np.ma.nomask
>>> mx
masked_array(data = [1 9 3 -99 5],
              mask = [False False False False False],
              fill_value = 999999)
```

Domain-aware functions

The masked array package also contains domain-aware functions:

```
>>> np.ma.log(np.array([1, 2, -1, -2, 3, -5]))
masked_array(data = [0.0 0.69314718056 -- -1.09861228867 --],
              mask = [False False True True False True],
              fill_value = 1e+20)
```

Note: Streamlined and more seamless support for dealing with missing data in arrays is making its way into Numpy 1.7. Stay tuned!

Example: Masked statistics

Canadian rangers were distracted when counting hares and lynxes in 1903-1910 and 1917-1918, and got the numbers are wrong. (Carrot farmers stayed alert, though.) Compute the mean populations over time, ignoring the invalid numbers.

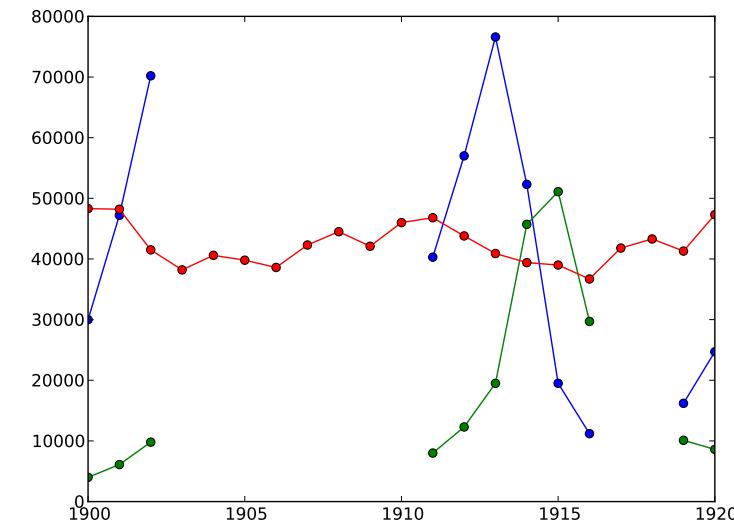
```
>>> data = np.loadtxt('.../data/populations.txt')
>>> populations = np.ma.masked_array(data[:,1:])
>>> year = data[:,0]
```

```
>>> bad_years = (((year >= 1903) & (year <= 1910))
...           | ((year >= 1917) & (year <= 1918)))
>>> populations[bad_years,0] = np.ma.masked
>>> populations[bad_years,1] = np.ma.masked
```

```
>>> populations.mean(axis=0)
masked_array(data = [40472.7272727 18627.2727273 42400.0],
             mask = [False False False],
             fill_value = 1e+20)
>>> populations.std(axis=0)
masked_array(data = [21087.656489 15625.7998142 3322.50622558],
             mask = [False False False],
             fill_value = 1e+20)
```

Note that Matplotlib knows about masked arrays:

```
>>> plt.plot(year, populations, 'o-')
>>> plt.show()
```

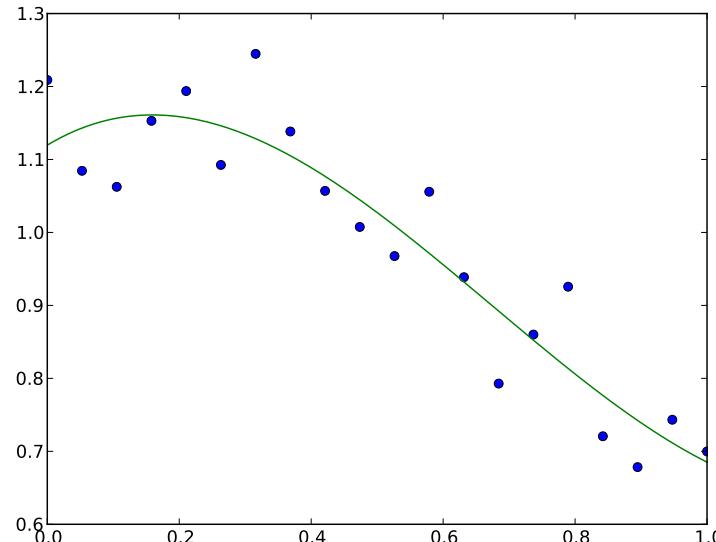


6.4.5 Polynomials

Numpy also contains polynomials in different bases:

For example, $3x^2 + 2x - 1$

```
>>> p = np.poly1d([3, 2, -1])
>>> p(0)
-1
>>> p.roots
array([-1.          ,  0.33333333])
>>> p.order
2
>>> x = np.linspace(0, 1, 20)
>>> y = np.cos(x) + 0.3*np.random.rand(20)
>>> p = np.poly1d(np.polyfit(x, y, 3))
>>> t = np.linspace(0, 1, 200)
>>> plt.plot(x, y, 'o', t, p(t), '-')
>>> plt.show()
```



See <http://docs.scipy.org/doc/numpy/reference/routines.polynomials.poly1d.html> for more.

More polynomials (with more bases)

Numpy also has a more sophisticated polynomial interface, which supports e.g. the Chebyshev basis.

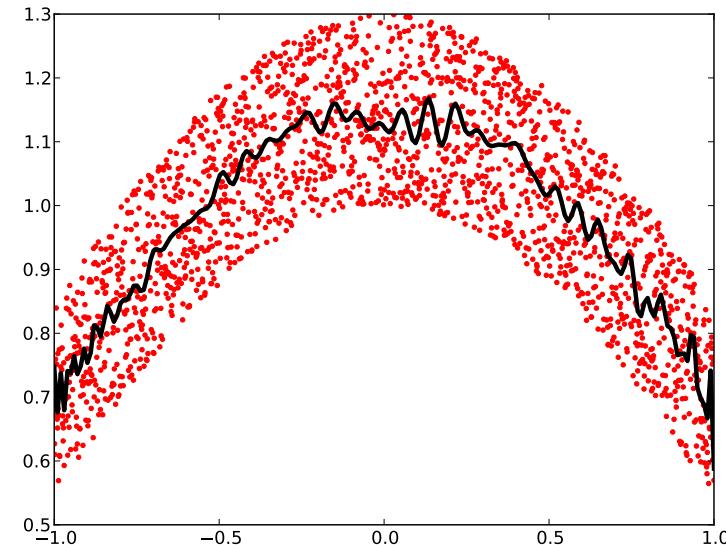
$3x^2 + 2x - 1$

```
>>> p = np.polynomial.Polynomial([-1, 2, 3]) # coefs in different order!
>>> p(0)
-1.0
>>> p.roots()
array([-1.          ,  0.33333333])
>>> p.order
2
```

Example using polynomials in Chebyshev basis, for polynomials in range [-1, 1]:

```
>>> x = np.linspace(-1, 1, 2000)
>>> y = np.cos(x) + 0.3*np.random.rand(2000)
>>> p = np.polynomial.Chebyshev.fit(x, y, 90)
```

```
>>> t = np.linspace(-1, 1, 200)
>>> plt.plot(x, y, 'r.')
>>> plt.plot(t, p(t), 'k-', lw=3)
>>> plt.show()
```



The Chebyshev polynomials have some advantages in interpolation.

6.4.6 Summary & Exercises

- There is a number of data types with different precisions. In some special cases you may need to care about this.
- Structured arrays contain data of a composite type. Lumping pieces of data together this way has various possible uses.
- Fourier transform routines are under `np.fft`
- Masked arrays can be used for missing data

- Polynomials are available in various bases

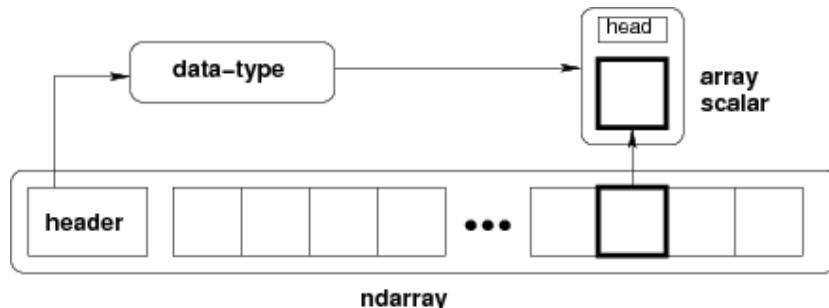
6.5.4. Under the hood

6.5.1 It's...

`ndarray =`

block of memory + indexing scheme + data type descriptor

- raw data
- how to locate an element
- how to interpret an element



6.5.2 Block of memory

```

>>> x = np.array([1, 2, 3, 4], dtype=np.int32)
>>> x.data
<read-write buffer for 0xa37bfd8, size 16, offset 0 at 0xa4eabe0>
>>> str(x.data)
'\x01\x00\x00\x00\x02\x00\x00\x00\x03\x00\x00\x04\x00\x00\x00\x00'
  
```

Memory address of the data:

```

>>> x.__array_interface__['data'][0]
159755776
  
```

Reminder: two ndarrays may share the same memory:

```

>>> x = np.array([1,2,3,4])
>>> y = x[:]
>>> x[0] = 9
>>> y
array([9, 2, 3, 4])
>>> y.base is x
True
  
```

Memory does not need to be owned by an ndarray:

```

>>> x = '\x01\x02\x03\x04'
>>> y = np.frombuffer(x, dtype=np.int8)
>>> y
array([1, 2, 3, 4], dtype=int8)
>>> y.data
  
```

```

<read-only buffer for 0xa588ba8, size 4, offset 0 at 0xa55cd60>
>>> y.base is x
True
  
```

```

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

The `owndata` and `writeable` flags indicate status of the memory block.

6.5.3 Indexing scheme: strides

The question

```

>>> x = np.array([[1, 2, 3],
   [4, 5, 6],
   [7, 8, 9]], dtype=np.int8)
>>> str(x.data)
'\x01\x02\x03\x04\x05\x06\x07\x08\x09'
  
```

At which byte in `x.data` does the item `x[1, 2]` begin?

The answer (in Numpy)

- `strides`: the number of bytes to jump to find the next element
- 1 stride per dimension

```

>>> x.strides
(3, 1)
>>> byte_offset = 3*1 + 1*2 # to find x[1,2]
>>> x.data[byte_offset]
'\x06'
>>> x[1,2]
6
  
```

- simple, flexible

C and Fortran order

```

>>> x = np.array([[1, 2, 3],
   [4, 5, 6],
   [7, 8, 9]], dtype=np.int16, order='C')
>>> x.strides
(6, 2)
>>> str(x.data)
'\x01\x00\x02\x00\x03\x00\x04\x00\x05\x00\x06\x00\x07\x00\x08\x00\t\x00'
  
```

- Need to jump 6 bytes to find the next row
- Need to jump 2 bytes to find the next column

```

>>> y = np.array(x, order='F')
>>> y.strides
(2, 6)
>>> str(y.data)
'\x01\x00\x04\x00\x07\x00\x02\x00\x05\x00\x08\x00\x03\x00\x06\x00\t\x00'
  
```

- Need to jump 2 bytes to find the next row

- Need to jump 6 bytes to find the next column
- Similarly to higher dimensions:
 - C: last dimensions vary fastest (= smaller strides)
 - F: first dimensions vary fastest

```
shape = (d1, d2, ..., dn)
strides = (s1, s2, ..., sn)
sjC = dj+1dj+2...dn × itemsize
sjF = d1d2...dj-1 × itemsize
```

Slicing

- *Everything* can be represented by changing only `shape`, `strides`, and possibly adjusting the data pointer!
- Never makes copies of the data

```
>>> x = np.array([1, 2, 3, 4, 5, 6], dtype=np.int32)
>>> y = x[::-1]
>>> y
array([6, 5, 4, 3, 2, 1])
>>> y.strides
(-4,)
```

```
>>> y = x[2:]
>>> y.__array_interface__['data'][0] - x.__array_interface__['data'][0]
8
```

```
>>> x = np.zeros((10, 10, 10), dtype=np.float)
>>> x.strides
(800, 80, 8)
>>> x[:, ::3, ::4].strides
(1600, 240, 32)
```

- Similarly, transposes never make copies (it just swaps strides)

```
>>> x = np.zeros((10, 10, 10), dtype=np.float)
>>> x.strides
(800, 80, 8)
>>> x.T.strides
(8, 80, 800)
```

Reshaping

But: not all reshaping operations can be represented by playing with strides.

```
>>> a = np.arange(6, dtype=np.int8).reshape(3, 2)
>>> b = a.T
>>> b.strides
(1, 2)
```

So far, so good. However:

```
>>> str(a.data)
'\x00\x01\x02\x03\x04\x05'
>>> b
array([[0, 2, 4],
```

```
[1, 3, 5]], dtype=int8)
>>> c = b.reshape(3*2)
>>> c
array([0, 2, 4, 1, 3, 5], dtype=int8)
```

Here, there is no way to represent the array `c` given one stride and the block of memory for `a`. Therefore, the `reshape` operation needs to make a copy here.

6.5.4 Summary

- Numpy array: block of memory + indexing scheme + data type description
- Indexing: strides
- `byte_position = np.sum(arr.strides * indices)`
- Various tricks can you do by playing with the strides (stuff for an advanced tutorial it is)

CHAPTER 7

Getting help and finding documentation

author Emmanuelle Gouillart

Rather than knowing all functions in Numpy and Scipy, it is important to find rapidly information throughout the documentation and the available help. Here are some ways to get information:

- In Ipython, help function opens the docstring of the function. Only type the beginning of the function's name and use tab completion to display the matching functions.

```
In [204]: help np.vander
np.vander      np.vdot      np.version    np.vvoid      np.vstack
np.var         np.vectorize  np void       np vsplit
```



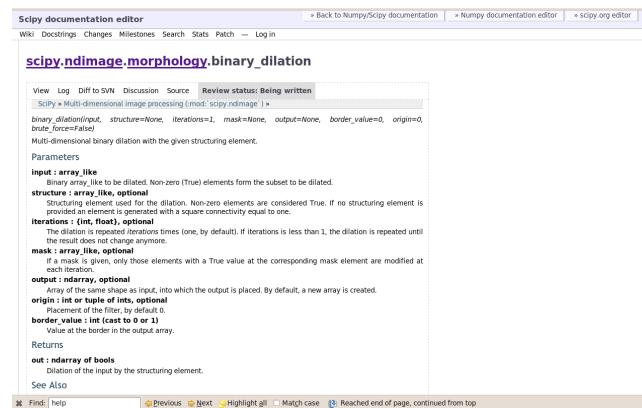
```
In [204]: help np.vander
```

In Ipython it is not possible to open a separated window for help and documentation; however one can always open a second Ipython shell just to display help and docstrings...

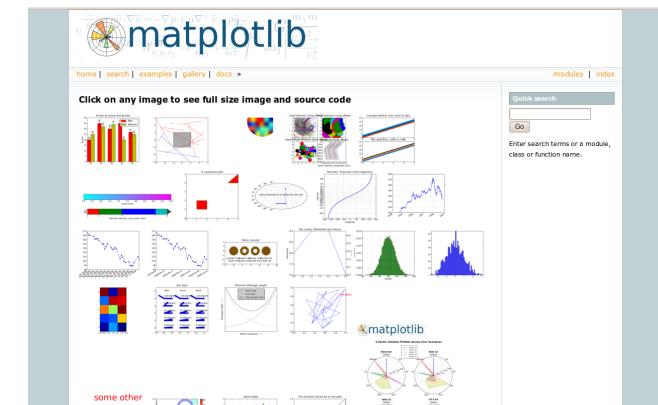
- Numpy's and Scipy's documentations can be browsed online on <http://docs.scipy.org/doc>. The search button is quite useful inside the reference documentation of the two packages (<http://docs.scipy.org/doc/numpy/reference/> and <http://docs.scipy.org/doc/scipy/reference/>).

Tutorials on various topics as well as the complete API with all docstrings are found on this website.

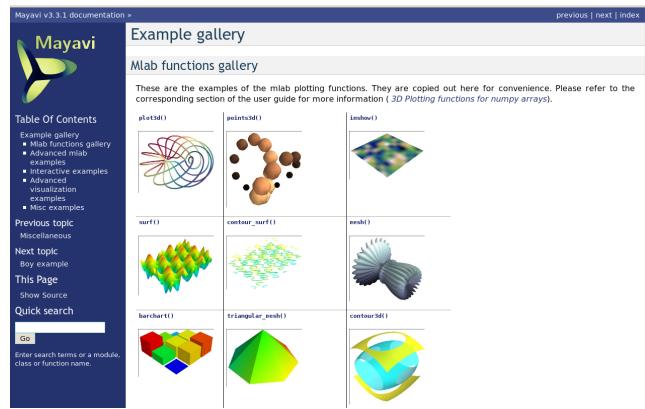
- Numpy's and Scipy's documentation is enriched and updated on a regular basis by users on a wiki <http://docs.scipy.org/scipy/>. As a result, some docstrings are clearer or more detailed on the wiki, and you may want to read directly the documentation on the wiki instead of the official documentation website. Note that anyone can create an account on the wiki and write better documentation; this is an easy way to contribute to an open-source project and improve the tools you are using!



- Scipy's cookbook <http://www.scipy.org/Cookbook> gives recipes on many common problems frequently encountered, such as fitting data points, solving ODE, etc.
- Matplotlib's website <http://matplotlib.sourceforge.net/> features a very nice **gallery** with a large number of plots, each of them shows both the source code and the resulting plot. This is very useful for learning by example. More standard documentation is also available.



- Mayavi's website <http://code.enthought.com/projects/mayavi/docs/development/html/mayavi/> also has a very nice gallery of examples <http://code.enthought.com/projects/mayavi/docs/development/html/mayavi/auto/examples.html> in which one can browse for different visualization solutions.



Finally, two more “technical” possibilities are useful as well:

- In Ipython, the magical function %psearch search for objects matching patterns. This is useful if, for example, one does not know the exact name of a function.

```
In [3]: import numpy as np
In [4]: %psearch np.diag*
np.diag
np.diagflat
np.diagonal
```

- numpy.lookfor looks for keywords inside the docstrings of specified modules.

```
In [45]: numpy.lookfor('convolution')
Search results for 'convolution'
-----
numpy.convolve
    Returns the discrete, linear convolution of two one-dimensional
    sequences.
numpy.bartlett
    Return the Bartlett window.
numpy.correlate
    Discrete, linear correlation of two 1-dimensional sequences.
In [46]: numpy.lookfor('remove', module='os')
Search results for 'remove'
-----
os.remove
    remove(path)
os.removedirs
    removedirs(path)
os.rmdir
    rmdir(path)
os.unlink
    unlink(path)
os.walk
    Directory tree generator.
```

- If everything listed above fails (and Google doesn’t have the answer)... don’t despair! Write to the mailing-list suited to your problem: you should have a quick answer if you describe your problem well. Experts on scientific python often give very enlightening explanations on the mailing-list.

– **Numpy discussion** (numpy-discussion@scipy.org): all about numpy arrays, manipulating them, indexing questions, etc.

- **SciPy Users List** (scipy-user@scipy.org): scientific computing with Python, high-level data processing, in particular with the scipy package.
- matplotlib-users@lists.sourceforge.net for plotting with matplotlib.

CHAPTER 8

Matplotlib

author Mike Müller

8.1 Introduction

`matplotlib` is probably the single most used Python package for 2D-graphics. It provides both a very quick way to visualize data from Python and publication-quality figures in many formats. We are going to explore `matplotlib` in interactive mode covering most common cases. We also look at the class library which is provided with an object-oriented interface.

8.2 IPython

IPython is an enhanced interactive Python shell that has lots of interesting features including named inputs and outputs, access to shell commands, improved debugging and many more. When we start it with the command line argument `-pylab`, it allows interactive `matplotlib` sessions that has Matlab/Mathematica-like functionality.

8.3 pylab

`pylab` provides a procedural interface to the `matplotlib` object-oriented plotting library. It is modeled closely after Matlab(TM). Therefore, the majority of plotting commands in `pylab` has Matlab(TM) analogs with similar arguments. Important commands are explained with interactive examples.

8.4 Simple Plots

Let's start an interactive session:

```
$ ipython -pylab
```

This brings us to the IPython prompt:

```
IPython 0.8.1 -- An enhanced Interactive Python.  
?          --> Introduction to IPython's features.  
%magic     --> Information about IPython's '%magic' % functions.  
help       --> Python's own help system.  
object?    --> Details about 'object'. ?object also works, ?? prints more.
```

```
Welcome to pylab, a matplotlib-based Python environment.  
For more information, type 'help(pylab)'.
```

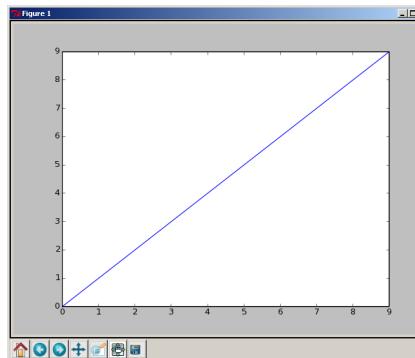
```
In [1]:
```

Now we can make our first, really simple plot:

```
In [1]: plot(range(10))  
Out[1]: [<matplotlib.lines.Line2D instance at 0x01AA26E8>]
```

```
In [2]:
```

The numbers form 0 through 9 are plotted:



Now we can interactively add features to or plot:

```
In [2]: xlabel('measured')  
Out[2]: <matplotlib.text.Text instance at 0x01A9D210>  
  
In [3]: ylabel('calculated')  
Out[3]: <matplotlib.text.Text instance at 0x01A9D918>  
  
In [4]: title('Measured vs. calculated')  
Out[4]: <matplotlib.text.Text instance at 0x01A9DF80>  
  
In [5]: grid(True)  
  
In [6]:
```

We get a reference to our plot:

```
In [6]: my_plot = gca()
```

and to our line we plotted, which is the first in the plot:

```
In [7]: line = my_plot.lines[0]
```

Now we can set properties using `set_something` methods:

```
In [8]: line.set_marker('o')
```

or the `setp` function:

```
In [9]: setp(line, color='g')  
Out[9]: [None]
```

To apply the new properties we need to redraw the screen:

```
In [10]: draw()
```

We can also add several lines to one plot:

```
In [1]: x = arange(100)
```

```
In [2]: linear = arange(100)
```

```
In [3]: square = [v * v for v in arange(0, 10, 0.1)]
```

```
In [4]: lines = plot(x, linear, x, square)
```

Let's add a legend:

```
In [5]: legend('linear', 'square')
Out[5]: <matplotlib.legend.Legend instance at 0x01BBC170>
```

This does not look particularly nice. We would rather like to have it at the left. So we clean the old graph:

```
In [6]: clf()
```

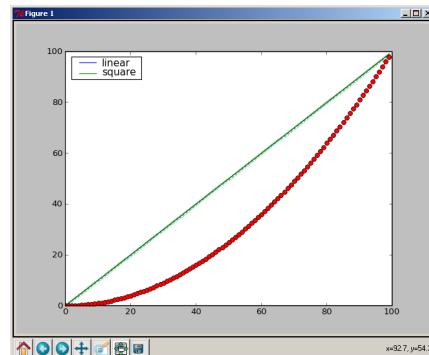
and print it anew providing new line styles (a green dotted line with crosses for the linear and a red dashed line with circles for the square graph):

```
In [7]: lines = plot(x, linear, 'g:+', x, square, 'r--o')
```

Now we add the legend at the upper left corner:

```
In [8]: l = legend(['linear', 'square'], loc='upper left')
```

The result looks like this:



8.4.1 Exercises

1. Plot a simple graph of a sinus function in the range 0 to 3 with a step size of 0.01.
2. Make the line red. Add diamond-shaped markers with size of 5.
3. Add a legend and a grid to the plot.

8.5 Properties

So far we have used properties for the lines. There are three possibilities to set them:

1) as keyword arguments at creation time: `plot(x, linear, 'g:+', x, square, 'r--o')`.

2. with the function `setp`: `setp(line, color='g')`.

3. using the `set_something` methods: `line.set_marker('o')`

Lines have several properties as shown in the following table:

Property	Value
alpha	alpha transparency on 0-1 scale
antialiased	True or False - use antialiased rendering
color	matplotlib color arg
data_clipping	whether to use numeric to clip data
label	string optionally used for legend
linestyle	one of - : -. -
linewidth	float, the line width in points
marker	one of +, o, s, v, x, >, etc
markeredgewidth	line width around the marker symbol
markeredgecolor	edge color if a marker is used
markerfacecolor	face color if a marker is used
markersize	size of the marker in points

There are many line styles that can be specified with symbols:

Symbol	Description
-	solid line
--	dashed line
-.	dash-dot line
:	dotted line
.	points
,	pixels
o	circle symbols
^	triangle up symbols
v	triangle down symbols
<	triangle left symbols
>	triangle right symbols
s	square symbols
+	plus symbols
x	cross symbols
D	diamond symbols
d	thin diamond symbols
1	tripod down symbols
2	tripod up symbols
3	tripod left symbols
4	tripod right symbols
h	hexagon symbols
H	rotated hexagon symbols
p	pentagon symbols
	vertical line symbols
_	horizontal line symbols
steps	use gnuplot style 'steps' # kwarg only

Colors can be given in many ways: one-letter abbreviations, gray scale intensity from 0 to 1, RGB in hex and tuple format as well as any legal html color name.

The one-letter abbreviations are very handy for quick work. With following you can get quite a few things done:

Abbreviation	Color
b	blue
g	green
r	red
c	cyan
m	magenta
y	yellow
k	black
w	white

Other objects also have properties. The following table list the text properties:

Property	Value
alpha	alpha transparency on 0-1 scale
color	matplotlib color arg
family	set the font family, eg sans-serif, cursive, fantasy
fontangle	the font slant, one of normal, italic, oblique
horizontalalignment	left, right or center
multialignment	left, right or center only for multiline strings
name	font name, eg, Sans, Courier, Helvetica
position	x,y location
variant	font variant, eg normal, small-caps
rotation	angle in degrees for rotated text
size	fontsize in points, eg, 8, 10, 12
style	font style, one of normal, italic, oblique
text	set the text string itself
verticalalignment	top, bottom or center
weight	font weight, e.g. normal, bold, heavy, light

8.5.1 Exercise

1. Apply different line styles to a plot. Change line color and thickness as well as the size and the kind of the marker. Experiment with different styles.

8.6 Text

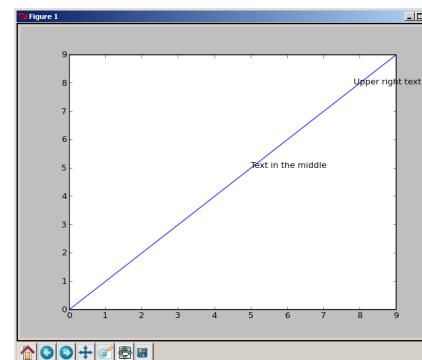
We've already used some commands to add text to our figure: `xlabel`, `ylabel`, and `title`.

There are two functions to put text at a defined position. `text` adds the text with data coordinates:

```
In [2]: plot(arange(10))
In [3]: t1 = text(5, 5, 'Text in the middle')
```

`figtext` uses figure coordinates from 0 to 1:

```
In [4]: t2 = figtext(0.8, 0.8, 'Upper right text')
```



matplotlib supports TeX mathematical expression. So `r'π'` will show up as:

$$\pi$$

If you want to get more control over where the text goes, you use annotations:

```
In [4]: ax = gca()
In [5]: ax.annotate('Here is something special', xy = (1, 1))
```

We will write the text at the position (1, 1) in terms of data. There are many optional arguments that help to customize the position of the text. The arguments `textcoords` and `xycoords` specifies what `x` and `y` mean:

argument	coordinate system
figure points	points from the lower left corner of the figure
figure pixels	pixels from the lower left corner of the figure
figure fraction	0,0 is lower left of figure and 1,1 is upper, right
axes points	points from lower left corner of axes
axes pixels	pixels from lower left corner of axes
axes fraction	0,1 is lower left of axes and 1,1 is upper right
data	use the axes data coordinate system

If we do not supply `xycoords`, the text will be written at `xy`.

Furthermore, we can use an arrow whose appearance can also be described in detail:

```
In [14]: plot(arange(10))
Out[14]: <matplotlib.lines.Line2D instance at 0x01BB15D0>

In [15]: ax = gca()

In [16]: ax.annotate('Here is something special', xy = (2, 1), xytext=(1,5))
Out[16]: <matplotlib.text.Annotation instance at 0x01BB1648>

In [17]: ax.annotate('Here is something special', xy = (2, 1), xytext=(1,5),
....: arrowprops={'facecolor': 'r'})
```

8.6.1 Exercise

1. Annotate a line at two places with text. Use green and red arrows and align it according to figure points and data.

8.7 Ticks

8.7.1 Where and What

Well formatted ticks are an important part of publishing-ready figures. matplotlib provides a totally configurable system for ticks. There are tick locators to specify where ticks should appear and tick formatters to make ticks look like the way you want. Major and minor ticks can be located and formatted independently from each other. Per default minor ticks are not shown, i.e. there is only an empty list for them because it is as NullLocator (see below).

8.7.2 Tick Locators

There are several locators for different kind of requirements:

Class	Description
NullLocator	no ticks
IndexLocator	locator for index plots (e.g. where <code>x = range(len(y))</code>)
LinearLocator	evenly spaced ticks from min to max
LogLocator	logarithmically ticks from min to max
MultipleLocator	ticks and range are a multiple of base; either integer or float
AutoLocator	choose a MultipleLocator and dynamically reassign

All of these locators derive from the base class `matplotlib.tickerLocator`. You can make your own locator deriving from it.

Handling dates as ticks can be especially tricky. Therefore, matplotlib provides special locators in `matplotlib.dates`:

Class	Description
MinuteLocator	locate minutes
HourLocator	locate hours
DayLocator	locate specified days of the month
WeekdayLocator	locate days of the week, e.g. MO, TU
MonthLocator	locate months, e.g. 10 for October
YearLocator	locate years that are multiples of base
RRuleLocator	locate using a <code>matplotlib.dates.rrule</code>

8.7.3 Tick Formatters

Similarly to locators, there are formatters:

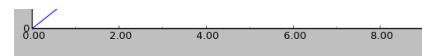
Class	Description
NullFormatter	no labels on the ticks
FixedFormatter	set the strings manually for the labels
FuncFormatter	user defined function sets the labels
FormatStrFormatter	use a sprint format string
IndexFormatter	cycle through fixed strings by tick position
ScalarFormatter	default formatter for scalars; autopick the fmt string
LogFormatter	formatter for log axes
DateFormatter	use an strftime string to format the date

All of these formatters derive from the base class `matplotlib.tickerFormatter`. You can make your own formatter deriving from it.

Now we set our major locator to 2 and the minor locator to 1. We also format the numbers as decimals using the `FormatStrFormatter`:

```
In [5]: major_locator = MultipleLocator(2)
In [6]: major_formatter = FormatStrFormatter('%5.2f')
In [7]: minor_locator = MultipleLocator(1)
In [8]: ax.xaxis.set_major_locator(major_locator)
In [9]: ax.xaxis.set_minor_locator(minor_locator)
In [10]: ax.xaxis.set_major_formatter(major_formatter)
In [10]: draw()
```

After we redraw the figure our x axis should look like this:



8.7.4 Exercises

1. Plot a graph with dates for one year with daily values at the x axis using the built-in module `datetime`.
2. Format the dates in such a way that only the first day of the month is shown.
3. Display the dates with and without the year. Show the month as number and as first three letters of the month name.

8.8 Figures, Subplots, and Axes

8.8.1 The Hierarchy

So far we have used implicit figure and axes creation. This is handy for fast plots. We can have more control over the display using `figure`, `subplot`, and `axes` explicitly. A `figure` in matplotlib means the whole window in the user interface. Within this `figure` there can be subplots. While `subplot` positions the plots in a regular grid, `axes` allows free placement within the `figure`. Both can be useful depending on your intention. We've already work with figures and subplots without explicitly calling them. When we call `plot` `matplotlib` calls `gca()` to get the current axes and `gca` in turn calls `gcf()` to get the current figure. If there is none it calls `figure()` to make one, strictly speaking, to make a subplot (111). Let's look at the details.

8.8.2 Figures

A `figure` is the windows in the GUI that has “Figure #” as title. Figures are numbered starting from 1 as opposed to the normal Python way starting from 0. This is clearly MATLAB-style. There are several parameters that determine how the figure looks like:

Argument	Default	Description
num	1	number of figure
figsize	figure.figsize	figure size in in inches (width, height)
dpi	figure.dpi	resolution in dots per inch
facecolor	figure.facecolor	color of the drawing background
edgecolor	figure.edgecolor	color of edge around the drawing background
frameon	True	draw figure frame or not

The defaults can be specified in the resource file and will be used most of the time. Only the number of the figure is frequently changed.

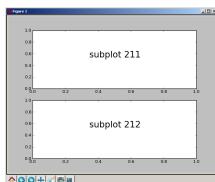
When you work with the GUI you can close a figure by clicking on the x in the upper right corner. But you can close a figure programmatically by calling `close`. Depending on the argument it closes (1) the current figure (no argument), (2) a specific figure (figure number or figure instance as argument), or (3) all figures (all as argument).

As with other objects, you can set figure properties also `setp` or with the `set_something` methods.

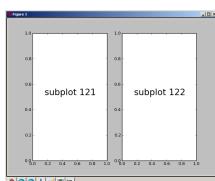
8.8.3 Subplots

With `subplot` you can arrange plots in regular grid. You need to specify the number of rows and columns and the number of the plot.

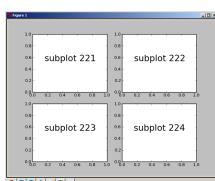
A plot with two rows and one column is created with `subplot(211)` and `subplot(212)`. The result looks like this:



If you want two plots side by side, you create one row and two columns with `subplot(121)` and `subplot(122)`. The result looks like this:



You can arrange as many figures as you want. A two-by-two arrangement can be created with `subplot(221)`, `subplot(222)`, `subplot(223)`, and `subplot(224)`. The result looks like this:



Frequently, you don't want all subplots to have ticks or labels. You can set the `xticklabels` or the `yticklabels` to an empty list (`[]`). Every subplot defines the methods `'is_first_row'`, `'is_first_col'`, `'is_last_row'`, and `'is_last_col'`. These can help to set ticks and labels only for the outer plots.

8.8.4 Axes

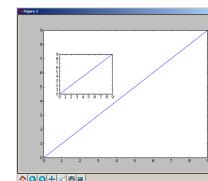
Axes are very similar to subplots but allow placement of plots at any location in the figure. So if we want to put a smaller plot inside a bigger one we do so with `axes`:

```
In [22]: plot(x)
Out[22]: [<matplotlib.lines.Line2D instance at 0x02C9CE90>]
```

```
In [23]: a = axes([0.2, 0.5, 0.25, 0.25])
```

```
In [24]: plot(x)
```

The result looks like this:



8.8.5 Exercises

1. Draw two figures, one 5 by 5, one 10 by 10 inches.
2. Add four subplots to one figure. Add labels and ticks only to the outermost axes.
3. Place a small plot in one bigger plot.

8.9 Other Types of Plots

8.9.1 Many More

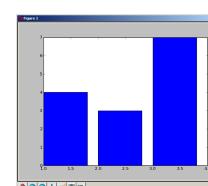
So far we have used only line plots. `matplotlib` offers many more types of plots. We will have a brief look at some of them. All functions have many optional arguments that are not shown here.

8.9.2 Bar Charts

The function `bar` creates a new bar chart:

```
bar([1, 2, 3], [4, 3, 7])
```

Now we have three bars starting at 1, 2, and 3 with height of 4, 3, 7 respectively:



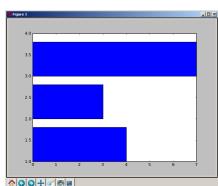
The default column width is 0.8. It can be changed with common methods by setting `width`. As it can be `color` and `bottom`, we can also set an error bar with `yerr` or `xerr`.

8.9.3 Horizontal Bar Charts

The function `barh` creates a vertical bar chart. Using the same data:

```
barh([1, 2, 3], [4, 3, 7])
```

We get:



8.9.4 Broken Horizontal Bar Charts

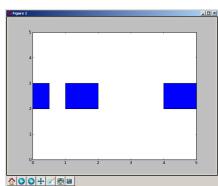
We can also have discontinuous vertical bars with `broken_barh`. We specify start and width of the range in y-direction and all start-width pairs in x-direction:

```
yrange = (2, 1)
xranges = ([0, 0.5], [1, 1], [4, 1])
broken_barh(xranges, yrange)
```

We changes the extension of the y-axis to make plot look nicer:

```
ax = gca()
ax.set_ylim(0, 5)
(0, 5)
draw()
```

and get this:



8.9.5 Box and Whisker Plots

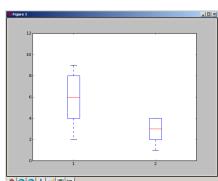
We can draw box and whisker plots:

```
boxplot((arange(2, 10), arange(1, 5)))
```

We want to have the whiskers well within the plot and therefore increase the y axis:

```
ax = gca()
ax.set_ylim(0, 12)
draw()
```

Our plot looks like this:



The range of the whiskers can be determined with the argument `whis`, which defaults to 1.5. The range of the whiskers is between the most extreme data point within `whis * (75% - 25%)` of the data.

8.9.6 Contour Plots

We can also do contour plots. We define arrays for the x and y coordinates:

```
x = y = arange(10)
```

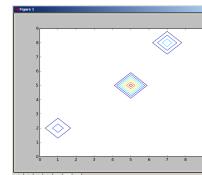
and also a 2D array for z:

```
z = ones((10, 10))
z[5,5] = 7
z[2,1] = 3
z[8,7] = 4
z
array([[ 1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.],
       [ 1.,  3.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.,  1.,  7.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.,  1.,  4.,  1.,  1.,  1.]])
```

Now we can make a simple contour plot:

```
contour(x, x, z)
```

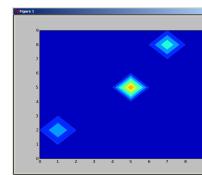
Our plot looks like this:



We can also fill the area. We just use numbers from 0 to 9 for the values v:

```
v = x
contourf(x, x, z, v)
```

Now our plot area is filled:



8.9.7 Histograms

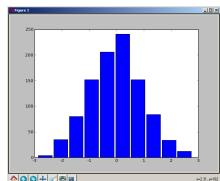
We can make histograms. Let's get some normally distributed random numbers from numpy:

```
import numpy as N
r_numbers = N.random.normal(size= 1000)
```

Now we make a simple histogram:

```
hist(r_numbers)
```

With 100 numbers our figure looks pretty good:



8.9.8 Loglog Plots

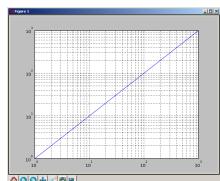
Plots with logarithmic scales are easy:

```
loglog(arange(1000))
```

We set the mayor and minor grid:

```
grid(True)
grid(True, which='minor')
```

Now we have loglog plot:



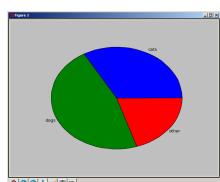
If we want only one axis with a logarithmic scale we can use `semilogx` or `semilogy`.

8.9.9 Pie Charts

Pie charts can also be created with a few lines:

```
data = [500, 700, 300]
labels = ['cats', 'dogs', 'other']
pie(data, labels=labels)
```

The result looks as expected:



8.9.10 Polar Plots

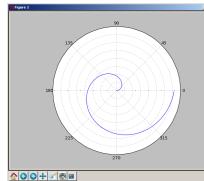
Polar plots are also possible. Let's define our `r` from 0 to 360 and our `theta` from 0 to 360 degrees. We need to convert them to radians:

```
r = arange(360)
theta = r / (180/pi)
```

Now plot in polar coordinates:

```
polar(theta, r)
```

We get a nice spiral:



8.9.11 Arrow Plots

Plotting arrows in 2D plane can be achieved with `quiver`. We define the x and y coordinates of the arrow shafts:

```
x = y = arange(10)
```

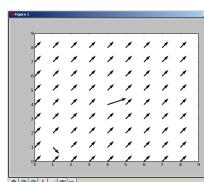
The x and y components of the arrows are specified as 2D arrays:

```
u = ones((10, 10))
v = ones((10, 10))
u[4, 4] = 3
v[1, 1] = -1
```

Now we can plot the arrows:

```
quiver(x, y, u, v)
```

All arrows point to the upper right, except two. The one at the location (4, 4) has 3 units in x-direction and the other at location (1, 1) has -1 unit in y direction:



8.9.12 Scatter Plots

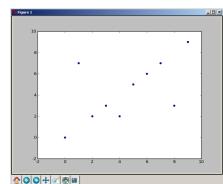
Scatter plots print x vs. y diagrams. We define x and y and make some point in y random:

```
x = arange(10)
y = arange(10)
y[1] = 7
y[4] = 2
y[8] = 3
```

Now make a scatter plot:

```
scatter(x, y)
```

The three different values for y break out of the line:



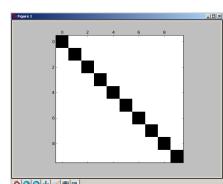
8.9.13 Sparsity Pattern Plots

Working with sparse matrices, it is often of interest as how the matrix looks like in terms of sparsity. We take an identity matrix as an example:

```
i = identity(10)
i
array([[1, 0, 0, 0, 0, 0, 0, 0, 0, 0],
       [0, 1, 0, 0, 0, 0, 0, 0, 0, 0],
       [0, 0, 1, 0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 1, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 1, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 1, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0, 1, 0, 0],
       [0, 0, 0, 0, 0, 0, 0, 0, 1, 0],
       [0, 0, 0, 0, 0, 0, 0, 0, 0, 1]])
```

Now we look at it more visually:

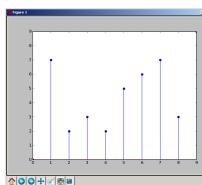
```
spy(i)
```



8.9.14 Stem Plots

Stem plots vertical lines at the given x location up to the specified y location. Let's reuse x and y from our scatter (see above):

```
stem(x, y)
```



8.9.15 Date Plots

There is a function for creating date plots. Let's define 10 dates starting at January 1st 2000 at 15.day intervals:

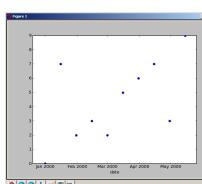
```
import datetime
d1 = datetime.datetime(2000, 1, 1)
delta = datetime.timedelta(15)
dates = [d1 + x * delta for x in range(10)]
[datetime.datetime(2000, 1, 1, 0, 0),
 datetime.datetime(2000, 1, 16, 0, 0),
 datetime.datetime(2000, 1, 31, 0, 0),
 datetime.datetime(2000, 2, 15, 0, 0),
 datetime.datetime(2000, 3, 1, 0, 0),
 datetime.datetime(2000, 3, 16, 0, 0),
 datetime.datetime(2000, 3, 31, 0, 0),
 datetime.datetime(2000, 4, 15, 0, 0),
 datetime.datetime(2000, 4, 30, 0, 0),
 datetime.datetime(2000, 5, 15, 0, 0)]
```

We reuse our data from the scatter plot (see above):

```
y
array([0, 7, 2, 3, 2, 5, 6, 7, 3, 9])
```

Now we can plot the dates at the x axis:

```
plot_date(dates, y)
```



8.10 The Class Library

So far we have used the `pylab` interface only. As the name suggests it is just wrapper around the class library. All `pylab` commands can be invoked via the class library using an object-oriented approach.

8.10.1 The Figure Class

The class `Figure` lives in the module `matplotlib.figure`. Its constructor takes these arguments:

```
figsize=None, dpi=None, facecolor=None, edgecolor=None,
linewidth=1.0, frameon=True, subplotpars=None
```

Comparing this with the arguments of `figure` in `pylab` shows significant overlap:

```
num=None, figsize=None, dpi=None, facecolor=None
edgecolor=None, frameon=True
```

Figure provides lots of methods, many of them have equivalents in `pylab`. The methods `add_axes` and `add_subplot` are called if new axes or subplot are created with `axes` or `subplot` in `pylab`. Also the method `gca` maps directly to `pylab` as do `legend`, `text` and many others.

There are also several `set_something` method such as `set_facecolor` or `set_edgecolor` that will be called through `pylab` to set properties of the figure. Figure also implements `get_something` methods such as `get_axes` or `get_facecolor` to get properties of the figure.

8.10.2 The Classes Axes and Subplot

In the class `Axes` we find most of the figure elements such as `Axis`, `Tick`, `Line2D`, or `Text`. It also sets the coordinate system. The class `Subplot` inherits from `Axes` and adds some more functionality to arrange the plots in a grid.

Analogous to `Figure`, it has methods to get and set properties and methods already encountered as functions in `pylab` such as `annotate`. In addition, `Axes` has methods for all types of plots shown in the previous section.

8.10.3 Other Classes

Other classes such as `text`, `Legend` or `Ticker` are setup very similarly. They can be understood mostly by comparing to the `pylab` interface.

8.10.4 Example

Let's look at an example for using the object-oriented API:

```
#file matplotlib/oo.py

from matplotlib.figure import Figure      #1

figsize = (8, 5)                         #2
fig = Figure(figsize=figsize)             #3
ax = fig.add_subplot(111)                  #4
line = ax.plot(range(10))[0]              #5
ax.set_title('Plotted with OO interface') #6
ax.set_xlabel('measured')
ax.set_ylabel('calculated')
ax.grid(True)                            #7
line.set_marker('o')                     #8

from matplotlib.backends.backend_agg import FigureCanvasAgg #9
canvas = FigureCanvasAgg(fig)              #10
canvas.print_figure("oo.png", dpi=80)       #11

import Tkinter as Tk                      #12
from matplotlib.backends.backend_tkagg import FigureCanvasTkAgg #13

root = Tk.Tk()                           #14
canvas2 = FigureCanvasTkAgg(fig, master=root) #15
canvas2.show()                            #16
canvas2.get_tk_widget().pack(side=Tk.TOP, fill=Tk.BOTH, expand=1) #17
Tk.mainloop()                            #18

from matplotlib import pylab_helpers      #19
```

```
import pylab                                #20
pylab_fig = pylab.figure(1, figsize=figsize) #21
figManager = __pylab_helpers.Gcf.get_active() #22
figManager.canvas.figure = fig               #23
pylab.show()                                #24
```

Since we are not in the interactive `pylab`-mode, we need to import the class `Figure` explicitly (#1).

We set the size of our figure to be 8 by 5 inches (#2). Now we initialize a new figure (#3) and add a subplot to the figure (#4). The 111 says one plot at position 1, 1 just as in MATLAB. We create a new plot with the numbers from 0 to 9 and at the same time get a reference to our line (#5). We can add several things to our plot. So we set a title and labels for the x and y axis (#6).

We also want to see the grid (#7) and would like to have little filled circles as markers (#8).

There are many different backends for rendering our figure. We use the Anti-Grain Geometry toolkit (<http://www.antigrain.com>) to render our figure. First, we import the backend (#9), then we create a new canvas that renders our figure (#10). We save our figure in a png-file with a resolution of 80 dpi (#11).

We can use several GUI toolkits directly. So we import Tkinter (#12) as well as the corresponding backend (#13). Now we have to do some basic GUI programming work. We make a root object for our GUI (#14) and feed it together with our figure to the backend to get our canvas (#15). We call the `show` method (#16), pack our widget (#17), and call the Tkinter mainloop to start the application (#18). You should see GUI window with the figure on your screen. After closing the screen, the next part, the script, will be executed.

We would like to create a screen display just as we would use `pylab`. Therefore we import a helper (#19) and `pylab` itself (#20). We create a normal figure with `pylab`` (#21) and get the corresponding figure manager (#22). Now let's set our figure we created above to be the current figure (#23) and let `pylab` show the result (#24). The lower part of the figure might be covered by the toolbar. If so, please adjust the `figsize` for `pylab` accordingly.

8.10.5 Exercises

1. Use the object-oriented API of `matplotlib` to create a png-file with a plot of two lines, one linear and square with a legend in it.

CHAPTER 9

Scipy : high-level scientific computing

authors Adrien Chauve, Andre Espaze, Emmanuelle Gouillart, Gaël Varoquaux

Scipy

The `scipy` package contains various toolboxes dedicated to common issues in scientific computing. Its different submodules correspond to different applications, such as interpolation, integration, optimization, image processing, statistics, special functions, etc.

`scipy` can be compared to other standard scientific-computing libraries, such as the GSL (GNU Scientific Library for C and C++), or Matlab's toolboxes. `scipy` is the core package for scientific routines in Python; it is meant to operate efficiently on `numpy` arrays, so that `numpy` and `scipy` work hand in hand.

Before implementing a routine, it is worth checking if the desired data processing is not already implemented in Scipy. As non-professional programmers, scientists often tend to **re-invent the wheel**, which leads to buggy, non-optimal, difficult-to-share and unmaintainable code. By contrast, Scipy's routines are optimized and tested, and should therefore be used when possible.

Warning: This tutorial is far from an introduction to numerical computing. As enumerating the different submodules and functions in `scipy` would be very boring, we concentrate instead on a few examples to give a general idea of how to use `scipy` for scientific computing.

To begin with

```
>>> import numpy as np
>>> import scipy
```

`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

9.1 Scipy builds upon Numpy

Numpy is required for running Scipy but also for using it. The most important type introduced to Python is the N dimensional array, and it can be seen that Scipy uses the same:

```
>>> scipy.ndarray is np.ndarray
True
```

Moreover most of the Scipy usual functions are provided by Numpy:

```
>>> scipy.cos is np.cos
True
```

If you would like to know the objects used from Numpy, have a look at the `scipy.__file__[:-1]` file. On version '0.6.0', the whole Numpy namespace is imported by the line `from numpy import *`.

9.2 File input/output: `scipy.io`

- Loading and saving 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, but numpy-specific, binary format:

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

9.3 Signal processing: `scipy.signal`

```
>>> from scipy import signal
```

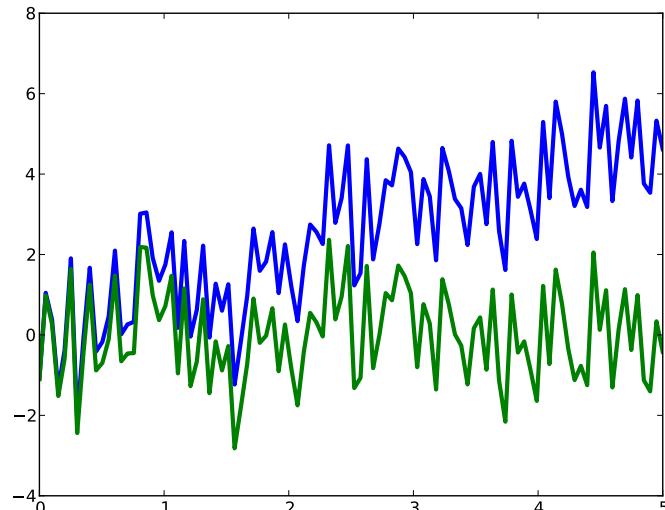
- Detrend: remove linear trend from signal:

```
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)
```

```
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)
```



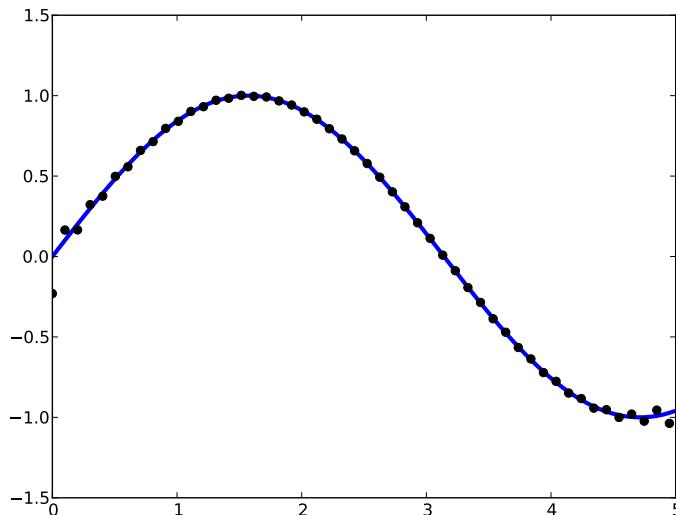
- Resample: resample a signal to n points using FFT.

```
t = np.linspace(0, 5, 100)
x = np.sin(t)

pl.plot(t, x, linewidth=3)
pl.plot(t[::2], signal.resample(x, 50), 'ko')
```

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

```
pl.plot(t, x, linewidth=3)
pl.plot(t[::2], signal.resample(x, 50), 'ko')
```



Notice how on the side of the window the resampling is less accurate and has a rippling effect.

- Signal has many window function: `hamming`, `bartlett`, `blackman`...
- Signal has filtering (Gaussian, median filter, Wiener), but we will discuss this in the image paragraph.

9.4 Special functions: `scipy.special`

Special functions are transcendental functions. The docstring of the module is well-written and we will not list them. Frequently used ones are:

- Bessel function, such as `special.jn` (nth integer order Bessel function)
- Elliptic function (`special.ellipj` for the Jacobian elliptic function, ...)
- Gamma function: `special.gamma`, also note `special.gammaln` which will give the log of Gamma to a higher numerical precision.
- Erf, the area under a Gaussian curve: `special.erf`

9.5 Statistics and random numbers: `scipy.stats`

The module `scipy.stats` contains statistical tools and probabilistic description of random processes. Random number generators for various random process can be found in `numpy.random`.

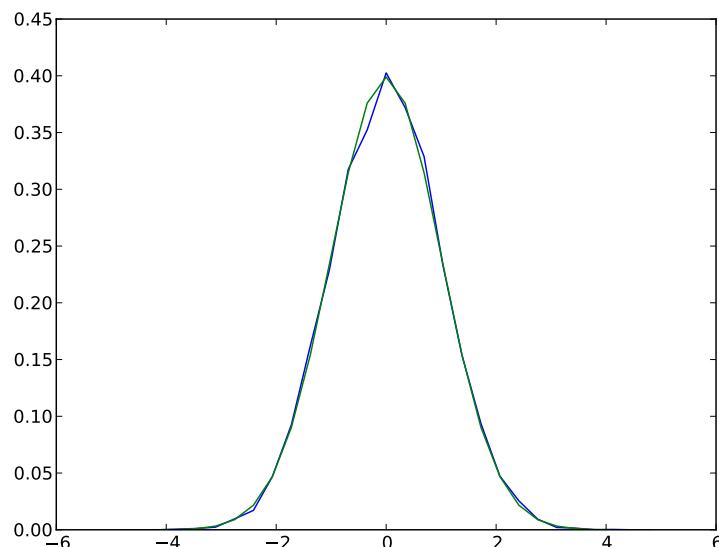
9.5.1 Histogram and probability density function

Given observations of a random process, their histogram is an estimator of the random process's PDF (probability density function):

```
>>> 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, normed=True)[0]
>>> 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)
```

```
from scipy import stats
import numpy as np
import pylab as pl
a = np.random.normal(size=10000)
bins = np.linspace(-5, 5, 30)
histogram, bins = np.histogram(a, bins=bins, normed=True)
bins = 0.5*(bins[1:] + bins[:-1])
from scipy import stats
b = stats.norm.pdf(bins)
pl.plot(bins, histogram)
pl.plot(bins, b)
```



If we know that the random process belongs to a given family of random processes, such as normal processes,

we can do a maximum-likelihood fit of the observations to estimate the parameters of the underlying distribution. Here we fit a normal process to the observed data:

```
>>> loc, std = stats.norm.fit(a)
>>> loc
0.003738964114102075
>>> std
0.97450996668871193
```

9.5.2 Percentiles

The median is the value with half of the observations below, and half above:

```
>>> np.median(a)
0.0071645570292782519
```

It is also called the percentile 50, because 50% of the observation are below it:

```
>>> stats.scoreatpercentile(a, 50)
0.0071645570292782519
```

Similarly, we can calculate the percentile 90:

```
>>> stats.scoreatpercentile(a, 90)
1.2729556087871292
```

The percentile is an estimator of the CDF: cumulative distribution function.

9.5.3 Statistical tests

A statistical test is a decision indicator. For instance, if we have 2 sets of observations, that we assume are generated from Gaussian processes, we can use a T-test to decide whether the two sets of observations are significantly different:

```
>>> a = np.random.normal(0, 1, size=100)
>>> b = np.random.normal(1, 1, size=10)
>>> stats.ttest_ind(a, b)
(-2.389876434401887, 0.018586471712806949)
```

The resulting output is composed of:

- The T statistic value: it is a number the sign of which is proportional to the difference between the two random processes and the magnitude is related to the significance of this difference.
- the *p value*: the probability of both process being identical. If it is close to 1, the two process are almost certainly identical. The closer it is to zero, the more likely it is that the processes have different mean.

9.6 Linear algebra operations: `scipy.linalg`

First, the linalg module provides standard linear algebra operations. The `det` function computes the determinant of a square matrix:

```
>>> from scipy import linalg
>>> arr = np.array([[1, 2],
...                 [3, 4]])
>>> linalg.det(arr)
-2.0
>>> arr = np.array([[3, 2],
...                 [6, 4]])
>>> linalg.det(arr)
```

```
0.0
>>> linalg.det(np.ones((3, 4)))
Traceback (most recent call last):
...
ValueError: expected square matrix
```

The `inv` function computes the inverse of a square matrix:

```
>>> arr = np.array([[1, 2],
...                 [3, 4]])
>>> iarr = linalg.inv(arr)
>>> iarr
array([[ -2. ,   1. ],
       [  1.5, -0.5]])
>>> np.allclose(np.dot(arr, iarr), np.eye(2))
True
```

Note that in case you use the matrix type, the inverse is computed when requesting the `I` attribute:

```
>>> ma = np.matrix(arr, copy=False)
>>> np.allclose(ma.I, iarr)
True
```

Finally computing the inverse of a singular matrix (its determinant is zero) will raise `LinAlgError`:

```
>>> arr = np.array([[3, 2],
...                 [6, 4]])
>>> linalg.inv(arr)
Traceback (most recent call last):
...
LinAlgError: singular matrix
```

More advanced operations are available like singular-value decomposition (SVD):

```
>>> arr = np.arange(12).reshape((3, 4)) + 1
>>> uarr, spec, vharr = linalg.svd(arr)
```

The resulting array spectrum is:

```
>>> spec
array([ 2.54368356e+01,   1.72261225e+00,   5.14037515e-16])
```

For the recomposition, an alias for manipulating matrix will first be defined:

```
>>> asmat = np.asmatrix
```

then the steps are:

```
>>> sarr = np.zeros((3, 4))
>>> sarr.put((0, 5, 10), spec)
>>> svd_mat = asmat(uarr) * asmat(sarr) * asmat(vharr)
>>> np.allclose(svd_mat, arr)
True
```

SVD is commonly used in statistics or signal processing. Many other standard decompositions (QR, LU, Cholesky, Schur), as well as solvers for linear systems, are available in `scipy.linalg`.

9.7 Numerical integration: `scipy.integrate`

The most generic integration routine is `scipy.integrate.quad`:

```
>>> from scipy.integrate import quad
>>> res, err = quad(np.sin, 0, np.pi/2)
```

```
>>> np.allclose(res, 1)
True
>>> np.allclose(err, 1 - res)
True
```

Others integration schemes are available with `fixed_quad`, `quadrature`, `romberg`.

`scipy.integrate` also features routines for Ordinary differential equations (ODE) integration. In particular, `scipy.integrate.odeint` is a general-purpose integrator using LSODA (Livermore solver for ordinary differential equations with automatic method switching for stiff and non-stiff problems), see the [ODEPACK Fortran library](#) for more details.

`odeint` solves first-order ODE systems of the form:

```
``dy/dt = rhs(y1, y2, ..., t0,...)``
```

As an introduction, let us solve the ODE $dy/dt = -2y$ between $t = 0 \dots 4$, with the initial condition $y(t=0) = 1$. First the function computing the derivative of the position needs to be defined:

```
>>> def calc_derivative(ypos, time, counter_arr):
...     counter_arr += 1
...     return -2*ypos
... 
```

An extra argument `counter_arr` has been added to illustrate that the function may be called several times for a single time step, until solver convergence. The counter array is defined as:

```
>>> counter = np.zeros((1,), np.uint16)
```

The trajectory will now be computed:

```
>>> from scipy.integrate import odeint
>>> time_vec = np.linspace(0, 4, 40)
>>> yvec, info = odeint(calc_derivative, 1, time_vec,
...                      args=(counter,), full_output=True)
```

Thus the derivative function has been called more than 40 times:

```
>>> counter
array([129], dtype=uint16)
```

and the cumulative iterations number for the 10 first convergences can be obtained by:

```
>>> info['nfe'][:10]
array([31, 35, 43, 49, 53, 57, 59, 63, 65, 69], dtype=int32)
```

The solver requires more iterations at start. The final trajectory is seen on the Matplotlib figure:

```
"""Solve the ODE dy/dt = -2y between t = 0..4, with the
initial condition y(t=0) = 1.

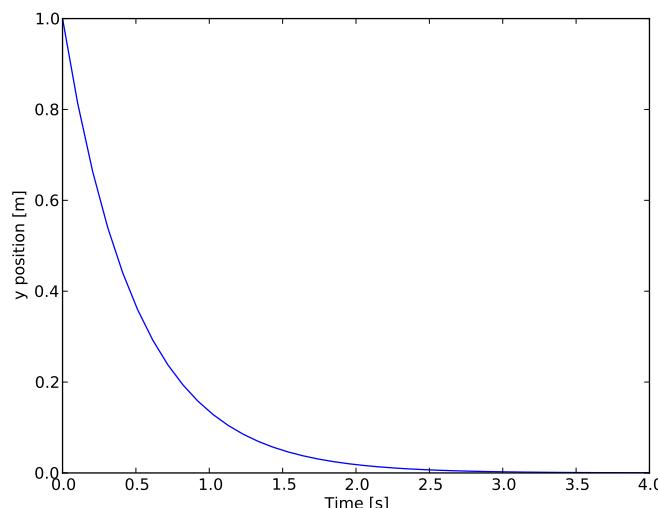
"""

import numpy as np
from scipy.integrate import odeint
import pylab as pl

def calc_derivative(ypos, time):
    return -2*ypos

time_vec = np.linspace(0, 4, 40)
yvec = odeint(calc_derivative, 1, time_vec)

pl.plot(time_vec, yvec)
pl.xlabel('Time [s]')
pl.ylabel('y position [m]')
```



Another example with `odeint` will be a damped spring-mass oscillator (2nd order oscillator). The position of a mass attached to a spring obeys the 2nd order ODE $y'' + 2 \epsilon \omega_0 y' + \omega_0^2 y = 0$ with $\omega_0^2 = k/m$ being k the spring constant, m the mass and $\epsilon = c/(2 m \omega_0)$ with c the damping coefficient. For a computing example, the parameters will be:

```
>>> mass = 0.5 # kg
>>> kspring = 4 # N/m
>>> cviscous = 0.4 # N s/m
```

so the system will be underdamped because:

```
>>> eps = cviscous / (2 * mass * np.sqrt(kspring/mass))
>>> eps < 1
True
```

For the `odeint` solver the 2nd order equation needs to be transformed in a system of two first-order equations for the vector $\mathbf{Y} = (y, y')$. It will be convenient to define $\nu = 2 \epsilon \omega_0$, $w_0 = c / m$ and $\omega_m = \omega_0^2 = k/m$:

```
>>> nu_coef = cviscous/mass
>>> om_coef = kspring/mass
```

Thus the function will calculate the velocity and acceleration by:

```
>>> def calc_der(yvec, time, nuc, omc):
...     return (yvec[1], -nuc * yvec[1] - omc * yvec[0])
...
>>> time_vec = np.linspace(0, 10, 100)
>>> yarr = odeint(calc_der, (1, 0), time_vec, args=(nu_coef, om_coef))
```

The final position and velocity are shown on the following Matplotlib figure:

```
"""Damped spring-mass oscillator
"""

import numpy as np
```

```
from scipy.integrate import odeint
import pylab as pl

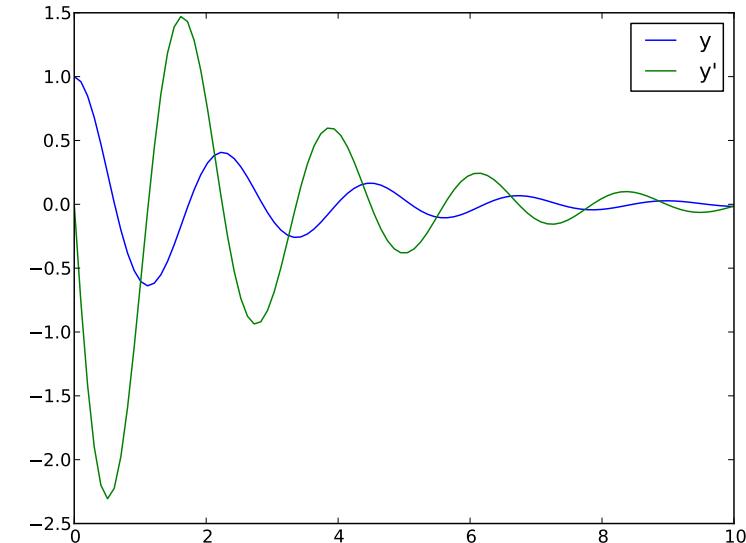
mass = 0.5
kspring = 4
cviscous = 0.4

nu_coef = cviscous / mass
om_coef = kspring / mass

def calc_der(yvec, time, nuc, omc):
    return (yvec[1], -nuc * yvec[1] - omc * yvec[0])

time_vec = np.linspace(0, 10, 100)
yarr = odeint(calc_der, (1, 0), time_vec, args=(nu_coef, om_coef))

pl.plot(time_vec, yarr[:, 0], label='y')
pl.plot(time_vec, yarr[:, 1], label="y'")
pl.legend()
```



There is no Partial Differential Equations (PDE) solver in `scipy`. Some PDE packages are written in Python, such as `fipy` or `SfePy`.

9.8 Fast Fourier transforms: `scipy.fftpack`

The `fftpack` module allows to compute fast Fourier transforms. As an illustration, an input signal may look like:

```
>>> time_step = 0.1
>>> period = 5.
```

```
>>> time_vec = np.arange(0, 20, time_step)
>>> sig = np.sin(2 * np.pi / period * time_vec) + \
...     np.cos(10 * np.pi * time_vec)
```

However the observer does not know the signal frequency, only the sampling time step of the signal `sig`. But the signal is supposed to come from a real function so the Fourier transform will be symmetric. The `fftfreq` function will generate the sampling frequencies and `fft` will compute the fast Fourier transform:

```
>>> from scipy import fftpack
>>> sample_freq = fftpack.fftfreq(sig.size, d=time_step)
>>> sig_fft = fftpack.fft(sig)
```

Nevertheless only the positive part will be used for finding the frequency because the resulting power is symmetric:

```
>>> pidxs = np.where(sample_freq > 0)
>>> freqs = sample_freq[pidxs]
>>> power = np.abs(sig_fft)[pidxs]
```

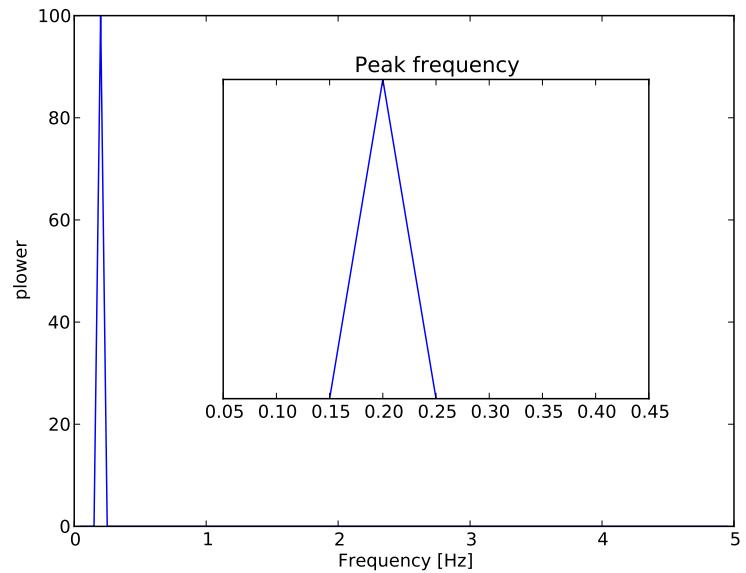
```
import numpy as np
from scipy import fftpack
import pylab as pl

time_step = 0.1
period = 5.

time_vec = np.arange(0, 20, time_step)
sig = np.sin(2 * np.pi / period * time_vec) + np.cos(10 * np.pi * time_vec)

sample_freq = fftpack.fftfreq(sig.size, d=time_step)
sig_fft = fftpack.fft(sig)
pidxs = np.where(sample_freq > 0)
freqs, power = sample_freq[pidxs], np.abs(sig_fft)[pidxs]
freq = freqs[power.argmax()]

pl.figure()
pl.plot(freqs, power)
pl.ylabel('power')
pl.xlabel('Frequency [Hz]')
axes = pl.axes([0.3, 0.3, 0.5, 0.5])
pl.title('Peak frequency')
pl.plot(freqs[:8], power[:8])
pl.setp(axes, yticks=[])
```



Thus the signal frequency can be found by:

```
>>> freq = freqs[power.argmax()]
>>> np.allclose(freq, 1./period)
True
```

Now only the main signal component will be extracted from the Fourier transform:

```
>>> sig_fft[np.abs(sample_freq) > freq] = 0
```

The resulting signal can be computed by the `ifft` function:

```
>>> main_sig = fftpack.ifft(sig_fft)
```

The result is shown on the Matplotlib figure:

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

time_step = 0.1
period = 5.

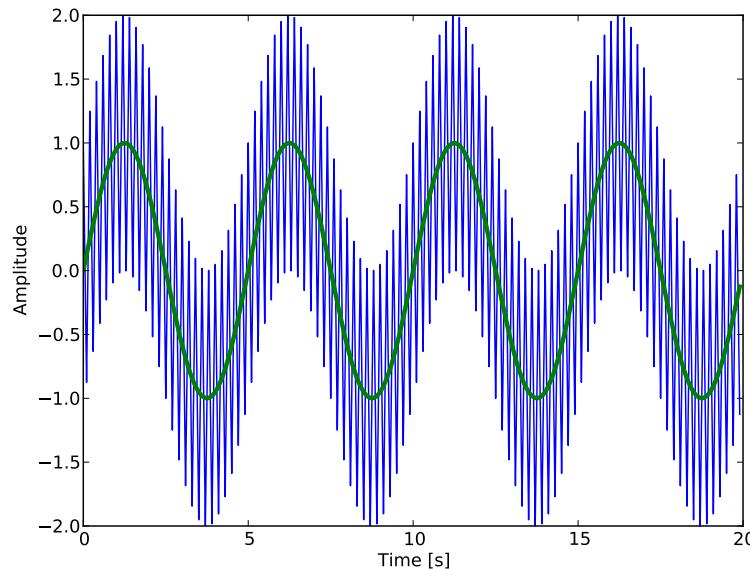
time_vec = np.arange(0, 20, time_step)
sig = np.sin(2 * np.pi / period * time_vec) + np.cos(10 * np.pi * time_vec)

sample_freq = fftpack.fftfreq(sig.size, d=time_step)
sig_fft = fftpack.fft(sig)
pidxs = np.where(sample_freq > 0)
freqs, power = sample_freq[pidxs], np.abs(sig_fft)[pidxs]
freq = freqs[power.argmax()]

sig_fft[np.abs(sample_freq) > freq] = 0
```

```
main_sig = fftpack.ifft(sig_fft)

pl.figure()
pl.plot(time_vec, sig)
pl.plot(time_vec, main_sig, linewidth=3)
pl.ylabel('Amplitude')
pl.xlabel('Time [s]')
```



9.9 Interpolation: `scipy.interpolate`

The `scipy.interpolate` is useful for fitting a function from experimental data and thus evaluating points where no measure exists. The module is based on the [FITPACK Fortran subroutines](#) from the [netlib](#) project.

By imagining experimental data close to a sinus function:

```
>>> measured_time = np.linspace(0, 1, 10)
>>> noise = (np.random.random(10)*2 - 1) * 1e-1
>>> measures = np.sin(2 * np.pi * measured_time) + noise
```

The `interp1d` class can built a linear interpolation function:

```
>>> from scipy.interpolate import interp1d
>>> linear_interp = interp1d(measured_time, measures)
```

Then the `linear_interp` instance needs to be evaluated on time of interest:

```
>>> computed_time = np.linspace(0, 1, 50)
>>> linear_results = linear_interp(computed_time)
```

A cubic interpolation can also be selected by providing the `kind` optional keyword argument:

```
>>> cubic_interp = interp1d(measured_time, measures, kind='cubic')
>>> cubic_results = cubic_interp(computed_time)
```

The results are now gathered on the following Matplotlib figure:

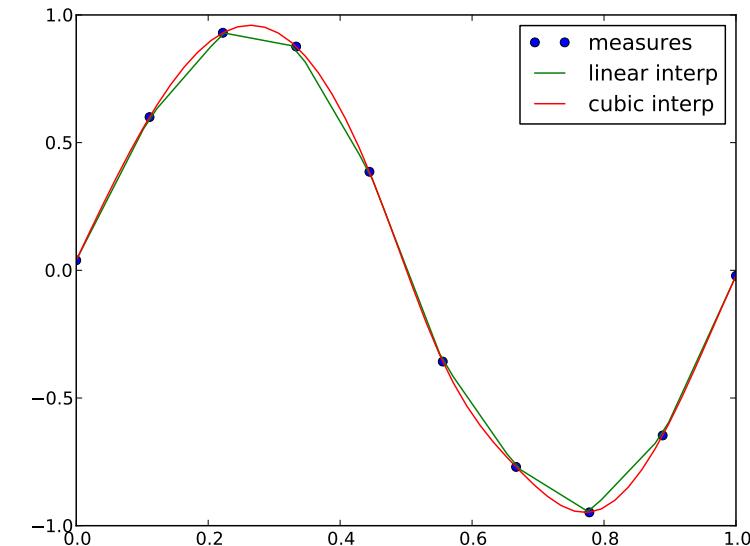
```
"""Generate the interpolation.png image for the interpolate
section of the Scipy tutorial
"""

import numpy as np
from scipy.interpolate import interp1d
import pylab as pl

measured_time = np.linspace(0, 1, 10)
noise = (np.random.random(10)*2 - 1) * 1e-1
measures = np.sin(2 * np.pi * measured_time) + noise

linear_interp = interp1d(measured_time, measures)
computed_time = np.linspace(0, 1, 50)
linear_results = linear_interp(computed_time)
cubic_interp = interp1d(measured_time, measures, kind='cubic')
cubic_results = cubic_interp(computed_time)

pl.plot(measured_time, measures, 'o', ms=6, label='measures')
pl.plot(computed_time, linear_results, label='linear interp')
pl.plot(computed_time, cubic_results, label='cubic interp')
pl.legend()
```



`scipy.interpolate.interp2d` is similar to `interp1d`, but for 2-D arrays. Note that for the `interp` family, the computed time must stay within the measured time range. See the summary exercise on [Maximum wind speed prediction at the Sprogø station](#) (page 135) for a more advance spline interpolation example.

9.10 Optimization and fit: `scipy.optimize`

Optimization is the problem of finding a numerical solution to a minimization or equality.

The `scipy.optimize` module provides useful algorithms for function minimization (scalar or multi-dimensional), curve fitting and root finding.

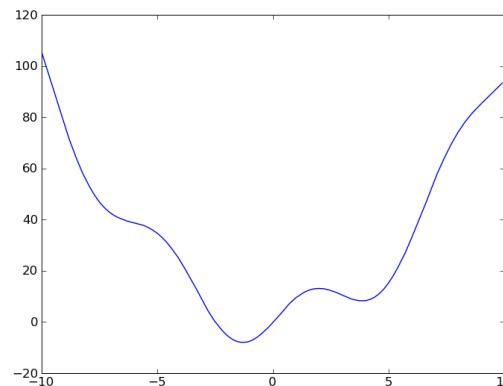
Example: Minimizing a scalar function using different algorithms

Let's define the following function:

```
>>> def f(x):
...     return x**2 + 10*np.sin(x)
```

and plot it:

```
>>> x = np.arange(-10,10,0.1)
>>> plt.plot(x, f(x))
>>> plt.show()
```



This function has a global minimum around -1.3 and a local minimum around 3.8.

9.10.1 Local (convex) optimization

The general and efficient way to find a minimum for this function is to conduct a gradient descent starting from a given initial point. The BFGS algorithm is a good way of doing this:

```
>>> optimize.fmin_bfgs(f, 0)
Optimization terminated successfully.
    Current function value: -7.945823
    Iterations: 5
    Function evaluations: 24
    Gradient evaluations: 8
array([-1.30644003])
```

This resolution takes 4.11ms on our computer.

The problem with this approach is that, if the function has local minima (is not convex), the algorithm may find these local minima instead of the global minimum depending on the initial point. If we don't know the neighborhood of the global minima to choose the initial point, we need to resort to costlier global optimization.

9.10.2 Global optimization

To find the global minimum, the simplest algorithm is the brute force algorithm, in which the function is evaluated on each point of a given grid:

```
>>> from scipy import optimize
>>> grid = (-10, 10, 0.1)
>>> optimize.brute(f, (grid,))
array([-1.30641113])
```

This approach take 20 ms on our computer.

This simple algorithm becomes very slow as the size of the grid grows, so you should use `optimize.brent` instead for scalar functions:

```
>>> optimize.brent(f)
-1.3064400120612139
```

To find the local minimum, let's add some constraints on the variable using `optimize.fminbound`:

```
>>> # search the minimum only between 0 and 10
>>> optimize.fminbound(f, 0, 10)
array([ 3.83746712])
```

You can find algorithms with the same functionalities for multi-dimensional problems in `scipy.optimize`.

See the summary exercise on [Non linear least squares curve fitting: application to point extraction in topographical lidar data](#) (page 140) for a more advanced example.

9.11 Image processing: `scipy.ndimage`

The submodule dedicated to image processing in `scipy` is `scipy.ndimage`.

```
>>> from scipy import ndimage
```

Image processing routines may be sorted according to the category of processing they perform.

9.11.1 Geometrical transformations on images

Changing orientation, resolution, ..

```
>>> import scipy
>>> lena = scipylena()
>>> shifted_lena = ndimage.shift(lena, (50, 50))
>>> shifted_lena2 = ndimage.shift(lena, (50, 50), mode='nearest')
>>> rotated_lena = ndimage.rotate(lena, 30)
>>> cropped_lena = lena[50:-50, 50:-50]
>>> zoomed_lena = ndimage.zoom(lena, 2)
>>> zoomed_lena.shape
(1024, 1024)
```



```
In [35]: subplot(151)
Out[35]: <matplotlib.axes.AxesSubplot object at 0x925f46c>

In [36]: imshow(shifted_lena, cmap=cm.gray)
Out[36]: <matplotlib.image.AxesImage object at 0x9593f6c>

In [37]: axis('off')
Out[37]: (-0.5, 511.5, 511.5, -0.5)

In [39]: # etc.
```

9.11.2 Image filtering

```
>>> lena = scipylena()
>>> import numpy as np
>>> noisy_lena = np.copy(lena)
>>> noisy_lena += lena.std()*0.5*np.random.standard_normal(lena.shape)
>>> blurred_lena = ndimage.gaussian_filter(noisy_lena, sigma=3)
>>> median_lena = ndimage.median_filter(blurred_lena, size=5)
>>> import scipy.signal
>>> wiener_lena = scipy.signal.wiener(blurred_lena, (5,5))
```



And many other filters in `scipy.ndimage.filters` and `scipy.signal` can be applied to images

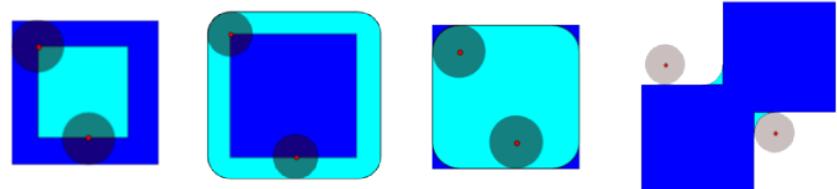
Exercise

Compare histograms for the different filtered images.

9.11.3 Mathematical morphology

Mathematical morphology is a mathematical theory that stems from set theory. It characterizes and transforms geometrical structures. Binary (black and white) images, in particular, can be transformed using this theory: the sets to be transformed are the sets of neighboring non-zero-valued pixels. The theory was also extended to gray-valued images.

Erosion Dilation Opening Closing



Elementary mathematical-morphology operations use a *structuring element* in order to modify other geometrical structures.

Let us first generate a structuring element

```
>>> el = ndimage.generate_binary_structure(2, 1)
>>> el
array([[False,  True, False],
       [ True,  True,  True],
       [False,  True, False]], dtype=bool)
>>> el.astype(np.int)
array([[0, 1, 0],
       [1, 1, 1],
       [0, 1, 0]])
```

- Erosion

```
>>> a = np.zeros((7,7), dtype=np.int)
>>> a[1:6, 2:5] = 1
>>> a
array([[0, 0, 0, 0, 0, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 0, 0, 0, 0, 0]])
>>> ndimage.binary_erosion(a.astype(a.dtype))
array([[0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0]])
>>> #Erosion removes objects smaller than the structure
>>> ndimage.binary_erosion(a, structure=np.ones((5,5))).astype(a.dtype)
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, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0]])
```

- Dilation

```
>>> a = np.zeros((5, 5))
>>> a[2, 2] = 1
>>> a
array([[0., 0., 0., 0., 0.],
```

```
[ 0.,  0.,  0.,  0.,  0.],
[ 0.,  0.,  1.,  0.,  0.],
[ 0.,  0.,  0.,  0.,  0.],
[ 0.,  0.,  0.,  0.,  0.])
>>> ndimage.binary_dilation(a).astype(a.dtype)
array([[ 0.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  1.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.],
       [ 0.,  1.,  1.,  1.,  0.],
       [ 0.,  0.,  1.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.]])
```

- **Opening**

```
>>> a = np.zeros((5,5), dtype=np.int)
>>> a[1:4, 1:4] = 1; a[4, 4] = 1
>>> a
array([[ 0,  0,  0,  0,  0],
       [ 0,  1,  1,  1,  0],
       [ 0,  1,  1,  1,  0],
       [ 0,  1,  1,  1,  0],
       [ 0,  0,  0,  0,  1]])
>>> # Opening removes small objects
>>> ndimage.binary_opening(a, structure=np.ones((3,3))).astype(np.int)
array([[ 0,  0,  0,  0,  0],
       [ 0,  1,  1,  1,  0],
       [ 0,  1,  1,  1,  0],
       [ 0,  1,  1,  1,  0],
       [ 0,  0,  0,  0,  0]])
>>> # Opening can also smooth corners
>>> ndimage.binary_opening(a).astype(np.int)
array([[ 0,  0,  0,  0,  0],
       [ 0,  0,  1,  0,  0],
       [ 0,  1,  1,  1,  0],
       [ 0,  0,  1,  0,  0],
       [ 0,  0,  0,  0,  0]])
```

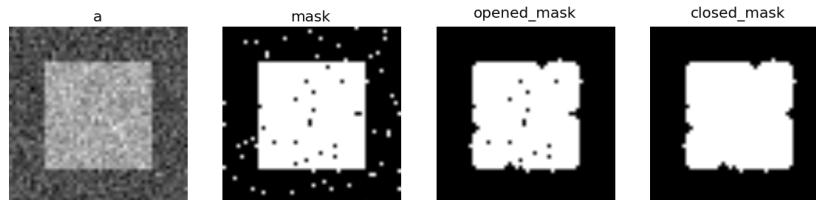
- **Closing:** `ndimage.binary_closing`

Exercise

Check that opening amounts to eroding, then dilating.

An opening operation removes small structures, while a closing operation fills small holes. Such operation can therefore be used to “clean” an image.

```
>>> a = np.zeros((50, 50))
>>> a[10:-10, 10:-10] = 1
>>> a += 0.25*np.random.standard_normal(a.shape)
>>> mask = a>=0.5
>>> opened_mask = ndimage.binary_opening(mask)
>>> closed_mask = ndimage.binary_closing(opened_mask)
```


Exercise

Check that the area of the reconstructed square is smaller than the area of the initial square. (The opposite would occur if the closing step was performed *before* the opening).

For **gray-valued** images, eroding (resp. dilating) amounts to replacing a pixel by the minimal (resp. maximal) value among pixels covered by the structuring element centered on the pixel of interest.

```
>>> a = np.zeros((7,7), dtype=np.int)
>>> a[1:6, 1:6] = 3
>>> a[4,4] = 2; a[2,3] = 1
>>> a
array([[ 0,  0,  0,  0,  0,  0,  0],
       [ 0,  3,  3,  3,  3,  3,  0],
       [ 0,  3,  3,  1,  3,  3,  0],
       [ 0,  3,  3,  3,  3,  3,  0],
       [ 0,  3,  3,  3,  2,  3,  0],
       [ 0,  3,  3,  3,  3,  3,  0],
       [ 0,  0,  0,  0,  0,  0,  0]])
>>> ndimage.grey_erosion(a, size=(3,3))
array([[ 0,  0,  0,  0,  0,  0,  0],
       [ 0,  0,  0,  0,  0,  0,  0],
       [ 0,  0,  1,  1,  1,  0,  0],
       [ 0,  0,  1,  1,  1,  0,  0],
       [ 0,  0,  3,  2,  2,  0,  0],
       [ 0,  0,  0,  0,  0,  0,  0],
       [ 0,  0,  0,  0,  0,  0,  0]])
```

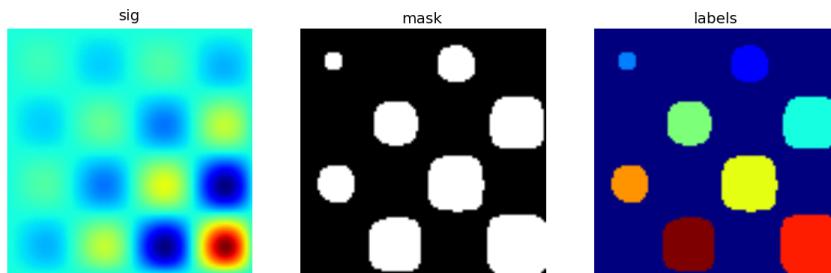
9.11.4 Measurements on images

Let us first generate a nice synthetic binary image.

```
>>> x, y = np.indices((100, 100))
>>> sig = np.sin(2*np.pi*x/50.)*np.sin(2*np.pi*y/50.)*(1+x*y/50.*x*x)
>>> mask = sig > 1
```

Now we look for various information about the objects in the image:

```
>>> labels, nb = ndimage.label(mask)
>>> nb
8
>>> areas = ndimage.sum(mask, labels, xrange(1, labels.max()+1))
>>> areas
[190.0, 45.0, 424.0, 278.0, 459.0, 190.0, 549.0, 424.0]
>>> maxima = ndimage.maximum(sig, labels, xrange(1, labels.max()+1))
>>> maxima
[1.8023823799830032, 1.1352760475048373, 5.5195407887291426,
 2.4961181804217221, 6.7167361922608864, 1.8023823799830032,
 16.765472169131161, 5.5195407887291426]
>>> ndimage.find_objects(labels==4)
[(slice(30, 48, None), slice(30, 48, None))]
>>> sl = ndimage.find_objects(labels==4)
>>> imshow(sig[sl[0]])
```



See the summary exercise on *Image processing application: counting bubbles and unmolten grains* (page 144) for a more advanced example.

9.12 Summary exercises on scientific computing

The summary exercises use mainly Numpy, Scipy and Matplotlib. They first aim at providing real life examples on scientific computing with Python. Once the groundwork is introduced, the interested user is invited to try some exercises.

9.12.1 Maximum wind speed prediction at the Sprogø station

The exercise goal is to predict the maximum wind speed occurring every 50 years even if no measure exists for such a period. The available data are only measured over 21 years at the Sprogø meteorological station located in Denmark. First, the statistical steps will be given and then illustrated with functions from the `scipy.interpolate` module. At the end the interested readers are invited to compute results from raw data and in a slightly different approach.

Statistical approach

The annual maxima are supposed to fit a normal probability density function. However such function is not going to be estimated because it gives a probability from a wind speed maxima. Finding the maximum wind speed occurring every 50 years requires the opposite approach, the result needs to be found from a defined probability. That is the quantile function role and the exercise goal will be to find it. In the current model, it is supposed that the maximum wind speed occurring every 50 years is defined as the upper 2% quantile.

By definition, the quantile function is the inverse of the cumulative distribution function. The latter describes the probability distribution of an annual maxima. In the exercise, the cumulative probability p_i for a given year i is defined as $p_i = i/(N+1)$ with $N = 21$, the number of measured years. Thus it will be possible to calculate the cumulative probability of every measured wind speed maxima. From those experimental points, the `scipy.interpolate` module will be very useful for fitting the quantile function. Finally the 50 years maxima is going to be evaluated from the cumulative probability of the 2% quantile.

Computing the cumulative probabilities

The annual wind speeds maxima have already been computed and saved in the numpy format in the file `max-speeds.npy`, thus they will be loaded by using numpy:

```
>>> import numpy as np
>>> max_speeds = np.load('data/max-speeds.npy')
>>> years_nb = max_speeds.shape[0]
```

Following the cumulative probability definition p_i from the previous section, the corresponding values will be:

```
>>> cprob = (np.arange(years_nb, dtype=np.float32) + 1) / (years_nb + 1)
```

and they are assumed to fit the given wind speeds:

```
>>> sorted_max_speeds = np.sort(max_speeds)
```

Prediction with UnivariateSpline

In this section the quantile function will be estimated by using the `UnivariateSpline` class which can represent a spline from points. The default behavior is to build a spline of degree 3 and points can have different weights according to their reliability. Variants are `InterpolatedUnivariateSpline` and `LSQUnivariateSpline` on which errors checking is going to change. In case a 2D spline is wanted, the `BivariateSpline` class family is provided. All those classes for 1D and 2D splines use the FITPACK Fortran subroutines, that's why a lower library access is available through the `splrep` and `splev` functions for respectively representing and evaluating a spline. Moreover interpolation functions without the use of FITPACK parameters are also provided for simpler use (see `interp1d`, `interp2d`, `barycentric_interpolate` and so on).

For the Sprogø maxima wind speeds, the `UnivariateSpline` will be used because a spline of degree 3 seems to correctly fit the data:

```
>>> from scipy.interpolate import UnivariateSpline
>>> quantile_func = UnivariateSpline(cprob, sorted_max_speeds)
```

The quantile function is now going to be evaluated from the full range of probabilities:

```
>>> nprob = np.linspace(0, 1, 1e2)
>>> fitted_max_speeds = quantile_func(nprob)
```

2%

In the current model, the maximum wind speed occurring every 50 years is defined as the upper 2% quantile. As a result, the cumulative probability value will be:

```
>>> fifty_prob = 1. - 0.02
```

So the storm wind speed occurring every 50 years can be guessed by:

```
>>> fifty_wind = quantile_func(fifty_prob)
>>> fifty_wind
array([ 32.9798925])
```

The results are now gathered on a Matplotlib figure:

```
"""Generate the image cumulative-wind-speed-prediction.png
for the interpolate section of scipy.rst.

"""

import numpy as np
from scipy.interpolate import UnivariateSpline
import pylab as pl

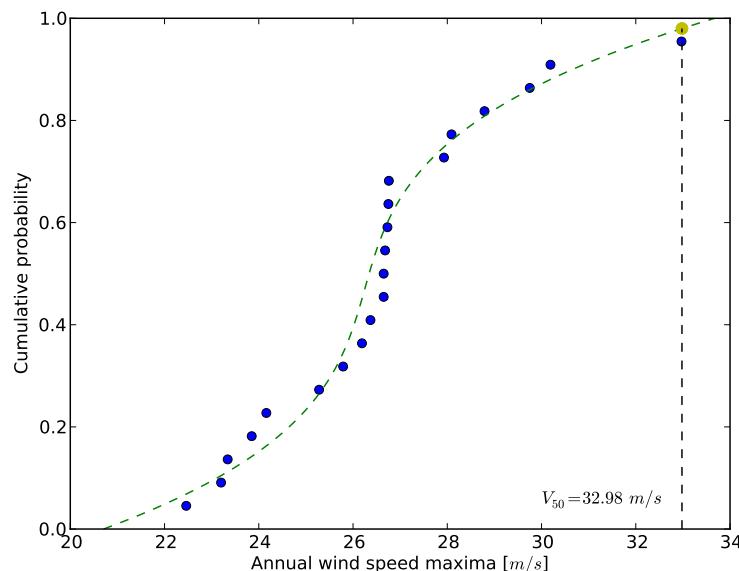
# since its called from intro/summary-exercises
# we need to ...
max_speeds = np.load('../data/max-speeds.npy')
years_nb = max_speeds.shape[0]

cprob = (np.arange(years_nb, dtype=np.float32) + 1) / (years_nb + 1)
sorted_max_speeds = np.sort(max_speeds)
speed_spline = UnivariateSpline(cprob, sorted_max_speeds)
nprob = np.linspace(0, 1, 1e2)
```

```
fitted_max_speeds = speed_spline(nprob)

fifty_prob = 1. - 0.02
fifty_wind = speed_spline(fifty_prob)

pl.figure()
pl.plot(sorted_max_speeds, cprob, 'o')
pl.plot(fitted_max_speeds, nprob, 'g--')
pl.plot([fifty_wind], [fifty_prob], 'o', ms=8., mfc='y', mec='y')
pl.text(30, 0.05, 'V50 = 32.98 m/s')
pl.plot([fifty_wind, fifty_wind], [pl.axis()[2], fifty_prob], 'k--')
pl.xlabel('Annual wind speed maxima [m/s]')
pl.ylabel('Cumulative probability')
```



Exercise with the Gumbell distribution

The interested readers are now invited to make an exercise by using the wind speeds measured over 21 years. The measurement period is around 90 minutes (the original period was around 10 minutes but the file size has been reduced for making the exercise setup easier). The data are stored in numpy format inside the file sprop-windspeeds.npy. Do not look at the source code for the plots until you have completed the exercise.

- The first step will be to find the annual maxima by using numpy and plot them as a matplotlib bar figure.

```
"""Generate the exercise results on the Gumbell distribution
"""

import numpy as np
from scipy.interpolate import UnivariateSpline
import pylab as pl

def gumbell_dist(arr):
```

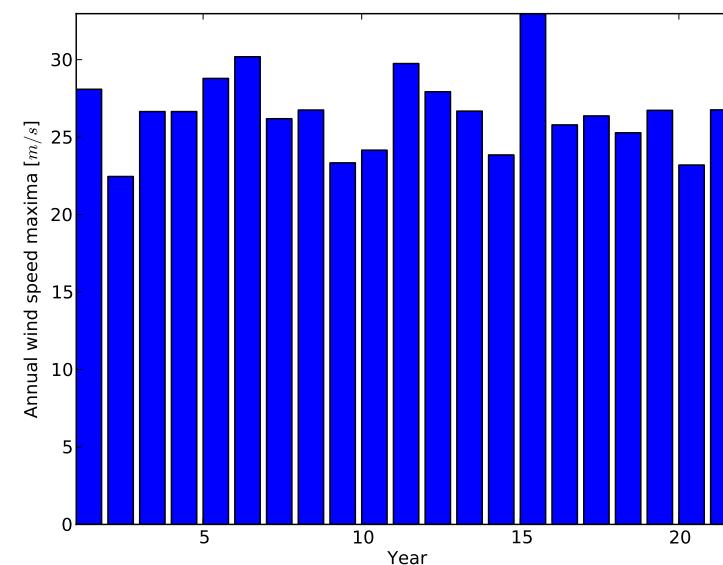
```
    return -np.log(-np.log(arr))

years_nb = 21
wspeeds = np.load('../data/sprop-windspeeds.npy')
max_speeds = np.array([arr.max() for arr in np.array_split(wspeeds, years_nb)])
sorted_max_speeds = np.sort(max_speeds)

cprob = (np.arange(years_nb, dtype=np.float32) + 1)/(years_nb + 1)
gprob = gumbell_dist(cprob)
speed_spline = UnivariateSpline(gprob, sorted_max_speeds, k=1)
nprob = gumbell_dist(np.linspace(1e-3, 1-1e-3, 1e2))
fitted_max_speeds = speed_spline(nprob)

fifty_prob = gumbell_dist(49./50.)
fifty_wind = speed_spline(fifty_prob)

pl.figure()
pl.bar(np.arange(years_nb) + 1, max_speeds)
pl.axis('tight')
pl.xlabel('Year')
pl.ylabel('Annual wind speed maxima [$m/s$]')
```



- The second step will be to use the Gumbell distribution on cumulative probabilities p_i defined as $-\log(-\log(p_i))$ for fitting a linear quantile function (remember that you can define the degree of the UnivariateSpline). Plotting the annual maxima versus the Gumbell distribution should give you the following figure.

```
"""Generate the exercise results on the Gumbell distribution
"""

import numpy as np
from scipy.interpolate import UnivariateSpline
import pylab as pl
```

```

def gumbell_dist(arr):
    return -np.log(-np.log(arr))

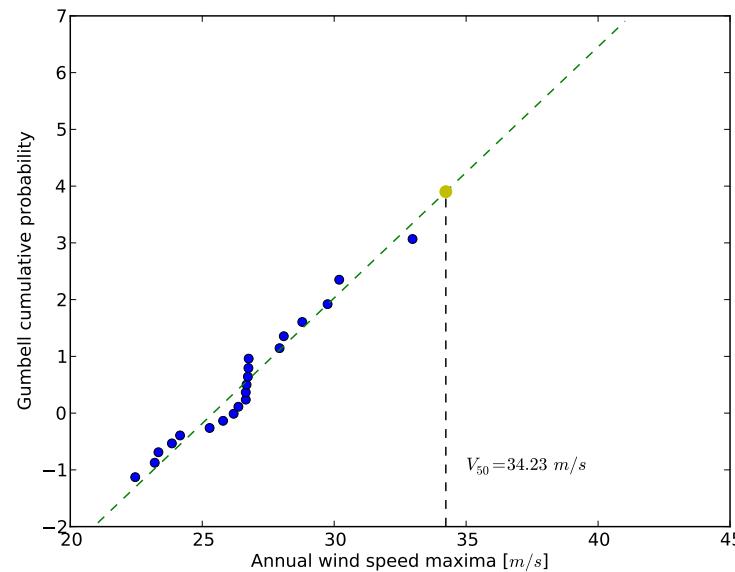
years_nb = 21
wspeeds = np.load('../data/sprop-windspeeds.npy')
max_speeds = np.array([arr.max() for arr in np.array_split(wspeeds, years_nb)])
sorted_max_speeds = np.sort(max_speeds)

cprob = (np.arange(years_nb, dtype=np.float32) + 1)/(years_nb + 1)
gprob = gumbell_dist(cprob)
speed_spline = UnivariateSpline(gprob, sorted_max_speeds, k=1)
nprob = gumbell_dist(np.linspace(1e-3, 1e-3, 1e2))
fitted_max_speeds = speed_spline(nprob)

fifty_prob = gumbell_dist(49./50.)
fifty_wind = speed_spline(fifty_prob)

pl.figure()
pl.plot(sorted_max_speeds, gprob, 'o')
pl.plot(fitted_max_speeds, nprob, 'g--')
pl.plot([fifty_wind], [fifty_prob], 'o', ms=8., mfc='y', mec='y')
pl.plot([fifty_wind, fifty_wind], [pl.axis()[2], fifty_prob], 'k--')
pl.text(35, -1, r'$V_{50} = %.2f \text{ m/s}' % fifty_wind)
pl.xlabel('Annual wind speed maxima [m/s]')
pl.ylabel('Gumbell cumulative probability')

```



- The last step will be to find 34.23 m/s for the maximum wind speed occurring every 50 years.

9.12.2 Non linear least squares curve fitting: application to point extraction in topographical lidar data

The goal of this exercise is to fit a model to some data. The data used in this tutorial are lidar data and are described in details in the following introductory paragraph. If you're impatient and want to practice now, please skip it and go directly to [Loading and visualization](#) (page 140).

Introduction

Lidars systems are optical rangefinders that analyze property of scattered light to measure distances. Most of them emit a short light impulsion towards a target and record the reflected signal. This signal is then processed to extract the distance between the lidar system and the target.

Topographical lidar systems are such systems embedded in airborne platforms. They measure distances between the platform and the Earth, so as to deliver information on the Earth's topography (see [\[Mallet09\]](#) (page 289) for more details).

In this tutorial, the goal is to analyze the waveform recorded by the lidar system¹. Such a signal contains peaks whose center and amplitude permit to compute the position and some characteristics of the hit target. When the footprint of the laser beam is around 1m on the Earth surface, the beam can hit multiple targets during the two-way propagation (for example the ground and the top of a tree or building). The sum of the contributions of each target hit by the laser beam then produces a complex signal with multiple peaks, each one containing information about one target.

One state of the art method to extract information from these data is to decompose them in a sum of Gaussian functions where each function represents the contribution of a target hit by the laser beam.

Therefore, we use the `scipy.optimize` module to fit a waveform to one or a sum of Gaussian functions.

Loading and visualization

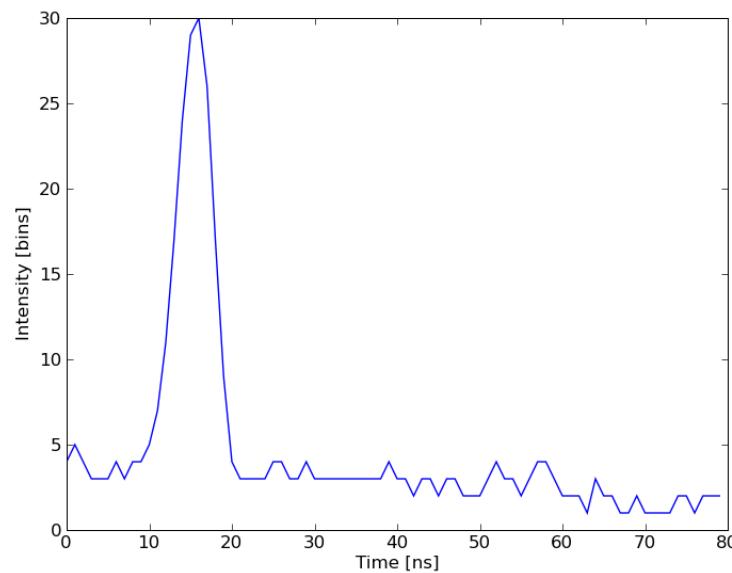
Load the first waveform using:

```
>>> import numpy as np
>>> waveform_1 = np.load('data/waveform_1.npy')
```

and visualize it:

```
>>> import matplotlib.pyplot as plt
>>> t = np.arange(len(waveform_1))
>>> plt.plot(t, waveform_1)
>>> plt.show()
```

¹ The data used for this tutorial are part of the demonstration data available for the FullAnalyze software and were kindly provided by the GIS DRAIX.



As you can notice, this waveform is a 80-bin-length signal with a single peak.

Fitting a waveform with a simple Gaussian model

The signal is very simple and can be modeled as a single Gaussian function and an offset corresponding to the background noise. To fit the signal with the function, we must:

- define the model
- propose an initial solution
- call `scipy.optimize.leastsq`

Model

A Gaussian function defined by

$$B + A \exp \left\{ - \left(\frac{t - \mu}{\sigma} \right)^2 \right\}$$

can be defined in python by:

```
>>> def model(t, coeffs):
...     return coeffs[0] + coeffs[1] * np.exp( - ((t-coeffs[2])/coeffs[3])**2 )
```

where

- `coeffs[0]` is B (noise)

- `coeffs[1]` is A (amplitude)
- `coeffs[2]` is μ (center)
- `coeffs[3]` is σ (width)

Initial solution

An approximative initial solution that we can find from looking at the graph is for instance:

```
>>> x0 = np.array([3, 30, 15, 1], dtype=float)
```

Fit

`scipy.optimize.leastsq` minimizes the sum of squares of the function given as an argument. Basically, the function to minimize is the residuals (the difference between the data and the model):

```
>>> def residuals(coeffs, y, t):
...     return y - model(t, coeffs)
```

So let's get our solution by calling `scipy.optimize.leastsq` with the following arguments:

- the function to minimize
- an initial solution
- the additional arguments to pass to the function

```
>>> from scipy.optimize import leastsq
>>> x, flag = leastsq(residuals, x0, args=(waveform_1, t))
>>> print x
[ 2.70363341  27.82020742  15.47924562  3.05636228]
```

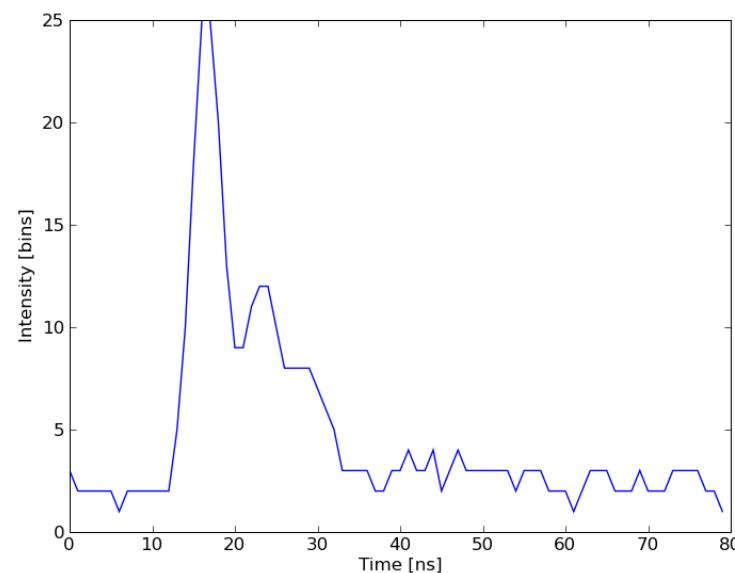
And visualize the solution:

```
>>> plt.plot(t, waveform_1, t, model(t, x))
>>> plt.legend(['waveform', 'model'])
>>> plt.show()
```

Remark: from `scipy` v0.8 and above, you should rather use `scipy.optimize.curve_fit` which takes the model and the data as arguments, so you don't need to define the residuals any more.

Going further

- Try with a more complex waveform (for instance `data/waveform_2.npy`) that contains three significant peaks. You must adapt the model which is now a sum of Gaussian functions instead of only one Gaussian peak.



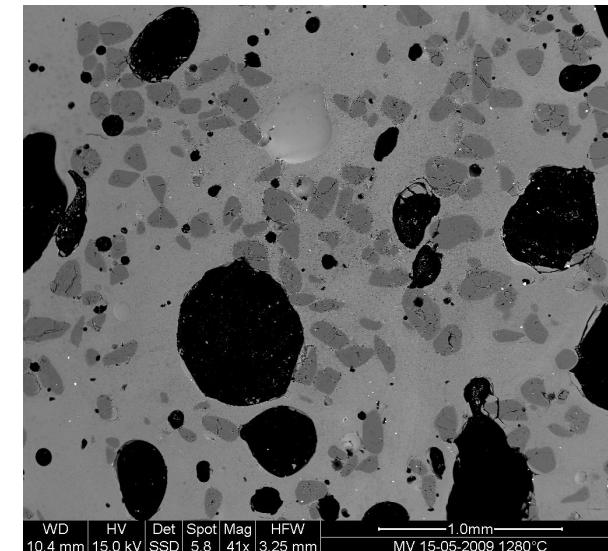
- In some cases, writing an explicit function to compute the Jacobian is faster than letting `leastsq` estimate it numerically. Create a function to compute the Jacobian of the residuals and use it as an input for `leastsq`.
- When we want to detect very small peaks in the signal, or when the initial guess is too far from a good solution, the result given by the algorithm is often not satisfying. Adding constraints to the parameters of the model enables to overcome such limitations. An example of *a priori* knowledge we can add is the sign of our variables (which are all positive).

With the following initial solution:

```
>>> x0 = np.array([3, 50, 20, 1], dtype=float)
```

compare the result of `scipy.optimize.leastsq` and what you can get with `scipy.optimize.fmin_slsqp` when adding boundary constraints.

9.12.3 Image processing application: counting bubbles and unmolten grains

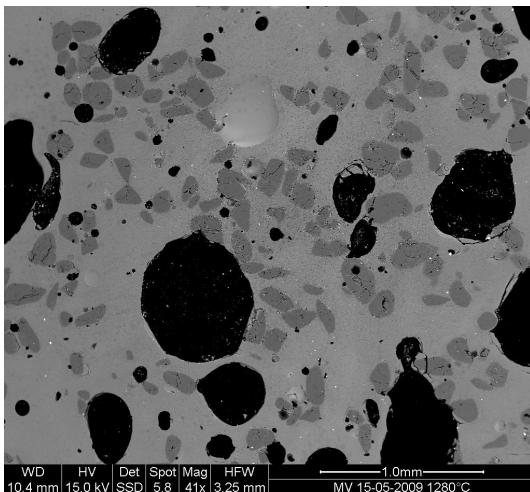


Statement of the problem

1. Open the image file MV_HFV_012.jpg and display it. Browse through the keyword arguments in the docstring of `imshow` to display the image with the "right" orientation (origin in the bottom left corner, and not the upper left corner as for standard arrays).

This Scanning Element Microscopy image shows a glass sample (light gray matrix) with some bubbles (on black) and unmolten sand grains (dark gray). We wish to determine the fraction of the sample covered by these three phases, and to estimate the typical size of sand grains and bubbles, their sizes, etc.

2. Crop the image to remove the lower panel with measure information.
3. Slightly filter the image with a median filter in order to refine its histogram. Check how the histogram changes.
4. Using the histogram of the filtered image, determine thresholds that allow to define masks for sand pixels, glass pixels and bubble pixels. Other option (homework): write a function that determines automatically the thresholds from the minima of the histogram.
5. Display an image in which the three phases are colored with three different colors.
6. Use mathematical morphology to clean the different phases.
7. Attribute labels to all bubbles and sand grains, and remove from the sand mask grains that are smaller than 10 pixels. To do so, use `ndimage.sum` or `np.bincount` to compute the grain sizes.
8. Compute the mean size of bubbles.

Proposed solution**9.12.4 Example of solution for the image processing exercise: unmolten grains in glass**

1. Open the image file MV_HFV_012.jpg and display it. Browse through the keyword arguments in the docstring of imshow to display the image with the “right” orientation (origin in the bottom left corner, and not the upper left corner as for standard arrays).

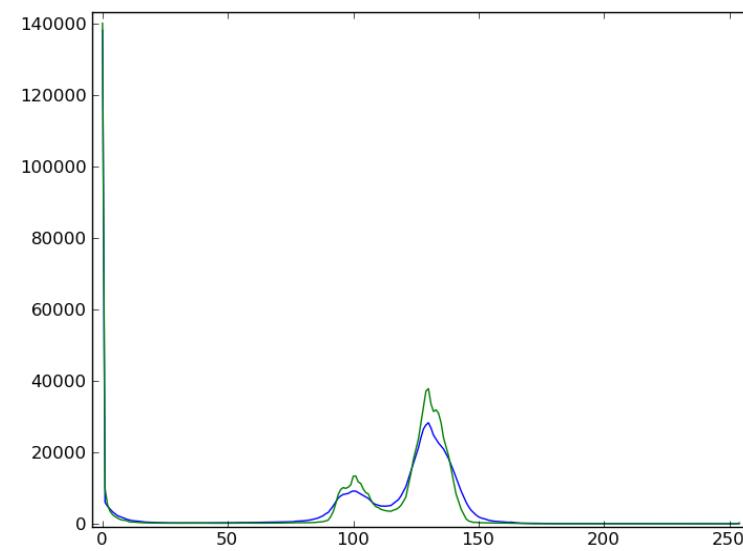
```
>>> dat = imread('MV_HFV_012.jpg')
```

2. Crop the image to remove the lower panel with measure information.

```
>>> dat = dat[60:]
```

3. Slightly filter the image with a median filter in order to refine its histogram. Check how the histogram changes.

```
>>> filtdat = ndimage.median_filter(dat, size=(7,7))
>>> hi_dat = np.histogram(dat, bins=np.arange(256))
>>> hi_filtdat = np.histogram(filtdat, bins=np.arange(256))
```

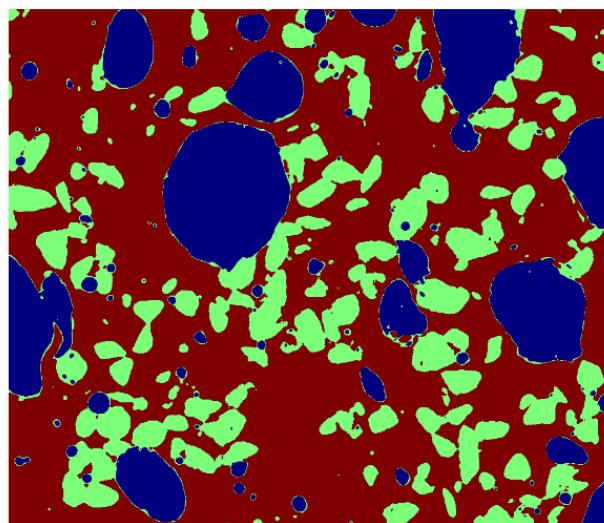


4. Using the histogram of the filtered image, determine thresholds that allow to define masks for sand pixels, glass pixels and bubble pixels. Other option (homework): write a function that determines automatically the thresholds from the minima of the histogram.

```
>>> void = filtdat <= 50
>>> sand = np.logical_and(filtdat>50, filtdat<=114)
>>> glass = filtdat > 114
```

5. Display an image in which the three phases are colored with three different colors.

```
>>> phases = void.astype(np.int) + 2*glass.astype(np.int) + \
            3*sand.astype(np.int)
```



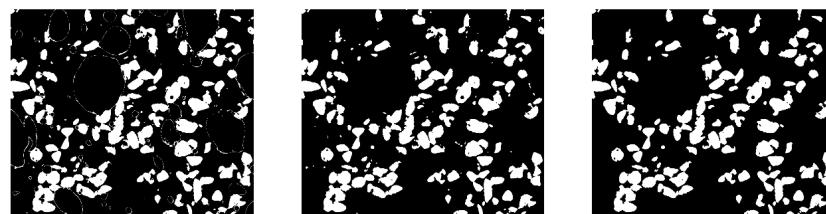
```
>>> mean_bubble_size, median_bubble_size
(1699.875, 65.0)
```

6. Use mathematical morphology to clean the different phases.

```
>>> sand_op = ndimage.binary_opening(sand, iterations=2)
```

7. Attribute labels to all bubbles and sand grains, and remove from the sand mask grains that are smaller than 10 pixels. To do so, use `ndimage.sum` or `np.bincount` to compute the grain sizes.

```
>>> sand_labels, sand_nb = ndimage.label(sand_op)
>>> sand_areas = np.array(ndimage.sum(sand_op, sand_labels,
...     np.arange(sand_labels.max()+1)))
>>> mask = sand_areas>100
>>> remove_small_sand = mask[sand_labels.ravel()].reshape(sand_labels.shape)
```



8. Compute the mean size of bubbles.

```
>>> bubbles_labels, bubbles_nb = ndimage.label(void)
>>> bubbles_areas = np.bincount(bubbles_labels.ravel())[1:]
>>> mean_bubble_size = bubbles_areas.mean()
>>> median_bubble_size = np.median(bubbles_areas)
```

Part IV

Advanced topics

Advanced Python Constructs

author Zbigniew Jędrzejewski-Szmek

This chapter is about some features of the Python language which can be considered advanced — in the sense that not every language has them, and also in the sense that they are more useful in more complicated programs or libraries, but not in the sense of being particularly specialized, or particularly complicated.

It is important to underline that this chapter is purely about the language itself — about features supported through special syntax complemented by functionality of the Python stdlib, which could not be implemented through clever external modules.

The process of developing the Python programming language, its syntax, is unique because it is very transparent, proposed changes are evaluated from various angles and discussed on public mailing lists, and the final decision takes into account the balance between the importance of envisioned use cases, the burden of carrying more language features, consistency with the rest of the syntax, and whether the proposed variant is the easiest to read, write, and understand. This process is formalised in Python Enhancement Proposals — [PEPs](#). As a result, features described in this chapter were added after it was shown that they indeed solve real problems and that their use is as simple as possible.

Chapters contents

- Iterators, generator expressions and generators (page 151)
 - Iterators (page 151)
 - Generator expressions (page 152)
 - Generators (page 152)
 - Bidirectional communication (page 153)
 - Chaining generators (page 155)
- Decorators (page 155)
 - Replacing or tweaking the original object (page 156)
 - Decorators implemented as classes and as functions (page 156)
 - Copying the docstring and other attributes of the original function (page 158)
 - Examples in the standard library (page 159)
 - Deprecation of functions (page 161)
 - A while-loop removing decorator (page 161)
 - A plugin registration system (page 162)
 - More examples and reading (page 163)
- Context managers (page 163)
 - Catching exceptions (page 164)
 - Using generators to define context managers (page 165)

10.1 Iterators, generator expressions and generators

10.1.1 Iterators

Simplicity

Duplication of effort is wasteful, and replacing the various home-grown approaches with a standard feature usually ends up making things more readable, and interoperable as well.

Guido van Rossum — Adding Optional Static Typing to Python

An iterator is an object adhering to the iterator protocol — basically this means that it has a `next` method, which, when called, returns the next item in the sequence, and when there's nothing to return, raises the `StopIteration` exception.

An iterator object allows to loop just once. It holds the state (position) of a single iteration, or from the other side, each loop over a sequence requires a single iterator object. This means that we can iterate over the same sequence more than once concurrently. Separating the iteration logic from the sequence allows us to have more than one way of iteration.

Calling the `__iter__` method on a container to create an iterator object is the most straightforward way to get hold of an iterator. The `iter` function does that for us, saving a few keystrokes.

```
>>> nums = [1,2,3]      # note that ... varies: these are different objects
>>> iter(nums)
<listiterator object at ...>
>>> nums.__iter__()
<listiterator object at ...>
>>> nums.__reversed__()
<listreverseiterator object at ...>
```

```
>>> it = iter(nums)
>>> next(it)          # next(obj) simply calls obj.next()
1
>>> it.next()
2
>>> next(it)
3
>>> next(it)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
StopIteration
```

When used in a loop, `StopIteration` is swallowed and causes the loop to finish. But with explicit invocation, we can see that once the iterator is exhausted, accessing it raises an exception.

Using the `for..in` loop also uses the `__iter__` method. This allows us to transparently start the iteration over a sequence. But if we already have the iterator, we want to be able to use it in an `for` loop in the same way. In order to achieve this, iterators in addition to `next` are also required to have a method called `__iter__` which returns the iterator (`self`).

Support for iteration is pervasive in Python: all sequences and unordered containers in the standard library allow this. The concept is also stretched to other things: e.g. `file` objects support iteration over lines.

```
>>> f = open('/etc/fstab')
>>> f is f.__iter__()
True
```

The `file` is an iterator itself and its `__iter__` method doesn't create a separate object: only a single thread of sequential access is allowed.

10.1.2 Generator expressions

A second way in which iterator objects are created is through **generator expressions**, the basis for **list comprehensions**. To increase clarity, a generator expression must always be enclosed in parentheses or an expression. If round parentheses are used, then a generator iterator is created. If rectangular parentheses are used, the process is short-circuited and we get a list.

```
>>> (i for i in nums)
<generator object <genexpr> at 0x...>
>>> [i for i in nums]
[1, 2, 3]
>>> list(i for i in nums)
[1, 2, 3]
```

In Python 2.7 and 3.x the list comprehension syntax was extended to **dictionary and set comprehensions**. A set is created when the generator expression is enclosed in curly braces. A dict is created when the generator expression contains "pairs" of the form `key:value`:

```
>>> {i for i in range(3)}
set([0, 1, 2])
>>> {i:i**2 for i in range(3)}
{0: 0, 1: 1, 2: 4}
```

If you are stuck at some previous Python version, the syntax is only a bit worse:

```
>>> set(i for i in 'abc')
set(['a', 'c', 'b'])
>>> dict((i, ord(i)) for i in 'abc')
{'a': 97, 'c': 99, 'b': 98}
```

Generator expression are fairly simple, not much to say here. Only one *gotcha* should be mentioned: in old Pythons the index variable (`i`) would leak, and in versions ≥ 3 this is fixed.

10.1.3 Generators

Generators

A generator is a function that produces a sequence of results instead of a single value.

David Beazley — A Curious Course on Coroutines and Concurrency

A third way to create iterator objects is to call a generator function. A **generator** is a function containing the keyword `yield`. It must be noted that the mere presence of this keyword completely changes the nature of the function: this `yield` statement doesn't have to be invoked, or even reachable, but causes the function to be marked as a generator. When a normal function is called, the instructions contained in the body start to be executed. When a generator is called, the execution stops before the first instruction in the body. An invocation of a generator function creates a generator object, adhering to the iterator protocol. As with normal function invocations, concurrent and recursive invocations are allowed.

When `next` is called, the function is executed until the first `yield`. Each encountered `yield` statement gives a value becomes the return value of `next`. After executing the `yield` statement, the execution of this function is suspended.

```
>>> def f():
...     yield 1
...     yield 2
>>> f()
<generator object f at 0x...>
>>> gen = f()
>>> gen.next()
1
```

```
>>> gen.next()
2
>>> gen.next()
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
StopIteration
```

Let's go over the life of the single invocation of the generator function.

```
>>> def f():
...     print("-- start --")
...     yield 3
...     print("-- middle --")
...     yield 4
...     print("-- finished --")
>>> gen = f()
>>> next(gen)
-- start --
3
>>> next(gen)
-- middle --
4
>>> next(gen)
-- finished --
Traceback (most recent call last):
...
StopIteration
```

Contrary to a normal function, where executing `f()` would immediately cause the first `print` to be executed, `gen` is assigned without executing any statements in the function body. Only when `gen.next()` is invoked by `next`, the statements up to the first `yield` are executed. The second `next` prints `-- middle --` and execution halts on the second `yield`. The third `next` prints `-- finished --` and falls off the end of the function. Since no `yield` was reached, an exception is raised.

What happens with the function after a `yield`, when the control passes to the caller? The state of each generator is stored in the generator object. From the point of view of the generator function, it looks almost as if it was running in a separate thread, but this is just an illusion: execution is strictly single-threaded, but the interpreter keeps and restores the state in between the requests for the `next` value.

Why are generators useful? As noted in the parts about iterators, a generator function is just a different way to create an iterator object. Everything that can be done with `yield` statements, could also be done with `next` methods. Nevertheless, using a function and having the interpreter perform its magic to create an iterator has advantages. A function can be much shorter than the definition of a class with the required `next` and `__iter__` methods. What is more important, it is easier for the author of the generator to understand the state which is kept in local variables, as opposed to instance attributes, which have to be used to pass data between consecutive invocations of `next` on an iterator object.

A broader question is why are iterators useful? When an iterator is used to power a loop, the loop becomes very simple. The code to initialise the state, to decide if the loop is finished, and to find the next value is extracted into a separate place. This highlights the body of the loop — the interesting part. In addition, it is possible to reuse the iterator code in other places.

10.1.4 Bidirectional communication

Each `yield` statement causes a value to be passed to the caller. This is the reason for the introduction of generators by [PEP 255](#) (implemented in Python 2.2). But communication in the reverse direction is also useful. One obvious way would be some external state, either a global variable or a shared mutable object. Direct communication is possible thanks to [PEP 342](#) (implemented in 2.5). It is achieved by turning the previously boring `yield` statement into an expression. When the generator resumes execution after a `yield` statement, the caller can call a method on the generator object to either pass a value `into` the generator, which then is returned by the `yield` statement, or a different method to inject an exception into the generator.

The first of the new methods is `send(value)`, which is similar to `next()`, but passes `value` into the generator to be used for the value of the `yield` expression. In fact, `g.next()` and `g.send(None)` are equivalent.

The second of the new methods is `throw(type, value=None, traceback=None)` which is equivalent to:

```
raise type, value, traceback
```

at the point of the `yield` statement.

Unlike `raise` (which immediately raises an exception from the current execution point), `throw()` first resumes the generator, and only then raises the exception. The word `throw` was picked because it is suggestive of putting the exception in another location, and is associated with exceptions in other languages.

What happens when an exception is raised inside the generator? It can be either raised explicitly or when executing some statements or it can be injected at the point of a `yield` statement by means of the `throw()` method. In either case, such an exception propagates in the standard manner: it can be intercepted by an `except` or `finally` clause, or otherwise it causes the execution of the generator function to be aborted and propagates in the caller.

For completeness' sake, it's worth mentioning that generator iterators also have a `close()` method, which can be used to force a generator that would otherwise be able to provide more values to finish immediately. It allows the generator `__del__` method to destroy objects holding the state of generator.

Let's define a generator which just prints what is passed in through `send` and `throw`.

```
>>> import itertools
>>> def g():
...     print '--start--'
...     for i in itertools.count():
...         print '--yielding {}--'.format(i)
...         try:
...             ans = yield i
...         except GeneratorExit:
...             print '--closing--'
...             raise
...         except Exception as e:
...             print '--yield raised {!r}--'.format(e)
...         else:
...             print '--yield returned {!r}--'.format(ans)
```

```
>>> it = g()
>>> next(it)
--start--
--yielding 0--
0
>>> it.send(11)
--yield returned 11--
--yielding 1--
1
>>> it.throw(IndexError)
--yield raised IndexError()--
--yielding 2--
2
>>> it.close()
--closing--
```

Note: `next` or `__next__`?

In Python 2.x, the iterator method to retrieve the next value is called `next`. It is invoked implicitly through the global function `next`, which means that it should be called `__next__`. Just like the global function `iter` calls `__iter__`. This inconsistency is corrected in Python 3.x, where `it.next` becomes `it.__next__`. For other generator methods — `send` and `throw` — the situation is more complicated, because they are not called implicitly by the interpreter. Nevertheless, there's a proposed syntax extension to allow `continue` to take an argument which will be passed to `send` of the loop's iterator. If this extension is accepted, it's likely that

`gen.send` will become `gen.__send__`. The last of generator methods, `close`, is pretty obviously named incorrectly, because it is already invoked implicitly.

10.1.5 Chaining generators

Note: This is a preview of PEP 380 (not yet implemented, but accepted for Python 3.3).

Let's say we are writing a generator and we want to yield a number of values generated by a second generator, a **subgenerator**. If yielding of values is the only concern, this can be performed without much difficulty using a loop such as

```
subgen = some_other_generator()
for v in subgen:
    yield v
```

However, if the subgenerator is to interact properly with the caller in the case of calls to `send()`, `throw()` and `close()`, things become considerably more difficult. The `yield` statement has to be guarded by a `try..except..finally` structure similar to the one defined in the previous section to "debug" the generator function. Such code is provided in [:pep:380#id13](#), here it suffices to say that new syntax to properly yield from a subgenerator is being introduced in Python 3.3:

```
yield from some_other_generator()
```

This behaves like the explicit loop above, repeatedly yielding values from `some_other_generator` until it is exhausted, but also forwards `send`, `throw` and `close` to the subgenerator.

10.2 Decorators

Summary

This amazing feature appeared in the language almost apologetically and with concern that it might not be that useful.

Bruce Eckel — An Introduction to Python Decorators

Since a function or a class are objects, they can be passed around. Since they are mutable objects, they can be modified. The act of altering a function or class object after it has been constructed but before it is bound to its name is called decorating.

There are two things hiding behind the name "decorator" — one is the function which does the work of decorating, i.e. performs the real work, and the other one is the expression adhering to the decorator syntax, i.e. an at-symbol and the name of the decorating function.

Function can be decorated by using the decorator syntax for functions:

```
@decorator      # ❷
def function(): # ❶
    pass
```

- A function is defined in the standard way. ❶
- An expression starting with @ placed before the function definition is the decorator ❷. The part after @ must be a simple expression, usually this is just the name of a function or class. This part is evaluated first, and after the function defined below is ready, the decorator is called with the newly defined function object as the single argument. The value returned by the decorator is attached to the original name of the function.

Decorators can be applied to functions and to classes. For classes the semantics are identical — the original class definition is used as an argument to call the decorator and whatever is returned is assigned under the original name.

Before the decorator syntax was implemented ([PEP 318](#)), it was possible to achieve the same effect by assigning the function or class object to a temporary variable and then invoking the decorator explicitly and then assigning

the return value to the name of the function. This sounds like more typing, and it is, and also the name of the decorated function doubling as a temporary variable must be used at least three times, which is prone to errors. Nevertheless, the example above is equivalent to:

```
def function():          # ❶
    pass
function = decorator(function) # ❷
```

Decorators can be stacked — the order of application is bottom-to-top, or inside-out. The semantics are such that the originally defined function is used as an argument for the first decorator, whatever is returned by the first decorator is used as an argument for the second decorator, ..., and whatever is returned by the last decorator is attached under the name of the original function.

The decorator syntax was chosen for its readability. Since the decorator is specified before the header of the function, it is obvious that it is not a part of the function body and its clear that it can only operate on the whole function. Because the expression is prefixed with @ it stands out and is hard to miss ("in your face", according to the PEP :)). When more than one decorator is applied, each one is placed on a separate line in an easy to read way.

10.2.1 Replacing or tweaking the original object

Decorators can either return the same function or class object or they can return a completely different object. In the first case, the decorator can exploit the fact that function and class objects are mutable and add attributes, e.g. add a docstring to a class. A decorator might do something useful even without modifying the object, for example register the decorated class in a global registry. In the second case, virtually anything is possible: when a something different is substituted for the original function or class, the new object can be completely different. Nevertheless, such behaviour is not the purpose of decorators: they are intended to tweak the decorated object, not do something unpredictable. Therefore, when a function is "decorated" by replacing it with a different function, the new function usually calls the original function, after doing some preparatory work. Likewise, when a class is "decorated" by replacing it with a new class, the new class is usually derived from the original class. When the purpose of the decorator is to do something "every time", like to log every call to a decorated function, only the second type of decorators can be used. On the other hand, if the first type is sufficient, it is better to use it, because it is simpler.

10.2.2 Decorators implemented as classes and as functions

The only *requirement* on decorators is that they can be called with a single argument. This means that decorators can be implemented as normal functions, or as classes with a `__call__` method, or in theory, even as lambda functions.

Let's compare the function and class approaches. The decorator expression (the part after @) can be either just a name, or a call. The bare-name approach is nice (less to type, looks cleaner, etc.), but is only possible when no arguments are needed to customise the decorator. Decorators written as functions can be used in those two cases:

```
>>> def simple_decorator(function):
...     print "doing decoration"
...     return function
>>> @simple_decorator
... def function():
...     print "inside function"
doing decoration
>>> function()
inside function
```

```
>>> def decorator_with_arguments(arg):
...     print "defining the decorator"
...     def _decorator(function):
...         # in this inner function, arg is available too
...         print "doing decoration,", arg
...         return function
```

```

...     return _decorator
>>> @decorator_with_arguments("abc")
... def function():
...     print "inside function"
defining the decorator
doing decoration, abc
>>> function()
inside function

```

The two trivial decorators above fall into the category of decorators which return the original function. If they were to return a new function, an extra level of nestedness would be required. In the worst case, three levels of nested functions.

```

>>> def replacing_decorator_with_args(arg):
...     print "defining the decorator"
...     def _decorator(function):
...         # in this inner function, arg is available too
...         print "doing decoration,", arg
...         def _wrapper(*args, **kwargs):
...             print "inside wrapper,", args, kwargs
...             return function(*args, **kwargs)
...         return _wrapper
...     return _decorator
>>> @replacing_decorator_with_args("abc")
... def function(*args, **kwargs):
...     print "inside function,", args, kwargs
...     return 14
defining the decorator
doing decoration, abc
>>> function(11, 12)
inside wrapper, (11, 12) {}
inside function, (11, 12) {}
14

```

The `_wrapper` function is defined to accept all positional and keyword arguments. In general we cannot know what arguments the decorated function is supposed to accept, so the wrapper function just passes everything to the wrapped function. One unfortunate consequence is that the apparent argument list is misleading.

Compared to decorators defined as functions, complex decorators defined as classes are simpler. When an object is created, the `__init__` method is only allowed to return `None`, and the type of the created object cannot be changed. This means that when a decorator is defined as a class, it doesn't make much sense to use the argumentless form: the final decorated object would just be an instance of the decorating class, returned by the constructor call, which is not very useful. Therefore it's enough to discuss class-based decorators where arguments are given in the decorator expression and the decorator `__init__` method is used for decorator construction.

```

>>> class decorator_class(object):
...     def __init__(self, arg):
...         # this method is called in the decorator expression
...         print "in decorator init,", arg
...         self.arg = arg
...     def __call__(self, function):
...         # this method is called to do the job
...         print "in decorator call,", self.arg
...         return function
>>> deco_instance = decorator_class('foo')
in decorator init, foo
>>> @deco_instance
... def function(*args, **kwargs):
...     print "in function,", args, kwargs
in decorator call, foo
>>> function()
in function, () {}

```

Contrary to normal rules ([PEP 8](#)) decorators written as classes behave more like functions and therefore their name often starts with a lowercase letter.

In reality, it doesn't make much sense to create a new class just to have a decorator which returns the original function. Objects are supposed to hold state, and such decorators are more useful when the decorator returns a new object.

```

>>> class replacing_decorator_class(object):
...     def __init__(self, arg):
...         # this method is called in the decorator expression
...         print "in decorator init,", arg
...         self.arg = arg
...     def __call__(self, function):
...         # this method is called to do the job
...         print "in decorator call,", self.arg
...         self.function = function
...         return self._wrapper
...     def _wrapper(self, *args, **kwargs):
...         print "in the wrapper,", args, kwargs
...         return self.function(*args, **kwargs)
>>> deco_instance = replacing_decorator_class('foo')
in decorator init, foo
>>> @deco_instance
... def function(*args, **kwargs):
...     print "in function,", args, kwargs
in decorator call, foo
>>> function(11, 12)
in the wrapper, (11, 12) {}
in function, (11, 12) {}

```

A decorator like this can do pretty much anything, since it can modify the original function object and mangle the arguments, call the original function or not, and afterwards mangle the return value.

10.2.3 Copying the docstring and other attributes of the original function

When a new function is returned by the decorator to replace the original function, an unfortunate consequence is that the original function name, the original docstring, the original argument list are lost. Those attributes of the original function can partially be “transplanted” to the new function by setting `__doc__` (the docstring), `__module__` and `__name__` (the full name of the function), and `__annotations__` (extra information about arguments and the return value of the function available in Python 3). This can be done automatically by using `functools.update_wrapper`.

`functools.update_wrapper(wrapper, wrapped)`

“Update a wrapper function to look like the wrapped function.”

```

>>> import functools
>>> def better_replacing_decorator_with_args(arg):
...     print "defining the decorator"
...     def _decorator(function):
...         print "doing decoration,", arg
...         def _wrapper(*args, **kwargs):
...             print "inside wrapper,", args, kwargs
...             return function(*args, **kwargs)
...         return functools.update_wrapper(_wrapper, function)
...     return _decorator
>>> @better_replacing_decorator_with_args("abc")
... def function():
...     "extensive documentation"
...     print "inside function"

```

```

...
    return 14
defining the decorator
doing decoration, abc
>>> function
<function function at 0x...>
>>> print function.__doc__
extensive documentation

```

One important thing is missing from the list of attributes which can be copied to the replacement function: the argument list. The default values for arguments can be modified through the `__defaults__`, `__kwdefaults__` attributes, but unfortunately the argument list itself cannot be set as an attribute. This means that `help(function)` will display a useless argument list which will be confusing for the user of the function. An effective but ugly way around this problem is to create the wrapper dynamically, using `eval`. This can be automated by using the external `decorator` module. It provides support the `decorator` decorator, which takes a wrapper and turns it into a decorator which preserves the function signature.

To sum things up, decorators should always use `functools.update_wrapper` or some other means of copying function attributes.

10.2.4 Examples in the standard library

First, it should be mentioned that there's a number of useful decorators available in the standard library. There are three decorators which really form a part of the language:

- `classmethod` causes a method to become a “class method”, which means that it can be invoked without creating an instance of the class. When a normal method is invoked, the interpreter inserts the instance object as the first positional parameter, `self`. When a class method is invoked, the class itself is given as the first parameter, often called `cls`.

Class methods are still accessible through the class' namespace, so they don't pollute the module's namespace. Class methods can be used to provide alternative constructors:

```

class Array(object):
    def __init__(self, data):
        self.data = data

    @classmethod
    def fromfile(cls, file):
        data = numpy.load(file)
        return cls(data)

```

This is cleaner then using a multitude of flags to `__init__`.

- `staticmethod` is applied to methods to make them “static”, i.e. basically a normal function, but accessible through the class namespace. This can be useful when the function is only needed inside this class (its name would then be prefixed with `_`), or when we want the user to think of the method as connected to the class, despite an implementation which doesn't require this.
- `property` is the pythonic answer to the problem of getters and setters. A method decorated with `property` becomes a getter which is automatically called on attribute access.

```

>>> class A(object):
...     @property
...     def a(self):
...         "an important attribute"
...         return "a value"
>>> A.a
<property object at 0x...>
>>> A().a
'a value'

```

In this example, `A.a` is an read-only attribute. It is also documented: `help(A)` includes the docstring for attribute `a` taken from the getter method. Defining `a` as a property allows it to be calculated on the fly, and

has the side effect of making it read-only, because no setter is defined.

To have a setter and a getter, two methods are required, obviously. Since Python 2.6 the following syntax is preferred:

```

class Rectangle(object):
    def __init__(self, edge):
        self.edge = edge

    @property
    def area(self):
        """Computed area.

        Setting this updates the edge length to the proper value.
        """
        return self.edge**2

    @area.setter
    def area(self, area):
        self.edge = area ** 0.5

```

The way that this works, is that the `property` decorator replaces the getter method with a property object. This object in turn has three methods, `getter`, `setter`, and `deleter`, which can be used as decorators. Their job is to set the getter, setter and deleter of the property object (stored as attributes `fget`, `fset`, and `fdel`). The getter can be set like in the example above, when creating the object. When defining the setter, we already have the property object under `area`, and we add the setter to it by using the `setter` method. All this happens when we are creating the class.

Afterwards, when an instance of the class has been created, the property object is special. When the interpreter executes attribute access, assignment, or deletion, the job is delegated to the methods of the property object.

To make everything crystal clear, let's define a “debug” example:

```

>>> class D(object):
...     @property
...     def a(self):
...         print "getting", 1
...         return 1
...     @a.setter
...     def a(self, value):
...         print "setting", value
...     @a.deleter
...     def a(self):
...         print "deleting"
>>> D.a
<property object at 0x...>
>>> D.a.fget
<function a at 0x...>
>>> D.a.fset
<function a at 0x...>
>>> D.a.fdel
<function a at 0x...>
>>> d = D()                               # ... varies, this is not the same 'a' function
>>> d.a
getting 1
1
>>> d.a = 2
setting 2
>>> del d.a
deleting
>>> d.a
getting 1
1

```

Properties are a bit of a stretch for the decorator syntax. One of the premises of the decorator syntax — that the name is not duplicated — is violated, but nothing better has been invented so far. It is just good style to use the same name for the getter, setter, and deleter methods.

Some newer examples include:

- `functools.lru_cache` memoizes an arbitrary function maintaining a limited cache of arguments:answer pairs (Python 3.2)
- `functools.total_ordering` is a class decorator which fills in missing ordering methods (`__lt__`, `__gt__`, `__le__`, ...) based on a single available one (Python 2.7).

10.2.5 Deprecation of functions

Let's say we want to print a deprecation warning on `stderr` on the first invocation of a function we don't like anymore. If we don't want to modify the function, we can use a decorator:

```
class deprecated(object):
    """Print a deprecation warning once on first use of the function.

    >>> @deprecated()
    ... def f():
    ...     pass
    >>> f()
    # doctest: +SKIP
    f is deprecated
    """
    def __call__(self, func):
        self.func = func
        self.count = 0
        return self._wrapper
    def _wrapper(self, *args, **kwargs):
        self.count += 1
        if self.count == 1:
            print self.func.__name__, 'is deprecated'
        return self.func(*args, **kwargs)
```

It can also be implemented as a function:

```
def deprecated(func):
    """Print a deprecation warning once on first use of the function.

    >>> @deprecated
    ... def f():
    ...     pass
    >>> f()
    # doctest: +SKIP
    f is deprecated
    """
    count = [0]
    def wrapper(*args, **kwargs):
        count[0] += 1
        if count[0] == 1:
            print func.__name__, 'is deprecated'
        return func(*args, **kwargs)
    return wrapper
```

10.2.6 A while-loop removing decorator

Let's say we have function which returns a lists of things, and this list created by running a loop. If we don't know how many objects will be needed, the standard way to do this is something like:

```
def find_answers():
    answers = []
    while True:
        ans = look_for_next_answer()
        if ans is None:
            break
        answers.append(ans)
    return answers
```

This is fine, as long as the body of the loop is fairly compact. Once it becomes more complicated, as often happens in real code, this becomes pretty unreadable. We could simplify this by using `yield` statements, but then the user would have to explicitly call `list(find_answers())`.

We can define a decorator which constructs the list for us:

```
@vectorized(generator_func):
    def wrapper(*args, **kwargs):
        return list(generator_func(*args, **kwargs))
    return functools.update_wrapper(wrapper, generator_func)
```

Our function then becomes:

```
@vectorized
def find_answers():
    while True:
        ans = look_for_next_answer()
        if ans is None:
            break
        yield ans
```

10.2.7 A plugin registration system

This is a class decorator which doesn't modify the class, but just puts it in a global registry. It falls into the category of decorators returning the original object:

```
class WordProcessor(object):
    PLUGINS = []
    def process(self, text):
        for plugin in self.PLUGINS:
            text = plugin().cleanup(text)
        return text

    @classmethod
    def plugin(cls, plugin):
        cls.PLUGINS.append(plugin)

@WordProcessor.plugin
class CleanMdashesExtension(object):
    def cleanup(self, text):
        return text.replace('&mdash;', u'\N{em dash}')
```

Here we use a decorator to decentralise the registration of plugins. We call our decorator with a noun, instead of a verb, because we use it to declare that our class is a plugin for `WordProcessor`. Method `plugin` simply appends the class to the list of plugins.

A word about the plugin itself: it replaces HTML entity for em-dash with a real Unicode em-dash character. It exploits the unicode literal notation to insert a character by using its name in the unicode database ("EM DASH"). If the Unicode character was inserted directly, it would be impossible to distinguish it from an en-dash in the source of a program.

10.2.8 More examples and reading

- [PEP 318](#) (function and method decorator syntax)
- [PEP 3129](#) (class decorator syntax)
- <http://wiki.python.org/moin/PythonDecoratorLibrary>
- <http://docs.python.org/dev/library/functools.html>
- <http://pypi.python.org/pypi/decorator>
- Bruce Eckel
 - Decorators I: Introduction to Python Decorators
 - Python Decorators II: Decorator Arguments
 - Python Decorators III: A Decorator-Based Build System

10.3 Context managers

A context manager is an object with `__enter__` and `__exit__` methods which can be used in the `with` statement:

```
with manager as var:
    do_something(var)
```

is in the simplest case equivalent to

```
var = manager.__enter__()
try:
    do_something(var)
finally:
    manager.__exit__()
```

In other words, the context manager protocol defined in [PEP 343](#) permits the extraction of the boring part of a `try..except..finally` structure into a separate class leaving only the interesting `do_something` block.

1. The `__enter__` method is called first. It can return a value which will be assigned to `var`. The `as`-part is optional: if it isn't present, the value returned by `__enter__` is simply ignored.
2. The block of code underneath `with` is executed. Just like with `try` clauses, it can either execute successfully to the end, or it can `break`, `continue` or `return`, or it can throw an exception. Either way, after the block is finished, the `__exit__` method is called. If an exception was thrown, the information about the exception is passed to `__exit__`, which is described below in the next subsection. In the normal case, exceptions can be ignored, just like in a `finally` clause, and will be rethrown after `__exit__` is finished.

Let's say we want to make sure that a file is closed immediately after we are done writing to it:

```
>>> class closing(object):
...     def __init__(self, obj):
...         self.obj = obj
...     def __enter__(self):
...         return self.obj
...     def __exit__(self, *args):
...         self.obj.close()
>>> with closing(open('/tmp/file', 'w')) as f:
...     f.write('the contents\n')
```

Here we have made sure that the `f.close()` is called when the `with` block is exited. Since closing files is such a common operation, the support for this is already present in the `file` class. It has an `__exit__` method which calls `close` and can be used as a context manager itself:

```
>>> with open('/tmp/file', 'a') as f:
...     f.write('more contents\n')
```

The common use for `try..finally` is releasing resources. Various different cases are implemented similarly: in the `__enter__` phase the resource is acquired, in the `__exit__` phase it is released, and the exception, if thrown, is propagated. As with files, there's often a natural operation to perform after the object has been used and it is most convenient to have the support built in. With each release, Python provides support in more places:

- all file-like objects:
 - `file` ↪ automatically closed
 - `fileinput`, `tempfile` (py >= 3.2)
 - `bz2.BZ2File`, `gzip.GzipFile`, `tarfile.TarFile`, `zipfile.ZipFile`
 - `ftplib`, `nntplib` ↪ close connection (py >= 3.2 or 3.3)
- locks
 - `multiprocessing.RLock` ↪ lock and unlock
 - `multiprocessing.Semaphore`
 - `memoryview` ↪ automatically release (py >= 3.2 and 2.7)
- `decimal.localcontext` ↪ modify precision of computations temporarily
- `_winreg.PyHKEY` ↪ open and close hive key
- `warnings.catch_warnings` ↪ kill warnings temporarily
- `contextlib.closing` ↪ the same as the example above, call `close`
- parallel programming
 - `concurrent.futures.ThreadPoolExecutor` ↪ invoke in parallel then kill thread pool (py >= 3.2)
 - `concurrent.futures.ProcessPoolExecutor` ↪ invoke in parallel then kill process pool (py >= 3.2)
 - `nogil` ↪ solve the GIL problem temporarily (cython only):()

10.3.1 Catching exceptions

When an exception is thrown in the `with`-block, it is passed as arguments to `__exit__`. Three arguments are used, the same as returned by `sys.exc_info()`: type, value, traceback. When no exception is thrown, `None` is used for all three arguments. The context manager can "swallow" the exception by returning a true value from `__exit__`. Exceptions can be easily ignored, because if `__exit__` doesn't use `return` and just falls of the end, `None` is returned, a false value, and therefore the exception is rethrown after `__exit__` is finished.

The ability to catch exceptions opens interesting possibilities. A classic example comes from unit-tests — we want to make sure that some code throws the right kind of exception:

```
class assert_raises(object):
    # based on pytest and unittest.TestCase
    def __init__(self, type):
        self.type = type
    def __enter__(self):
        pass
    def __exit__(self, type, value, traceback):
        if type is None:
            raise AssertionError('exception expected')
        if issubclass(type, self.type):
            return True # swallow the expected exception
        raise AssertionError('wrong exception type')
```

```
with assert_raises(KeyError):
    {}['foo']
```

10.3.2 Using generators to define context managers

When discussing [generators](#) (page 152), it was said that we prefer generators to iterators implemented as classes because they are shorter, sweeter, and the state is stored as local, not instance, variables. On the other hand, as described in [Bidirectional communication](#) (page 153), the flow of data between the generator and its caller can be bidirectional. This includes exceptions, which can be thrown into the generator. We would like to implement context managers as special generator functions. In fact, the generator protocol was designed to support this use case.

```
@contextlib.contextmanager
def some_generator(<arguments>):
    <setup>
    try:
        yield <value>
    finally:
        <cleanup>
```

The `contextlib.contextmanager` helper takes a generator and turns it into a context manager. The generator has to obey some rules which are enforced by the wrapper function — most importantly it must `yield` exactly once. The part before the `yield` is executed from `__enter__`, the block of code protected by the context manager is executed when the generator is suspended in `yield`, and the rest is executed in `__exit__`. If an exception is thrown, the interpreter hands it to the wrapper through `__exit__` arguments, and the wrapper function then throws it at the point of the `yield` statement. Through the use of generators, the context manager is shorter and simpler.

Let's rewrite the `closing` example as a generator:

```
@contextlib.contextmanager
def closing(obj):
    try:
        yield obj
    finally:
        obj.close()
```

Let's rewrite the `assert_raises` example as a generator:

```
@contextlib.contextmanager
def assert_raises(type):
    try:
        yield
    except type:
        return
    except Exception as value:
        raise AssertionError('wrong exception type')
    else:
        raise AssertionError('exception expected')
```

Here we use a decorator to turn generator functions into context managers!

Advanced Numpy

author Pauli Virtanen

Numpy is at the base of Python's scientific stack of tools. Its purpose is simple: implementing efficient operations on many items in a block of memory. Understanding how it works in detail helps in making efficient use of its flexibility, taking useful shortcuts, and in building new work based on it.

This tutorial aims to cover:

- Anatomy of Numpy arrays, and its consequences. Tips and tricks.
- Universal functions: what, why, and what to do if you want a new one.
- Integration with other tools: Numpy offers several ways to wrap any data in an ndarray, without unnecessary copies.
- Recently added features, and what's in them for me: PEP 3118 buffers, generalized ufuncs, ...

Prerequisites

- Numpy (>= 1.2; preferably newer...)
- Cython (>= 0.12, for the Ufunc example)
- PIL (used in a couple of examples)
- Source codes:
– <http://pav.iki.fi/tmp/advnumpy-ex.zip>

In this section, numpy will be imported as follows:

```
>>> import numpy as np
```

- Life of ndarray (page 167)
 - It's... (page 167)
 - Block of memory (page 168)
 - Data types (page 169)
 - Indexing scheme: strides (page 173)
 - Findings in dissection (page 179)
- Universal functions (page 179)
 - What they are? (page 179)
 - Exercise: building an ufunc from scratch (page 180)
 - Solution: building an ufunc from scratch (page 183)
 - Generalized ufuncs (page 186)
- Interoperability features (page 188)
 - Sharing multidimensional, typed data (page 188)
 - The old buffer protocol (page 188)
 - The old buffer protocol (page 188)
 - Array interface protocol (page 189)
 - The new buffer protocol: PEP 3118 (page 190)
 - PEP 3118 – details (page 191)
- Siblings: `chararray`, `maskedarray`, `matrix` (page 195)
- Summary (page 196)
- Contributing to Numpy/Scipy (page 196)
 - Why (page 196)
 - Reporting bugs (page 196)
 - Contributing to documentation (page 197)
 - Contributing features (page 198)
 - How to help, in general (page 199)

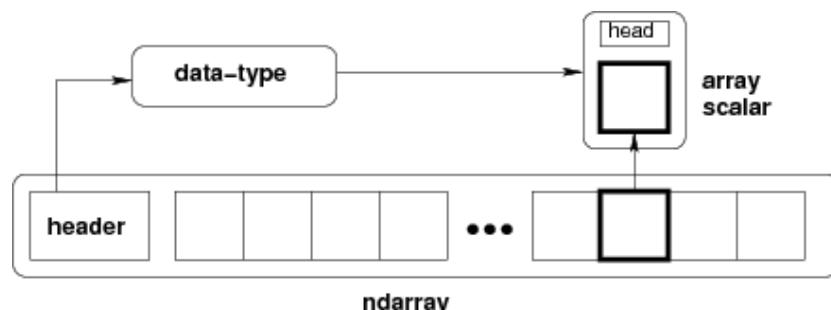
11.1 Life of ndarray

11.1.1 It's...

`ndarray =`

block of memory + indexing scheme + data type descriptor

- raw data
- how to locate an element
- how to interpret an element



```
typedef struct PyArrayObject {
    PyObject_HEAD
```

```
/* Block of memory */
char *data;

/* Data type descriptor */
PyArray_Descr *descr;

/* Indexing scheme */
int nd;
npy_intp *dimensions;
npy_intp *strides;

/* Other stuff */
PyObject *base;
int flags;
PyObject *weakreflist;
} PyArrayObject;
```

11.1.2 Block of memory

```
>>> x = np.array([1, 2, 3, 4], dtype=np.int32)
>>> x.data
<read-write buffer for 0xa37bfd8, size 16, offset 0 at 0xa4eabe0>
>>> str(x.data)
'\x01\x00\x00\x00\x02\x00\x00\x00\x03\x00\x00\x00\x04\x00\x00\x00'
```

Memory address of the data:

```
>>> x.__array_interface__['data'][0]
159755776
```

Reminder: two ndarrays may share the same memory:

```
>>> x = np.array([1,2,3,4])
>>> y = x[:-1]
>>> x[0] = 9
>>> y
array([9, 2, 3])
```

Memory does not need to be owned by an ndarray:

```
>>> x = '1234'
>>> y = np.frombuffer(x, dtype=np.int8)
>>> y.data
<read-only buffer for 0xa588ba8, size 4, offset 0 at 0xa55cd60>
>>> y.base is x
True
```

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

The `owndata` and `writeable` flags indicate status of the memory block.

11.1.3 Data types

The descriptor

`dtype` describes a single item in the array:

type	scalar type of the data, one of: int8, int16, float64, <i>et al.</i> (fixed size) str, unicode, void (flexible size)
itemsize	size of the data block
byteorder	byte order: big-endian > / little-endian < / not applicable
fields	sub-types, if it's a structured data type
shape	shape of the array, if it's a sub-array

```
>>> np.dtype(int).type
<type 'numpy.int32'>
>>> np.dtype(int).itemsize
4
>>> np.dtype(int).byteorder
'='
```

Example: reading .wav files

The .wav file header:

chunk_id	"RIFF"
chunk_size	4-byte unsigned little-endian integer
format	"WAVE"
fmt_id	"fmt "
fmt_size	4-byte unsigned little-endian integer
audio_fmt	2-byte unsigned little-endian integer
num_channels	2-byte unsigned little-endian integer
sample_rate	4-byte unsigned little-endian integer
byte_rate	4-byte unsigned little-endian integer
block_align	2-byte unsigned little-endian integer
bits_per_sample	2-byte unsigned little-endian integer
data_id	"data"
data_size	4-byte unsigned little-endian integer

- 44-byte block of raw data (in the beginning of the file)
- ... followed by `data_size` bytes of actual sound data.

The .wav file header as a Numpy *structured* data type:

```
>>> wav_header_dtype = np.dtype([
    ("chunk_id", (str, 4)),      # flexible-sized scalar type, item size 4
    ("chunk_size", "<u4"),       # little-endian unsigned 32-bit integer
    ("format", "S4"),           # 4-byte string
    ("fmt_id", "S4"),
    ("fmt_size", "<u4"),
    ("audio_fmt", "<u2"),       #
    ("num_channels", "<u2"),    # .. more of the same ...
    ("sample_rate", "<u4"),
    ("byte_rate", "<u4"),
    ("block_align", "<u2"),
    ("bits_per_sample", "<u2"),
    ("data_id", ("S1", (2, 2))), # sub-array, just for fun!
    ("data_size", "u4"),
    #
    # the sound data itself cannot be represented here:
```

```
    # it does not have a fixed size
])
```

See Also:

`wavreader.py`

```
>>> wav_header_dtype['format']
dtype('|S4')
>>> wav_header_dtype.fields
<dictproxy object at 0x85e9704>
>>> wav_header_dtype.fields['format']
(dtype('|S4'), 8)
```

- The first element is the sub-dtype in the structured data, corresponding to the name `format`
- The second one is its offset (in bytes) from the beginning of the item

Note: Mini-exercise, make a "sparse" dtype by using offsets, and only some of the fields:

```
>>> wav_header_dtype = np.dtype(dict(
    names=['format', 'sample_rate', 'data_id'],
    offsets=[offset_1, offset_2, offset_3], # counted from start of structure in bytes
    formats=list of dtypes for each of the fields,
))
```

and use that to read the sample rate, and `data_id` (as sub-array).

```
>>> f = open('test.wav', 'r')
>>> wav_header = np.fromfile(f, dtype=wav_header_dtype, count=1)
>>> f.close()
>>> print(wav_header)
[ ('RIFF', 17402L, 'WAVE', 'fmt ', 16L, 1, 1, 16000L, 32000L, 2, 16,
  ['d', 'a'], ['t', 'a']), 17366L]
>>> wav_header['sample_rate']
array([16000], dtype=uint32)
```

Let's try accessing the sub-array:

```
>>> wav_header['data_id']
array([[[['d', 'a'],
          ['t', 'a']]],
       dtype='|S1')
>>> wav_header.shape
(1,)
>>> wav_header['data_id'].shape
(1, 2, 2)
```

When accessing sub-arrays, the dimensions get added to the end!

Note: There are existing modules such as `wavfile`, `audiolab`, etc. for loading sound data...

Casting and re-interpretation/views

casting

- on assignment
- on array construction
- on arithmetic
- etc.
- and manually: `.astype(dtype)`

data re-interpretation

- manually: `.view(dtype)`

Casting

- Casting in arithmetic, in nutshell:
 - only type (not value!) of operands matters
 - largest “safe” type able to represent both is picked
 - scalars can “lose” to arrays in some situations
- Casting in general copies data

```
>>> x = np.array([1, 2, 3, 4], dtype=np.float)
>>> x
array([ 1.,  2.,  3.,  4.])
>>> y = x.astype(np.int8)
>>> y
array([1, 2, 3, 4], dtype=int8)
>>> y + 1
array([2, 3, 4, 5], dtype=int8)
>>> y + 256
array([1, 2, 3, 4], dtype=int8)
>>> y + 256.0
array([ 257.,  258.,  259.,  260.])
>>> y + np.array([256], dtype=np.int32)
array([258, 259, 260, 261])
```

- Casting on setitem: dtype of the array is not changed on item assignment

```
>>> y[:] = y + 1.5
>>> y
array([2, 3, 4, 5], dtype=int8)
```

Note: Exact rules: see documentation: <http://docs.scipy.org/doc/numpy/reference/ufuncs.html#casting-rules>

Re-interpretation / viewing

- Data block in memory (4 bytes)

0x01		0x02		0x03		0x04
------	--	------	--	------	--	------

- 4 of uint8, OR,
- 4 of int8, OR,
- 2 of int16, OR,
- 1 of int32, OR,
- 1 of float32, OR,
- ...

How to switch from one to another?

- Switch the dtype:

```
>>> x = np.array([1, 2, 3, 4], dtype=np.uint8)
>>> x.dtype = "<i2"
>>> x
array([ 513, 1027], dtype=int16)
>>> 0x0201, 0x0403
(513, 1027)
```

0x01	0x02		0x03	0x04
------	------	--	------	------

Note: little-endian: least significant byte is on the *left* in memory

- Create a new view:

```
>>> y = x.view("<i4")
>>> y
array([67305985])
>>> 0x04030201
67305985
```

0x01	0x02	0x03	0x04
------	------	------	------

Note:

- `.view()` makes *views*, does not copy (or alter) the memory block
- only changes the dtype (and adjusts array shape)

```
>>> x[1] = 5
>>> y
array([328193])
>>> y.base is x
True
```

Mini-exercise: data re-interpretation

See Also:

[view-colors.py](#)

You have RGBA data in an array

```
>>> x = np.zeros((10, 10, 4), dtype=np.int8)
>>> x[:, :, 0] = 1
>>> x[:, :, 1] = 2
>>> x[:, :, 2] = 3
>>> x[:, :, 3] = 4
```

where the last three dimensions are the R, B, and G, and alpha channels.

How to make a (10, 10) structured array with field names ‘r’, ‘g’, ‘b’, ‘a’ without copying data?

```
>>> y = ...
```

```
>>> assert (y['r'] == 1).all()
>>> assert (y['g'] == 2).all()
>>> assert (y['b'] == 3).all()
>>> assert (y['a'] == 4).all()
```

Solution

```
>>> y = x.view([('r', 'i1'),
                ('g', 'i1'),
                ('b', 'i1'),
                ('a', 'i1')])
                )[:, :, 0]
```

Warning: Another array taking exactly 4 bytes of memory:

```
>>> y = np.array([[1, 3], [2, 4]], dtype=np.uint8).transpose()
>>> x = y.copy()
>>> x
array([[1, 2],
       [3, 4]], dtype=uint8)
>>> y
array([[1, 2],
       [3, 4]], dtype=uint8)
>>> x.view(np.int16)
array([[ 513],
       [1027]], dtype=int16)
>>> 0x0201, 0x0403
(513, 1027)
>>> y.view(np.int16)
array([[ 769, 1026]], dtype=int16)
```

- What happened?
- ... we need to look into what `x[0, 1]` actually means

```
>>> 0x0301, 0x0402
(769, 1026)
```

11.1.4 Indexing scheme: strides

Main point

The question

```
>>> x = np.array([[1, 2, 3],
                  [4, 5, 6],
                  [7, 8, 9]], dtype=np.int8)
>>> str(x.data)
'\x01\x02\x03\x04\x05\x06\x07\x08\t'
```

At which byte in `x.data` does the item `x[1, 2]` begin?

The answer (in Numpy)

- **strides:** the number of bytes to jump to find the next element
- 1 stride per dimension

```
>>> x.strides
(3, 1)
>>> byte_offset = 3*1 + 1*2    # to find x[1,2]
>>> x.data[byte_offset]
'\x06'
>>> x[1,2]
6
```

- simple, **flexible**

C and Fortran order

```
>>> x = np.array([[1, 2, 3],
                  [4, 5, 6],
                  [7, 8, 9]], dtype=np.int16, order='C')
```

```
>>> x.strides
(6, 2)
>>> str(x.data)
'\x01\x00\x02\x00\x03\x00\x04\x00\x05\x00\x06\x00\x07\x00\x08\x00\t\x00'
```

- Need to jump 6 bytes to find the next row
- Need to jump 2 bytes to find the next column

```
>>> y = np.array(x, order='F')
>>> y.strides
(2, 6)
>>> str(y.data)
'\x01\x00\x04\x00\x07\x00\x02\x00\x05\x00\x08\x00\x03\x00\x06\x00\t\x00'
```

- Need to jump 2 bytes to find the next row
- Need to jump 6 bytes to find the next column
- Similarly to higher dimensions:
 - C: last dimensions vary fastest (= smaller strides)
 - F: first dimensions vary fastest

$$\text{shape} = (d_1, d_2, \dots, d_n)$$

$$\text{strides} = (s_1, s_2, \dots, s_n)$$

$$s_j^C = d_{j+1}d_{j+2}\dots d_n \times \text{itemsize}$$

$$s_j^F = d_1d_2\dots d_{j-1} \times \text{itemsize}$$

Note: Now we can understand the behavior of `.view()`:

```
>>> y = np.array([[1, 3], [2, 4]], dtype=np.uint8).transpose()
>>> x = y.copy()
```

Transposition does not affect the memory layout of the data, only strides

```
>>> x.strides
(2, 1)
>>> y.strides
(1, 2)
```

```
>>> str(x.data)
'\x01\x02\x03\x04'
>>> str(y.data)
'\x01\x03\x02\x04'
```

- the results are different when interpreted as 2 of int16
- `.copy()` creates new arrays in the C order (by default)

Slicing with integers

- *Everything* can be represented by changing only shape, strides, and possibly adjusting the data pointer!
- Never makes copies of the data

```
>>> x = np.array([1, 2, 3, 4, 5, 6], dtype=np.int32)
>>> y = x[::-1]
>>> y
array([6, 5, 4, 3, 2, 1])
```

```
>>> y.strides
(-4,)

>>> y = x[2:]
>>> y.__array_interface__['data'][0] - x.__array_interface__['data'][0]
8

>>> x = np.zeros((10, 10, 10), dtype=np.float)
>>> x.strides
(800, 80, 8)
>>> x[::-2, ::3, ::4].strides
(1600, 240, 32)
```

Example: fake dimensions with strides**Stride manipulation**

```
>>> from numpy.lib.stride_tricks import as_strided
>>> help(as_strided)
as_strided(x, shape=None, strides=None)
    Make an ndarray from the given array with the given shape and strides
```

Warning: `as_strided` does **not** check that you stay inside the memory block bounds...

```
>>> x = np.array([1, 2, 3, 4], dtype=np.int16)
>>> as_strided(x, strides=(2*2,), shape=(2,))
array([1, 3], dtype=int16)
>>> x[::-2]
array([1, 3], dtype=int16)
```

See Also:

[stride-fakedims.py](#)

Exercise

```
array([1, 2, 3, 4], dtype=np.int8)
-> array([[1, 2, 3, 4],
          [1, 2, 3, 4],
          [1, 2, 3, 4]], dtype=np.int8)
```

using only `as_strided`:

```
Hint: byte_offset = stride[0]*index[0] + stride[1]*index[1] + ...
```

Spoiler

Stride can also be 0:

```
>>> x = np.array([1, 2, 3, 4], dtype=np.int8)
>>> y = as_strided(x, strides=(0, 1), shape=(3, 4))
>>> y
array([[1, 2, 3, 4],
       [1, 2, 3, 4],
       [1, 2, 3, 4]], dtype=int8)
>>> y.base.base is x
True
```

Broadcasting

- Doing something useful with it: outer product of [1, 2, 3, 4] and [5, 6, 7]

```
>>> x = np.array([1, 2, 3, 4], dtype=np.int16)
>>> x2 = as_strided(x, strides=(0, 1*2), shape=(3, 4))
>>> x2
array([[1, 2, 3, 4],
       [1, 2, 3, 4],
       [1, 2, 3, 4]], dtype=int16)
```

```
>>> y = np.array([5, 6, 7], dtype=np.int16)
>>> y2 = as_strided(y, strides=(1*2, 0), shape=(3, 4))
>>> y2
array([[5, 5, 5, 5],
       [6, 6, 6, 6],
       [7, 7, 7, 7]], dtype=int16)
```

```
>>> x2 * y2
array([[ 5, 10, 15, 20],
       [ 6, 12, 18, 24],
       [ 7, 14, 21, 28]], dtype=int16)
```

... seems somehow familiar ...

```
>>> x = np.array([1, 2, 3, 4], dtype=np.int16)
>>> y = np.array([5, 6, 7], dtype=np.int16)
>>> x[np.newaxis, :] * y[:, np.newaxis]
array([[ 5, 10, 15, 20],
       [ 6, 12, 18, 24],
       [ 7, 14, 21, 28]], dtype=int16)
```

- Internally, array **broadcasting** is indeed implemented using 0-strides.

More tricks: diagonals**See Also:**

[stride-diagonals.py](#)

Challenge

Pick diagonal entries of the matrix: (assume C memory order)

```
>>> x = np.array([[1, 2, 3],
                  [4, 5, 6],
                  [7, 8, 9]], dtype=np.int32)
```

```
>>> x_diag = as_strided(x, shape=(3,), strides=(???,))
```

Pick the first super-diagonal entries [2, 6].

And the sub-diagonals?

(**Hint to the last two:** slicing first moves the point where striding starts from.)

Solution

Pick diagonals:

```
>>> x_diag = as_strided(x, shape=(3,), strides=((3+1)*x.itemsize,))
>>> x_diag
array([1, 5, 9])
```

Slice first, to adjust the data pointer:

```
>>> as_strided(x[0,1:], shape=(2,), strides=((3+1)*x.itemsize,))
array([2, 6])

>>> as_strided(x[1:,0], shape=(2,), strides=((3+1)*x.itemsize,))
array([4, 8])
```

Note:

```
>>> y = np.diag(x, k=1)
>>> y
array([2, 6])
```

However,

```
>>> y.flags.owndata
True
```

It makes a copy?! Room for improvement... (bug #xxx)

See Also:

[stride-diagonals.py](#)

Challenge

Compute the tensor trace

```
>>> x = np.arange(5*5*5*5).reshape(5,5,5,5)
>>> s = 0
>>> for i in xrange(5):
>>>     for j in xrange(5):
>>>         s += x[j,i,j,i]
```

by striding, and using sum() on the result.

```
>>> y = as_strided(x, shape=(5, 5), strides=(TODO, TODO))
>>> s2 = ...
>>> assert s == s2
```

Solution

```
>>> y = as_strided(x, shape=(5, 5), strides=((5*5*5+5)*x.itemsize,
                                              (5*5+1)*x.itemsize))
>>> s2 = y.sum()
```

CPU cache effects

Memory layout can affect performance:

```
In [1]: x = np.zeros((20000,))

In [2]: y = np.zeros((20000*67,))[:,67]

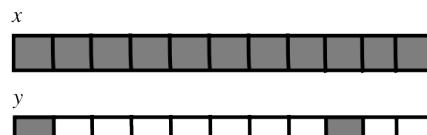
In [3]: x.shape, y.shape
((20000,), (20000,))

In [4]: %timeit x.sum()
100000 loops, best of 3: 0.180 ms per loop

In [5]: %timeit y.sum()
100000 loops, best of 3: 2.34 ms per loop

In [6]: x.strides, y.strides
((8,), (536,))
```

Smaller strides are faster?



cache block size

- CPU pulls data from main memory to its cache in blocks
- If many array items consecutively operated on fit in a single block (small stride):
 - ⇒ fewer transfers needed
 - ⇒ faster

See Also:

[numexpr](#) is designed to mitigate cache effects in array computing.

Example: inplace operations (caveat emptor)

- Sometimes,

```
>>> a -= b
```

is not the same as

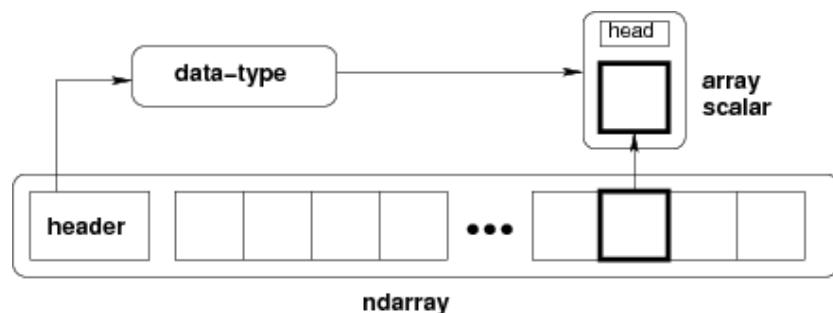
```
>>> a -= b.copy()
```

```
>>> x = np.array([[1, 2], [3, 4]])
>>> x -= x.transpose()
>>> x
array([[ 0, -1],
       [ 4,  0]])
```

```
>>> y = np.array([[1, 2], [3, 4]])
>>> y -= y.T.copy()
>>> y
array([[ 0, -1],
       [ 1,  0]])
```

- `x` and `x.transpose()` share data
- `x -= x.transpose()` modifies the data element-by-element...
- because `x` and `x.transpose()` have different striding, modified data reappears on the RHS

11.1.5 Findings in dissection



- *memory block*: may be shared, `.base`, `.data`
- *data type descriptor*: structured data, sub-arrays, byte order, casting, viewing, `.astype()`, `.view()`
- *strided indexing*: strides, C/F-order, slicing w/ integers, `as_strided`, broadcasting, stride tricks, `diag`, CPU cache coherence

11.2 Universal functions

11.2.1 What they are?

- Ufunc performs and elementwise operation on all elements of an array.

Examples:

```
np.add, np.subtract, scipy.special.*, ...
```

- Automatically support: broadcasting, casting, ...
- The author of an ufunc only has to supply the elementwise operation, Numpy takes care of the rest.
- The elementwise operation needs to be implemented in C (or, e.g., Cython)

Parts of an Ufunc

1. Provided by user

```
void ufunc_loop(void **args, int *dimensions, int *steps, void *data)
{
    /*
     * int8 output = elementwise_function(int8 input_1, int8 input_2)
     *
     * This function must compute the ufunc for many values at once,
     * in the way shown below.
     */
    char *input_1 = (char*)args[0];
    char *input_2 = (char*)args[1];
    char *output = (char*)args[2];
    int i;

    for (i = 0; i < dimensions[0]; ++i) {
        *output = elementwise_function(*input_1, *input_2);
        input_1 += steps[0];
        input_2 += steps[1];
        output += steps[2];
    }
}
```

```
    input_2 += steps[1];
    output += steps[2];
}
}
```

2. The Numpy part, built by

```
char types[3]

types[0] = NPY_BYTE /* type of first input arg */
types[1] = NPY_BYTE /* type of second input arg */
types[2] = NPY_BYTE /* type of third input arg */

PyObject *python_ufunc = PyUFunc_FromFuncAndData(
    ufunc_loop,
    NULL,
    types,
    1, /* ntypes */
    2, /* num_inputs */
    1, /* num_outputs */
    identity_element,
    name,
    docstring,
    unused)
```

- A ufunc can also support multiple different input-output type combinations.

... can be made slightly easier

3. `ufunc_loop` is of very generic form, and Numpy provides pre-made ones

```
PyUfunc_f_f float elementwise_func(float input_1)
PyUfunc_ff_ffloat elementwise_func(float input_1, float input_2)
PyUfunc_d_d double elementwise_func(double input_1)
PyUfunc_dd_ddouble elementwise_func(double input_1, double input_2)
PyUfunc_D_D elementwise_func(npy_cdouble *input, npy_cdouble* output)
PyUfunc_DD_Delementwise_func(npy_cdouble *in1, npy_cdouble *in2,
    npy_cdouble* out)
```

- Only `elementwise_func` needs to be supplied
- ... except when your elementwise function is not in one of the above forms

11.2.2 Exercise: building an ufunc from scratch

The Mandelbrot fractal is defined by the iteration

$$z \leftarrow z^2 + c$$

where $c = x + iy$ is a complex number. This iteration is repeated – if z stays finite no matter how long the iteration runs, c belongs to the Mandelbrot set.

- Make ufunc called `mandel(z0, c)` that computes:

```
z = z0
for k in range(iterations):
    z = z*z + c
```

say, 100 iterations or until $z.\text{real}^{**2} + z.\text{imag}^{**2} > 1000$. Use it to determine which c are in the Mandelbrot set.

- Our function is a simple one, so make use of the `PyUFunc_*` helpers.

- Write it in Cython

See Also:

`mandel.pyx`, `mandelplot.py`

```
#  
# Fix the parts marked by TODO  
#  
  
#  
# Compile this file by (Cython >= 0.12 required because of the complex vars)  
#  
#     cython mandel.pyx  
#     python setup.py build_ext -i  
#  
# and try it out with, in this directory,  
#  
#     >>> import mandel  
#     >>> mandel.mandel(0, 1 + 2j)  
#  
  
# The elementwise function  
# -----  
  
cdef void mandel_single_point(double complex *z_in,  
                               double complex *c_in,  
                               double complex *z_out) nogil:  
    #  
    # The Mandelbrot iteration  
    #  
  
    # Some points of note:  
    #  
    # - It's *NOT* allowed to call any Python functions here.  
    #  
    # The Ufunc loop runs with the Python Global Interpreter Lock released.  
    # Hence, the ``nogil``.  
    #  
    # - And so all local variables must be declared with ``cdef``  
    #  
    # - Note also that this function receives *pointers* to the data  
    #  
  
    cdef double complex z = z_in[0]  
    cdef double complex c = c_in[0]  
    cdef int k # the integer we use in the for loop  
  
    #  
    # TODO: write the Mandelbrot iteration for one point here,  
    #       as you would write it in Python.  
    #  
    #       Say, use 100 as the maximum number of iterations, and 1000  
    #       as the cutoff for z.real**2 + z.imag**2.  
    #  
  
    TODO: mandelbrot iteration should go here  
  
    # Return the answer for this point  
    z_out[0] = z
```

```
# Boilerplate Cython definitions  
#  
# The litany below is particularly long, but you don't really need to  
# read this part; it just pulls in stuff from the Numpy C headers.  
# -----  
  
cdef extern from "numpy/arrayobject.h":  
    void import_array()  
    ctypedef int npy_intp  
    cdef enum NPY_TYPES:  
        NPY_DOUBLE  
        NPY_CDOUBLE  
        NPY_LONG  
  
cdef extern from "numpy/ufuncobject.h":  
    void import_ufunc()  
    ctypedef void (*PyUFuncGenericFunction)(char**, npy_intp*, npy_intp*, void*)  
    object PyUFunc_FromFuncAndData(PyUFuncGenericFunction* func, void** data,  
                                   char* types, int ntypes, int nin, int tout,  
                                   int identity, char* name, char* doc, int c)  
  
    # List of pre-defined loop functions  
  
    void PyUFunc_f_f_As_d_d(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_d_d(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_f_f(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_g_g(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_F_F_As_D_D(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_F_F(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_D_D(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_G_G(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_ff_f_As_dd_d(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_ff_f(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_dd_d(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_gg_g(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_FF_F_As_DD_D(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_DD_D(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_FF_F(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
    void PyUFunc_GG_G(char** args, npy_intp* dimensions, npy_intp* steps, void* func)  
  
    # Required module initialization  
    # -----  
  
    import_array()  
    import_ufunc()  
  
    # The actual ufunc declaration  
    # -----  
  
    cdef PyUFuncGenericFunction loop_func[1]  
    cdef char input_output_types[3]  
    cdef void *elementwise_funcs[1]  
  
    #  
    # Reminder: some pre-made Ufunc loops:  
    #  
    # ===== ===== ===== ===== ===== ===== ===== =====  
    # ``PyUfunc_f_f`` ``float elementwise_func(float input_1)``  
    # ``PyUfunc_ff_f`` ``float elementwise_func(float input_1, float input_2)``  
    # ``PyUfunc_d_d`` ``double elementwise_func(double input_1)``  
    # ``PyUfunc_dd_d`` ``double elementwise_func(double input_1, double input_2)``
```

```

# ``PyUfunc_D_D``  ``elementwise_func(complex_double *input, complex_double* complex_double)``
# ``PyUfunc_DD_D``  ``elementwise_func(complex_double *in1, complex_double *in2, complex_double* out)``
# =====
#
# The full list is above.
#
#
# Type codes:
#
# NPY_BOOL, NPY_BYTE, NPY_UBYTE, NPY_SHORT, NPY USHORT, NPY_INT, NPY_UINT,
# NPY_LONG, NPY ULONG, NPY LONGLONG, NPY ULONGLONG, NPY_FLOAT, NPY_DOUBLE,
# NPY_LONGLONG, NPY_CFLOAT, NPY_CDOUBLE, NPY_CLONGDOUBLE, NPY_DATETIME,
# NPY_TIMEDELTA, NPY_OBJECT, NPY_STRING, NPY_UNICODE, NPY_VOID
#
loop_func[0] = ... TODO: suitable PyUFunc_* ...
input_output_types[0] = ... TODO ...
... TODO: fill in rest of input_output_types ...

# This thing is passed as the ``data`` parameter for the generic
# PyUFunc_* loop, to let it know which function it should call.
elementwise_funcs[0] = <void*>mandel_single_point

# Construct the ufunc:

mandel = PyUFunc_FromFuncAndData(
    loop_func,
    elementwise_funcs,
    input_output_types,
    1, # number of supported input types
    TODO, # number of input args
    TODO, # number of output args
    0, # 'identity' element, never mind this
    "mandel", # function name
    "mandel(z, c) -> computes z*z + c", # docstring
    0 # unused
)

```

Reminder: some pre-made Ufunc loops:

```

PyUfunc_f_ float elementwise_func(float input_1)
PyUfunc_ff_ ffloat elementwise_func(float input_1, float input_2)
PyUfunc_d_ double elementwise_func(double input_1)
PyUfunc_dd_ double elementwise_func(double input_1, double input_2)
PyUfunc_D_D elementwise_func(complex_double *input, complex_double* output)
PyUfunc_DD_D elementwise_func(complex_double *in1, complex_double *in2,
                               complex_double* out)

```

Type codes:

```

NPY_BOOL, NPY_BYTE, NPY_UBYTE, NPY_SHORT, NPY USHORT, NPY_INT, NPY_UINT,
NPY_LONG, NPY ULONG, NPY LONGLONG, NPY ULONGLONG, NPY_FLOAT, NPY_DOUBLE,
NPY_LONGLONG, NPY_CFLOAT, NPY_CDOUBLE, NPY_CLONGDOUBLE, NPY_DATETIME,
NPY_TIMEDELTA, NPY_OBJECT, NPY_STRING, NPY_UNICODE, NPY_VOID

```

11.2.3 Solution: building an ufunc from scratch

```

# The elementwise function
# ----

cdef void mandel_single_point(double complex *z_in,

```

```

double complex *c_in,
double complex *z_out) nogil:
#
# The Mandelbrot iteration
#
#
# Some points of note:
#
# - It's *NOT* allowed to call any Python functions here.
#
# The Ufunc loop runs with the Python Global Interpreter Lock released.
# Hence, the ``nogil``.
#
# - And so all local variables must be declared with ``cdef``
#
# - Note also that this function receives *pointers* to the data;
#   the "traditional" solution to passing complex variables around
#
cdef double complex z = z_in[0]
cdef double complex c = c_in[0]
cdef int k # the integer we use in the for loop

# Straightforward iteration

for k in range(100):
    z = z*z + c
    if z.real**2 + z.imag**2 > 1000:
        break

# Return the answer for this point
z_out[0] = z

# Boilerplate Cython definitions
#
# You don't really need to read this part, it just pulls in
# stuff from the Numpy C headers.
#
# ----

cdef extern from "numpy/arrayobject.h":
    void import_array()
    ctypedef int npy_intp
    cdef enum NPY_TYPES:
        NPY_CDOUBLE

cdef extern from "numpy/ufuncobject.h":
    void import_ufunc()
    ctypedef void (*PyUFuncGenericFunction)(char**, npy_intp*, npy_intp*, void*)
    object PyUFunc_FromFuncAndData(PyUFuncGenericFunction* func, void** data,
                                   char* types, int ntypes, int nin, int nout,
                                   int identity, char* name, char* doc, int c)

    void PyUFunc_DD_D(char**, npy_intp*, npy_intp*, void*)

# Required module initialization
# ----

import_array()
import_ufunc()

```

```
# The actual ufunc declaration
# -----
cdef PyUFuncGenericFunction loop_func[1]
cdef char input_output_types[3]
cdef void *elementwise_funcs[1]

loop_func[0] = PyUFunc_DD_D

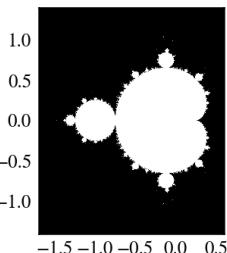
input_output_types[0] = NPY_CDOUBLE
input_output_types[1] = NPY_CDOUBLE
input_output_types[2] = NPY_CDOUBLE

elementwise_funcs[0] = <void*>mandel_single_point

mandel = PyUFunc_FromFuncAndData(
    loop_func,
    elementwise_funcs,
    input_output_types,
    1, # number of supported input types
    2, # number of input args
    1, # number of output args
    0, # 'identity' element, never mind this
    "mandel", # function name
    "mandel(z, c) -> computes iterated z*z + c", # docstring
    0 # unused
)
```

```
import numpy as np
import mandel
x = np.linspace(-1.7, 0.6, 1000)
y = np.linspace(-1.4, 1.4, 1000)
c = x[None,:] + 1j*y[:,None]
z = mandel.mandel(c, c)

import matplotlib.pyplot as plt
plt.imshow(np.abs(z)**2 < 1000, extent=[-1.7, 0.6, -1.4, 1.4])
plt.gray()
plt.show()
```



Note: Most of the boilerplate could be automated by these Cython modules:

<http://wiki.cython.org/MarkLodato/CreatingUfuncs>

Several accepted input types

E.g. supporting both single- and double-precision versions

```
cdef void mandel_single_point(double complex *z_in,
                               double complex *c_in,
                               double complex *z_out) nogil:
    ...

cdef void mandel_single_point_singleprec(float complex *z_in,
                                         float complex *c_in,
                                         float complex *z_out) nogil:
    ...

cdef PyUFuncGenericFunction loop_funcs[2]
cdef char input_output_types[3*2]
cdef void *elementwise_funcs[1*2]

loop_funcs[0] = PyUFunc_DD_D
input_output_types[0] = NPY_CDOUBLE
input_output_types[1] = NPY_CDOUBLE
input_output_types[2] = NPY_CDOUBLE
elementwise_funcs[0] = <void*>mandel_single_point

loop_funcs[1] = PyUFunc_FF_F
input_output_types[3] = NPY_CFLOAT
input_output_types[4] = NPY_CFLOAT
input_output_types[5] = NPY_CFLOAT
elementwise_funcs[1] = <void*>mandel_single_point_singleprec

mandel = PyUFunc_FromFuncAndData(
    loop_funcs,
    elementwise_funcs,
    input_output_types,
    2, # number of supported input types  -----
    2, # number of input args
    1, # number of output args
    0, # 'identity' element, never mind this
    "mandel", # function name
    "mandel(z, c) -> computes iterated z*z + c", # docstring
    0 # unused
)
```

11.2.4 Generalized ufuncs

ufunc

```
output = elementwise_function(input)
```

Both `output` and `input` can be a single array element only.

generalized ufunc

`output` and `input` can be arrays with a fixed number of dimensions

For example, matrix trace (sum of diag elements):

input shape = (n, n)	output shape = () i.e. scalar
(n, n) -> ()	

Matrix product:

```
input_1 shape = (m, n)
input_2 shape = (n, p)
output shape = (m, p)

(m, n), (n, p) -> (m, p)
```

- This is called the “*signature*” of the generalized ufunc
- The dimensions on which the g-ufunc acts, are “*core dimensions*”

Status in Numpy

- g-ufuncs are in Numpy already ...
- new ones can be created with `PyUFunc_FromFuncAndDataAndSignature`
- ... but we don't ship with public g-ufuncs, except for testing, ATM

```
>>> import numpy.core.umath_tests as ut
>>> ut.matrix_multiply.signature
'(m, n), (n, p)->(m, p)'
```

```
>>> x = np.ones((10, 2, 4))
>>> y = np.ones((10, 4, 5))
>>> ut.matrix_multiply(x, y).shape
(10, 2, 5)
```

- the last two dimensions became *core dimensions*, and are modified as per the *signature*
- otherwise, the g-ufunc operates “elementwise”
- matrix multiplication this way could be useful for operating on many small matrices at once

Generalized ufunc loop

Matrix multiplication $(m, n), (n, p) \rightarrow (m, p)$

```
void gufunc_loop(void **args, int *dimensions, int *steps, void *data)
{
    char *input_1 = (char*)args[0]; /* these are as previously */
    char *input_2 = (char*)args[1];
    char *output = (char*)args[2];

    int input_1_stride_m = steps[3]; /* strides for the core dimensions */
    int input_1_stride_n = steps[4]; /* are added after the non-core */
    int input_2_strides_n = steps[5]; /* steps */
    int input_2_strides_p = steps[6];
    int output_strides_n = steps[7];
    int output_strides_p = steps[8];

    int m = dimension[1]; /* core dimensions are added after */
    int n = dimension[2]; /* the main dimension; order as in */
    int p = dimension[3]; /* signature */

    int i;

    for (i = 0; i < dimensions[0]; ++i) {
        matmul_for_strided_matrices(input_1, input_2, output,
                                     strides for each array...);

        input_1 += steps[0];
        input_2 += steps[1];
    }
}
```

```
        output += steps[2];
    }
}
```

11.3 Interoperability features

11.3.1 Sharing multidimensional, typed data

Suppose you

1. Write a library than handles (multidimensional) binary data,
2. Want to make it easy to manipulate the data with Numpy, or whatever other library,
3. ... but would **not** like to have Numpy as a dependency.

Currently, 3 solutions:

1. the “old” buffer interface
2. the array interface
3. the “new” buffer interface ([PEP 3118](#))

11.3.2 The old buffer protocol

- Only 1-D buffers
- No data type information
- C-level interface; `PyBufferProcs tp_as_buffer` in the type object
- But it's integrated into Python (e.g. strings support it)

Mini-exercise using PIL (Python Imaging Library):

See Also:

`pilbuffer.py`

```
>>> import Image
>>> x = np.zeros((200, 200, 4), dtype=np.int8)
```

- TODO: RGBA images consist of 32-bit integers whose bytes are [RR,GG,BB,AA].
 - Fill `x` with opaque red [255,0,0,255]
 - Mangle it to (200,200) 32-bit integer array so that PIL accepts it

```
>>> img = Image.frombuffer("RGBA", (200, 200), data)
>>> img.save('test.png')
```

Q:

Check what happens if `x` is now modified, and `img` saved again.

11.3.3 The old buffer protocol

```
import numpy as np
import Image

# Let's make a sample image, RGBA format
```

```

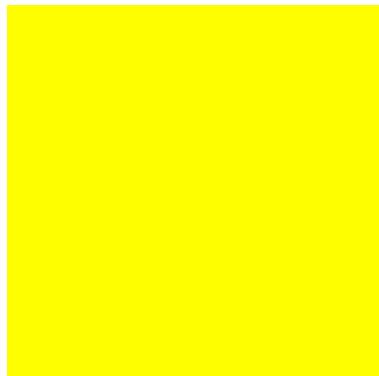
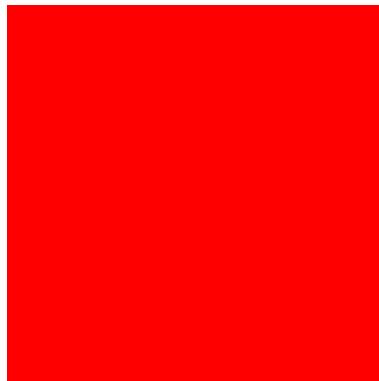
x = np.zeros((200, 200, 4), dtype=np.int8)
x[:, :, 0] = 254 # red
x[:, :, 3] = 255 # opaque

data = x.view(np.int32) # Check that you understand why this is OK!

img = Image.frombuffer("RGBA", (200, 200), data)
img.save('test.png')

#
# Modify the original data, and save again.
#
# It turns out that PIL, which knows next to nothing about Numpy,
# happily shares the same data.
#
x[:, :, 1] = 254
img.save('test2.png')

```



11.3.4 Array interface protocol

- Multidimensional buffers

- Data type information present
- Numpy-specific approach; slowly deprecated (but not going away)
- Not integrated in Python otherwise

See Also:

Documentation: <http://docs.scipy.org/doc/numpy/reference/arrays.interface.html>

```

>>> x = np.array([[1, 2], [3, 4]])
>>> x.__array_interface__
{'data': (171694552, False), # memory address of data, is readonly?
 'descr': [("'", '<i4'], # data type descriptor
 'typestr': '<i4',
 'strides': None, # same, in another form
 'shape': (2, 2),
 'version': 3,
}

```

```

>>> import Image
>>> img = Image.open('test.png')
>>> img.__array_interface__
{'data': a very long string,
 'shape': (200, 200, 4),
 'typestr': '|u1'}
>>> x = np.asarray(img)
>>> x.shape
(200, 200, 4)
>>> x.dtype
dtype('uint8')

```

Note: A more C-friendly variant of the array interface is also defined.

11.3.5 The new buffer protocol: PEP 3118

- Multidimensional buffers
- Data type information present
- C-level interface; extensions to `tp_as_buffer`
- Integrated into Python (>= 2.6)
- Replaces the “old” buffer interface in Python 3
- Next releases of Numpy (>= 1.5) will also implement it fully
- Demo in Python 3 / Numpy dev version:

```

Python 3.1.2 (r312:79147, Apr 15 2010, 12:35:07)
[GCC 4.4.3] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy as np
>>> np.__version__
'2.0.0.dev8469+15dcfb'

```

- Memoryview object exposes some of the stuff Python-side

```

>>> x = np.array([[1, 2], [3, 4]])
>>> y = memoryview(x)
>>> y.format
'l'
>>> y.itemsize
4
>>> y.ndim

```

```

2
>>> y.readonly
False
>>> y.shape
(2, 2)
>>> y.strides
(8, 4)

```

- Roundtrips work

```

>>> z = np.asarray(y)
>>> z
array([[1, 2],
       [3, 4]])
>>> x[0,0] = 9
>>> z
array([[9, 2],
       [3, 4]])

```

- Interoperability with the built-in Python array module

```

>>> import array
>>> x = array.array('h', b'1212')      # 2 of int16, but no Numpy!
>>> y = np.asarray(x)
>>> y
array([12849, 12849], dtype=int16)
>>> y.base
<memory at 0xa225acc>

```

11.3.6 PEP 3118 – details

- Suppose: you have a new Python extension type `MyObject` (defined in C)
- ... and want it to interoperable with a (2, 2) array of `int32`

See Also:

`myobject.c`, `myobject_test.py`, `setup_myobject.py`

```

static PyBufferProcs myobject_as_buffer = {
    (getbufferproc)myobject_getbuffer,
    (releasebufferproc)myobject_releasebuffer,
};

/* ... and stick this to the type object */

static int
myobject_getbuffer(PyObject *obj, Py_buffer *view, int flags)
{
    PyMyObjectObject *self = (PyMyObjectObject*)obj;

    /* Called when something requests that a MyObject-type object
     * provides a buffer interface */

    view->buf = self->buffer;
    view->readonly = 0;
    view->format = "i";
    view->shape = malloc(sizeof(Py_ssize_t) * 2);
    view->strides = malloc(sizeof(Py_ssize_t) * 2);
    view->suboffsets = NULL;

    TODO: Just fill in view->len, view->itemsize, view->strides[0] and 1,
    view->shape[0] and 1, and view->ndim.

```

```

/* Note: if correct interpretation *requires* strides or shape,
you need to check flags for what was requested, and raise
appropriate errors.

```

```

The same if the buffer is not readable.
*/

```

```

view->obj = (PyObject*)self;
Py_INCREF(self);

```

```

return 0;
}

```

```

static void

```

```

myobject_releasebuffer(PyMemoryViewObject *self, Py_buffer *view)
{

```

```

    if (view->shape) {
        free(view->shape);
        view->shape = NULL;
    }

```

```

    if (view->strides) {
        free(view->strides);
        view->strides = NULL;
    }
}

```

```

/*

```

```

 * Sample implementation of a custom data type that exposes an array
 * interface. (And does nothing else : )
 *
 * Requires Python >= 3.1
 */

```

```

/*
 * Mini-exercises:
 *
 * - make the array strided
 * - change the data type
 *
 */

```

```

#define PY_SSIZE_T_CLEAN
#include <Python.h>
#include "structmember.h"

```

```

typedef struct {
    PyObject_HEAD
    int buffer[4];
} PyMyObjectObject;

```

```

static int
myobject_getbuffer(PyObject *obj, Py_buffer *view, int flags)
{
    PyMyObjectObject *self = (PyMyObjectObject*)obj;

    /* Called when something requests that a MyObject-type object
     * provides a buffer interface */

    view->buf = self->buffer;
    view->readonly = 0;
}

```

```

view->buf = self->buffer;
view->readonly = 0;

```

```

view->format = "i";
view->len = 4;
view->itemsize = sizeof(int);
view->ndim = 2;
view->shape = malloc(sizeof(Py_ssize_t) * 2);
view->shape[0] = 2;
view->shape[1] = 2;
view->strides = malloc(sizeof(Py_ssize_t) * 2);
view->strides[0] = 2*sizeof(int);
view->strides[1] = sizeof(int);
view->suboffsets = NULL;

/* Note: if correct interpretation requires* strides or shape,
   you need to check flags for what was requested, and raise
   appropriate errors.

   The same if the buffer is not readable.
 */

view->obj = (PyObject*)self;
Py_INCREF(self);

return 0;
}

static void
myobject_releasebuffer(PyMemoryViewObject *self, Py_buffer *view)
{
    if (view->shape) {
        free(view->shape);
        view->shape = NULL;
    }
    if (view->strides) {
        free(view->strides);
        view->strides = NULL;
    }
}

static PyBufferProcs myobject_as_buffer = {
    (getbufferproc)myobject_getbuffer,
    (releasebufferproc)myobject_releasebuffer,
};

/*
 * Standard stuff follows
 */
PyTypeObject PyMyObject_Type;

static PyObject *
myobject_new(PyTypeObject *subtype, PyObject *args, PyObject *kwds)
{
    PyMyObjectObject *self;
    static char *kwlist[] = {NULL};
    if (!PyArg_ParseTupleAndKeywords(args, kwds, "", kwlist)) {
        return NULL;
    }
    self = (PyMyObjectObject *)
        PyObject_New(PyMyObjectObject, &PyMyObject_Type);
    self->buffer[0] = 1;
    self->buffer[1] = 2;
    self->buffer[2] = 3;
}

```

```

NULL,
NULL,
NULL
};

PyObject *PyInit_myobject(void) {
    PyObject *m, *d;

    if (PyType_Ready(&PyMyObject_Type) < 0)
        return NULL;
}

m = PyModule_Create(&moduledef);

d = PyModule_GetDict(m);

Py_INCREF(&PyMyObject_Type);
PyDict_SetItemString(d, "MyObject", (PyObject *)&PyMyObject_Type);

return m;
}

```

11.4 Siblings: chararray, maskedarray, matrix

chararray — vectorized string operations

```

>>> x = np.array(['a', 'bbb', 'ccc']).view(np.chararray)
>>> x.lstrip(' ')
chararray(['a', 'bbb', 'ccc'],
          dtype='|S5')
>>> x.upper()
chararray(['A', 'BBB', 'CCC'],
          dtype='|S5')

```

Note: `.view()` has a second meaning: it can make an ndarray an instance of a specialized ndarray subclass

MaskedArray — dealing with (propagation of) missing data

- For floats one could use NaN's, but masks work for all types

```

>>> x = np.ma.array([1, 2, 3, 4], mask=[0, 1, 0, 1])
>>> x
masked_array(data = [1 -- 3 --],
              mask = [False True False True],
              fill_value = 999999)

```

```

>>> y = np.ma.array([1, 2, 3, 4], mask=[0, 1, 1, 1])
>>> x + y
masked_array(data = [2 -- -- --],
              mask = [False True True True],
              fill_value = 999999)

```

- Masking versions of common functions

```

>>> np.ma.sqrt([1, -1, 2, -2])
masked_array(data = [1.0 -- 1.41421356237 --],
              mask = [False True False True],
              fill_value = 1e+20)

```

Note: There's more to them!

recarray — purely convenience

```

>>> arr = np.array([('a', 1), ('b', 2)], dtype=[('x', 'S1'), ('y', int)])
>>> arr2 = arr.view(np.recarray)
>>> arr2.x
chararray(['a', 'b'],
          dtype='|S1')
>>> arr2.y
array([1, 2])

```

matrix — convenience?

- always 2-D
- * is the matrix product, not the elementwise one

```

>>> np.matrix([[1, 0], [0, 1]]) * np.matrix([[1, 2], [3, 4]])
matrix([[1, 2],
        [3, 4]])

```

11.5 Summary

- Anatomy of the ndarray: data, dtype, strides.
- Universal functions: elementwise operations, how to make new ones
- Ndarray subclasses
- Various buffer interfaces for integration with other tools
- Recent additions: PEP 3118, generalized ufuncs

11.6 Contributing to Numpy/Scipy

Get this tutorial: <http://www.euroscipy.org/talk/882>

11.6.1 Why

- “There's a bug?”
- “I don't understand what this is supposed to do?”
- “I have this fancy code. Would you like to have it?”
- “I'd like to help! What can I do?”

11.6.2 Reporting bugs

- Bug tracker (prefer [this](#))
 - <http://projects.scipy.org/numpy>
 - <http://projects.scipy.org/scipy>
 - Click the “Register” link to get an account

- Mailing lists (scipy.org/Mailing_Lists)
 - If you're unsure
 - No replies in a week or so? Just file a bug ticket.

Good bug report

```
Title: numpy.random.permutations fails for non-integer arguments

I'm trying to generate random permutations, using numpy.random.permutations

When calling numpy.random.permutation with non-integer arguments
it fails with a cryptic error message:

>>> np.random.permutation(12)
array([10,  9,  4,  7,  3,  8,  0,  6,  5,  1, 11,  2])
>>> np.random.permutation(long(12))
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
  File "mtrand.pyx", line 3311, in mtrand.RandomState.permutation
  File "mtrand.pyx", line 3254, in mtrand.RandomState.shuffle
TypeError: len() of unsized object

This also happens with long arguments, and so
np.random.permutation(X.shape[0]) where X is an array fails on 64
bit windows (where shape is a tuple of longs).

It would be great if it could cast to integer or at least raise a
proper error for non-integer types.

I'm using Numpy 1.4.1, built from the official tarball, on Windows
64 with Visual studio 2008, on Python.org 64-bit Python.
```

0. What are you trying to do?
1. Small code snippet reproducing the bug (if possible)
 - What actually happens
 - What you'd expect
2. Platform (Windows / Linux / OSX, 32/64 bits, x86/PPC, ...)
3. Version of Numpy/Scipy

```
>>> print numpy.__version__
```

Check that the following is what you expect

```
>>> print numpy.__file__
```

In case you have old/broken Numpy installations lying around.

If unsure, try to remove existing Numpy installations, and reinstall...

11.6.3 Contributing to documentation

1. Documentation editor
 - <http://docs.scipy.org/numpy>
 - Registration
 - Register an account

- Subscribe to `scipy-dev` mailing list (subscribers-only)
- Problem with mailing lists: you get mail
 - * But: **you can turn mail delivery off**
 - * “change your subscription options”, at the bottom of <http://mail.scipy.org/mailman/listinfo/scipy-dev>
- Send a mail @ `scipy-dev` mailing list; ask for activation:

```
To: scipy-dev@scipy.org

Hi,

I'd like to edit Numpy/Scipy docstrings. My account is XXXXX

Cheers,
N. N.
```

- Check the style guide:
 - <http://docs.scipy.org/numpy/>
 - Don't be intimidated; to fix a small thing, just fix it
 - Edit
2. Edit sources and send patches (as for bugs)
 3. Complain on the mailing list

11.6.4 Contributing features

0. Ask on mailing list, if unsure where it should go
1. Write a patch, add an enhancement ticket on the bug tracket
2. OR, create a Git branch implementing the feature + add enhancement ticket.
 - Especially for big/invasive additions
 - <http://projects.scipy.org/numpy/wiki/GitMirror>
 - http://www.spheredev.org/wiki/Git_for_the_lazy

```
# Clone numpy repository
git clone --origin svn http://projects.scipy.org/git/numpy.git numpy
cd numpy
```

```
# Create a feature branch
git checkout -b name-of-my-feature-branch svn/trunk
<edit stuff>
git commit -a
```

- Create account on <http://github.com> (or anywhere)
- Create a new repository @ Github
- Push your work to github

```
git remote add github git@github:YOURUSERNAME/YOURREPOSITORYNAME.git
git push github name-of-my-feature-branch
```

11.6.5 How to help, in general

- Bug fixes always welcome!
 - What irks you most
 - Browse the tracker
- Documentation work
 - API docs: improvements to docstrings
 - * Know some Scipy module well?
 - *User guide*
 - * Needs to be done eventually.
 - * Want to think? Come up with a Table of Contents
- Ask on communication channels:
 - numpy-discussion list
 - scipy-dev list

Debugging code

author Gaël Varoquaux

This tutorial explores tool to understand better your code base: debugging, to find and fix bugs.

It is not specific to the scientific Python community, but the strategies that we will employ are tailored to its needs.

Prerequisites

- Numpy
- IPython
- nosetests (<http://readthedocs.org/docs/nose/en/latest/>)
- line_profiler (http://packages.python.org/line_profiler/)
- pyflakes (<http://pypi.python.org/pypi/pyflakes>)
- gdb for the C-debugging part.

Chapters contents

- Avoiding bugs (page 200)
 - Coding best practices to avoid getting in trouble (page 200)
 - pyflakes: fast static analysis (page 201)
 - * Running pyflakes on the current edited file (page 201)
 - * A type-as-go spell-checker like integration (page 202)
- Debugging workflow (page 202)
- Using the Python debugger (page 203)
 - Invoking the debugger (page 203)
 - * Postmortem (page 203)
 - * Step-by-step execution (page 205)
 - * Other ways of starting a debugger (page 206)
 - Debugger commands and interaction (page 207)
 - Debugging segmentation faults using gdb (page 207)

12.1 Avoiding bugs

12.1.1 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 (not mathematics names)

12.1.2 pyflakes: fast static analysis

There are several static analysis tools in Python; to name a few: `pylint`, `pychecker`, and `pyflakes`. Here we focus on `pyflakes`, which is the simplest tool.

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

Integrating `pyflakes` in your editor is highly recommended, it **does yield productivity gains**.

Running pyflakes on the current edited file

You can bind a key to run `pyflakes` in the current buffer.

- **In kate** Menu: 'settings -> configure kate
 - In plugins enable 'external tools'
 - In external Tools', add `pyflakes`:

```
kdialog --title "pyflakes %filename" --msgbox "$(pyflakes %filename)"
```

- **In TextMate**

Menu: TextMate -> Preferences -> Advanced -> Shell variables, add a shell variable:

```
TM_PYCHECKER=/Library/Frameworks/Python.framework/Versions/Current/bin/pyflakes
```

Then Ctrl-Shift-V is binded to a `pyflakes` report

- **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
```

- **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.
  " Pyflakes"
  ;; The minor mode bindings.
  ' ([f5] . pyflakes-thisfile)
)

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

A type-as-go spell-checker like integration

```
869
870     def _compute_log_likelihood(obs):
871         return self._log_emissionprob[:, obs].T
872
```

- **In vim** Use the `pyflakes.vim` plugin:
 1. download the zip file from http://www.vim.org/scripts/script.php?script_id=2441
 2. extract the files in `vim/ftplugin/python`
 3. make sure your `vimrc` has "filetype plugin indent on"
- **In emacs** Use the `flymake` mode with `pyflakes`, documented on <http://www.plope.com/Members/chrism/flymake-mode>: add the following to your `.emacs` file:

```
(when (load "flymake" t)
  (defun flymake-pyflakes-init ()
    (let* ((temp-file (flymake-init-create-temp-buffer-copy
                       'flymake-create-temp-inplace))
           (local-file (file-relative-name
                        temp-file
                        (file-name-directory buffer-file-name))))
      (list "pyflakes" (list local-file))))
  (add-to-list 'flymake-allowed-file-name-masks
              '("^\.\.py$" flymake-pyflakes-init)))
  (add-hook 'find-file-hook 'flymake-find-file-hook))
```

12.2 Debugging workflow

If you do have a non trivial bug, this is when debugging strategies kick in. There is no silver bullet. Yet, strategies help:

For debugging a given problem, the favorable situation is when the problem is isolated in a small number of lines of code, outside framework or application code, with short modify-run-fail cycles

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.

=> isolate a small reproducible failure: a test case

3. Change one thing at a time and re-run the failing test case.
4. Use the debugger to understand what is going wrong.
5. Take notes and be patient. It may take a while.

Note: Once you have gone through this process: isolated a tight piece of code reproducing the bug and fix the bug using this piece of code, add the corresponding code to your test suite.

12.3 Using the Python debugger

The python debugger, pdb: <http://docs.python.org/library/pdb.html>, 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.

print

Yes, print statements do work as a debugging tool. However to inspect runtime, it is often more efficient to use the debugger.

12.3.1 Invoking the debugger

Ways to launch the debugger:

1. Postmortem, launch debugger after module errors.
2. Launch the module with the debugger.
3. Call the debugger inside the module

Postmortem

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

Here we debug the file index_error.py. When running it, an IndexError is raised. Type %debug and drop into the debugger.

```
In [1]: %run index_error.py
-----
IndexError                                 Traceback (most recent call last)
/home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/index_error.py in <module>()
6
```

```
7 if __name__ == '__main__':
----> 8     index_error()
9
/home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/index_error.py in index_error()
3     def index_error():
4         lst = list('foobar')
----> 5         print lst[len(lst)]
6
7 if __name__ == '__main__':
8     index_error()
IndexError: list index out of range
In [2]: %debug
> /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/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()
9
ipdb> len(lst)
6
ipdb> print lst[len(lst)-1]
r
ipdb> quit
In [3]:
```

Post-mortem debugging without IPython

In some situations you cannot use IPython, for instance to debug a script that wants to be called from the command line. In this case, you can call the script with `python -m pdb script.py`:

```
$ python -m pdb index_error.py
> /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/index_error.py(1)<module>
-> """Small snippet to raise an IndexError."""
(Pdb) continue
Traceback (most recent call last):
File "/usr/lib/python2.6/pdb.py", line 1296, in main
    pdb._runscript(mainpyfile)
File "/usr/lib/python2.6/pdb.py", line 1215, in _runscript
    self.run(statement)
File "/usr/lib/python2.6/bdb.py", line 372, in run
    exec cmd in globals, locals
File "<string>", line 1, in <module>
    index_error()
File "index_error.py", line 5, in index_error
    print lst[len(lst)]
IndexError: list index out of range
Uncaught exception. Entering post mortem debugging
Running 'cont' or 'step' will restart the program
> /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/index_error.py(5)index_error
-> print lst[len(lst)]
(Pdb)
```

Step-by-step execution

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

For instance we are trying to debug `wiener_filtering.py`. Indeed the code runs, but the filtering does not work well.

- Run the script with the debugger:

```
In [1]: %run -d wiener_filtering.py
*** Blank or comment
*** Blank or comment
*** Blank or comment
Breakpoint 1 at /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/wiener_
NOTE: Enter 'c' at the ipdb> prompt to start your script.
> <string>(1)<module>()
```

- Enter the `wiener_filtering.py` file and set a break point at line 34:

```
ipdb> n
> /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/wiener_filtering.py
    3
1--> 4 import numpy as np
    5 import scipy as sp

ipdb> b 34
Breakpoint 2 at /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/wiener_
```

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

```
ipdb> c
> /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/wiener_filtering.py
    33 """
2--> 34     noisy_img = noisy_img
    35     denoised_img = local_mean(noisy_img, size=size)
```

- Step into code with `n(ext)` and `s(tep)`: next jumps to the next statement in the current execution context, while `step` will go across execution contexts, i.e. enable exploring inside function calls:

```
ipdb> s
> /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/wiener_filtering.py
    2     34     noisy_img = noisy_img
---> 35     denoised_img = local_mean(noisy_img, size=size)
    36     l_var = local_var(noisy_img, size=size)

ipdb> n
> /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/wiener_filtering.py
    35     denoised_img = local_mean(noisy_img, size=size)
---> 36     l_var = local_var(noisy_img, size=size)
    37     for i in range(3):
```

- Step a few lines and explore the local variables:

```
ipdb> n
> /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/wiener_filtering.py
    36     l_var = local_var(noisy_img, size=size)
---> 37     for i in range(3):
    38         res = noisy_img - denoised_img
ipdb> print l_var
[[5868 5379 5316 ..., 5071 4799 5149]
 [5013 363 437 ..., 346 262 4355]
 [5379 410 344 ..., 392 604 3377]
 ...
 [ 435 362 308 ..., 275 198 1632]
 [ 548 392 290 ..., 248 263 1653]
 [ 466 789 736 ..., 1835 1725 1940]]
ipdb> print l_var.min()
0
```

Oh dear, nothing but integers, and 0 variation. Here is our bug, we are doing integer arithmetic.

Raising exception on numerical errors

When we run the `wiener_filtering.py` file, the following warnings are raised:

```
In [2]: %run wiener_filtering.py
Warning: divide by zero encountered in divide
Warning: divide by zero encountered in divide
Warning: divide by zero encountered in divide
```

We can turn these warnings in exception, which enables us to do post-mortem debugging on them, and find our problem more quickly:

```
In [3]: np.seterr(all='raise')
Out[3]: {'divide': 'print', 'invalid': 'print', 'over': 'print', 'under': 'ignore'}
```

Other ways of starting a debugger

- Raising an exception as a poor man break point

If you find it tedious to note the line number to set a break point, you can simply raise an exception at the point that you want to inspect and use IPython's `%debug`. Note that in this case you cannot step or continue the execution.

- Debugging test failures using nosetests

You can run nosetests `--pdb` to drop in post-mortem debugging on exceptions, and nosetests `--pdb-failure` to inspect test failures using the debugger.

In addition, you can use the IPython interface for the debugger in nose by installing the nose plugin `ipdb-plugin`. You can then pass `--ipdb` and `--ipdb-failure` options to nosetests.

- **Calling the debugger explicitly**

Insert the following line where you want to drop in the debugger:

```
import pdb; pdb.set_trace()
```

Warning: When running nosetests, the output is captured, and thus it seems that the debugger does not work. Simply run the nosetests with the `-s` flag.

Graphical debuggers

For stepping through code and inspecting variables, you might find it more convenient to use a graphical debugger such as `winpdb`.

Alternatively, `pudb` is a good semi-graphical debugger with a text user interface in the console.

12.3.2 Debugger commands and interaction

<code>l(list)</code>	Lists the code at the current position
<code>u(p)</code>	Walk up the call stack
<code>d(own)</code>	Walk down the call stack
<code>n(ext)</code>	Execute the next line (does not go down in new functions)
<code>s(tep)</code>	Execute the next statement (goes down in new functions)
<code>bt</code>	Print the call stack
<code>a</code>	Print the local variables
<code>!command</code>	Execute the given Python command (by opposition to pdb commands)

Warning: Debugger commands are not Python code

You cannot name the variables the way you want. For instance, if in you cannot override the variables in the current frame with the same name: **use different names than your local variable when typing code in the debugger.**

12.4 Debugging segmentation faults using gdb

If you have a segmentation fault, you cannot debug it with pdb, as it crashes the Python interpreter before it can drop in the debugger. Similarly, if you have a bug in C code embedded in Python, pdb is useless. For this we turn to the gnu debugger, `gdb`, available on Linux.

Before we start with gdb, let us add a few Python-specific tools to it. For this we add a few macros to our `gdbinit`. The optimal choice of macro depends on your Python version and your gdb version. I have added a simplified version in `gdbinit`, but feel free to read [DebuggingWithGdb](#).

To debug with gdb the Python script `segfault.py`, we can run the script in gdb as follows:

```
$ gdb python
...
(gdb) run segfault.py
Starting program: /usr/bin/python segfault.py
[Thread debugging using libthread_db enabled]

Program received signal SIGSEGV, Segmentation fault.
_strided_byte_copy (dst=0x8537478 "\360\343G", outstrides=4, src=
 0x86c0690 <Address 0x86c0690 out of bounds>, instrides=32, N=3,
```

```
      elsize=4)
      at numpy/core/src/multiarray/ctors.c:365
365      _FAST_MOVE(Int32);
(gdb)
```

We get a segfault, and gdb captures it for post-mortem debugging in the C level stack (not the Python call stack). We can debug the C call stack using gdb's commands:

```
(gdb) up
#1 0x004af4f5 in _copy_from_same_shape (dest=<value optimized out>,
    src=<value optimized out>, myfunc=0x496780 <_strided_byte_copy>,
    swap=0)
at numpy/core/src/multiarray/ctors.c:748
748      myfunc(dst->dataptr, dest->strides[maxaxis],
```

As you can see, right now, we are in the C code of numpy. We would like to know what is the Python code that triggers this segfault, so we go up the stack until we hit the Python execution loop:

```
(gdb) up
#8 0x080ddd23 in call_function (f=
  Frame 0x85371ec, for file /home/varoquau/usr/lib/python2.6/site-packages/numpy/core/arrayprint.py
  at ../Python/ceval.c:3750
3750  ..../Python/ceval.c: No such file or directory.
  in ../Python/ceval.c

(gdb) up
#9 PyEval_EvalFrameEx (f=
  Frame 0x85371ec, for file /home/varoquau/usr/lib/python2.6/site-packages/numpy/core/arrayprint.py
  at ../Python/ceval.c:2412
2412  in ../Python/ceval.c
(gdb)
```

Once we are in the Python execution loop, we can use our special Python helper function. For instance we can find the corresponding Python code:

```
(gdb) pyframe
/home/varoquau/usr/lib/python2.6/site-packages/numpy/core/arrayprint.py (158): _leading_trailing
(gdb)
```

This is numpy code, we need to go up until we find code that we have written:

```
(gdb) up
...
(gdb) up
#34 0x080dc97a in PyEval_EvalFrameEx (f=
  Frame 0x82f064c, for file segfault.py, line 11, in print_big_array (small_array=<numpy.ndarray>
1630  ..../Python/ceval.c: No such file or directory.
  in ../Python/ceval.c
(gdb) pyframe
segfault.py (12): print_big_array
```

The corresponding code is:

```
1 def print_big_array(small_array):
2     big_array = make_big_array(small_array)
3     print big_array[-10:]
4     return big_array
```

Thus the segfault happens when printing `big_array[-10:]`. The reason is simply that `big_array` has been allocated with its end outside the program memory.

Note: For a list of Python-specific commands defined in the `gdbinit`, read the source of this file.

Wrap up exercise

The following script is well documented and hopefully legible. It seeks to answer a problem of actual interest for numerical computing, but it does not work... Can you debug it?

Python source code: `to_debug.py`

Optimizing code

author Gaël Varoquaux

Donald Knuth

"Premature optimization is the root of all evil"

This chapter deals with strategies to make Python code go faster.

Prerequisites

- `line_profiler` (http://packages.python.org/line_profiler/)

Chapters contents

- Optimization workflow (page 210)
- Profiling Python code (page 211)
 - `Timeit` (page 211)
 - `Profiler` (page 211)
 - `Line-profiler` (page 212)
- Making code go faster (page 213)
 - Algorithmic optimization (page 213)
 - * Example of the SVD (page 213)
- Writing faster numerical code (page 214)

13.1 Optimization workflow

1. Make it work: write the code in a simple **legible** ways.
2. Make it work reliably: write automated test cases, make really sure that your algorithm is right and that if you break it, the tests will capture the breakage.
3. Optimize the code by profiling simple use-cases to find the bottlenecks and speeding up these bottlenecks, finding a better algorithm or implementation. Keep in mind that a trade off should be found between profiling on a realistic example and the simplicity and speed of execution of the code. For efficient work, it is best to work with profiling runs lasting around 10s.

13.2 Profiling Python code

No optimization without measuring!

- **Measure:** profiling, timing
- You'll have surprises: the fastest code is not always what you think

13.2.1 Timeit

In IPython, use `timeit` (<http://docs.python.org/library/timeit.html>) to time elementary 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
```

Use this to guide your choice between strategies.

Note: For long running calls, using `%time` instead of `%timeit`; it is less precise but faster

13.2.2 Profiler

Useful when you have a large program to profile, for example the following file:

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

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 IPython we can time the script:

```
In [1]: %run -t demo.py
IPython CPU timings (estimated):
  User : 14.3929 s.
  System: 0.256016 s.
```

and profile it:

```
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' object}
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)
			...		

Clearly the svd (in `decomp.py`) is what takes most of our time, a.k.a. the bottleneck. We have to find a way to make this step go faster, or to avoid this step (algorithmic optimization). Spending time on the rest of the code is useless.

13.2.3 Line-profiler

The profiler is great: it tells us which function takes most of the time, but not where it is called.

For this, we use the `line_profiler`: in the source file, we decorate a few functions that we want to inspect with `@profile` (no need to import it):

```
@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)
```

Then we run the script using the `kernprof.py` program, with switches `-l` and `-v`:

```
~ $ 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 line.

13.3 Making code go faster

Once we have identified the bottlenecks, we need to make the corresponding code go faster.

13.3.1 Algorithmic optimization

The first thing to look for is algorithmic optimization: are there ways to compute less, or better?

For a high-level view of the problem, a good understanding of the maths behind the algorithm helps. However, it is not uncommon to find simple changes, like **moving computation or memory allocation outside a for loop**, that bring in big gains.

Example of the SVD

In both examples above, the SVD - Singular Value Decomposition - is what takes most of the time. Indeed, the computational cost of this algorithm is roughly n^3 in the size of the input matrix.

However, in both of these example, we are not using all the output of the SVD, but only the first few rows of its first return argument. If we use the svd implementation of scipy, we can ask for an incomplete version of the SVD. Note that implementations of linear algebra in scipy are richer than those in numpy and should be preferred.

```

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

```

Real incomplete SVDs, e.g. computing only the first 10 eigenvectors, can be computed with arpack, available in `scipy.sparse.linalg.eigsh`.

Computational linear algebra

For certain algorithms, many of the bottlenecks will be linear algebra computations. In this case, using the right function to solve the right problem is key. For instance, an eigenvalue problem with a symmetric matrix is easier to solve than with a general matrix. Also, most often, you can avoid inverting a matrix and use a less costly (and more numerically stable) operation.

Know your computational linear algebra. When in doubt, explore `scipy.linalg`, and use `%timeit` to try out different alternatives on your data.

13.4 Writing faster numerical code

A complete discussion on advanced use of numpy is found in chapter [Advanced Numpy](#) (page 166), or in the article [The NumPy array: a structure for efficient numerical computation](#) by van der Walt et al. Here we discuss only some commonly encountered tricks to make code faster.

- **Vectorizing for loops**

Find tricks to avoid for loops using numpy arrays. For this, masks and indices arrays can be useful.

- **Broadcasting**

Use [broadcasting](#) (page 176) to do operations on arrays as small as possible before combining them.

- **In place operations**

```

In [1]: a = np.zeros(1e7)

In [2]: %timeit global a ; a = 0*a
10 loops, best of 3: 111 ms per loop

In [3]: %timeit global a ; a *= 0
10 loops, best of 3: 48.4 ms per loop

```

note: we need `global a` in the `timeit` so that it work, as it is assigning to `a`, and thus considers it as a local variable.

- **Be easy on the memory: use views, and not copies**

Copying big arrays is as costly as making simple numerical operations on them:

```

In [1]: a = np.zeros(1e7)

In [2]: %timeit a.copy()
10 loops, best of 3: 124 ms per loop

In [3]: %timeit a + 1
10 loops, best of 3: 112 ms per loop

```

- **Beware of cache effects**

Memory access is cheaper when it is grouped: accessing a big array in a continuous way is much faster than random access. This implies amongst other things that **smaller strides are faster** (see [CPU cache effects](#) (page 177)):

```

In [1]: c = np.zeros((1e4, 1e4), order='C')

In [2]: %timeit c.sum(axis=0)
1 loops, best of 3: 3.89 s per loop

In [3]: %timeit c.sum(axis=1)
1 loops, best of 3: 188 ms per loop

In [4]: c.strides
Out[4]: (80000, 8)

```

This is the reason why Fortran ordering or C ordering may make a big difference on operations. Using `numexpr` can be useful to automatically optimize code for such effects.

- **Use compiled code**

The last resort, once you are sure that all the high-level optimizations have been explored, is to transfer the hot spots, i.e. the few lines or functions in which most of the time is spent, to compiled code. For compiled code, the preferred option is to use [Cython](#): it is easy to transform exiting Python code in compiled code, and with a good use of the [numpy support](#) yields efficient code on numpy arrays, for instance by unrolling loops.

Warning: For all the above: profile and time your choices. Don't base your optimization on theoretical considerations.

Sparse Matrices in SciPy

author Robert Cimrman

14.1 Introduction

(dense) matrix is:

- mathematical object
- data structure for storing a 2D array of values

important features:

- **memory allocated once for all items**
 - usually a contiguous chunk, think NumPy ndarray
- *fast* access to individual items (*)

14.1.1 Why Sparse Matrices?

- the memory, that grows like $n \times 2$
- small example (double precision matrix):

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> x = np.linspace(0, 1e6, 10)
>>> plt.plot(x, 8.0 * (x**2) / 1e6, lw=5)
>>> plt.xlabel('size n')
>>> plt.ylabel('memory [MB]')
>>> plt.show()
```

14.1.2 Sparse Matrices vs. Sparse Matrix Storage Schemes

- sparse matrix is a matrix, which is *almost empty*
- storing all the zeros is wasteful -> store only nonzero items
- think **compression**
- pros: huge memory savings
- cons: depends on actual storage scheme, (*) usually does not hold

14.1.3 Typical Applications

- solution of partial differential equations (PDEs)
 - the *finite element method*
 - mechanical engineering, electrotechnics, physics, ...
- graph theory
 - nonzero at (i, j) means that node i is connected to node j
- ...

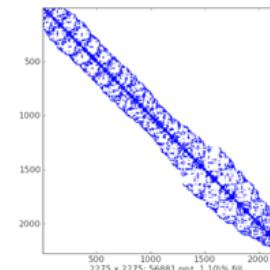
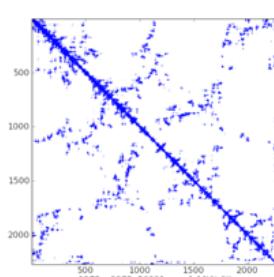
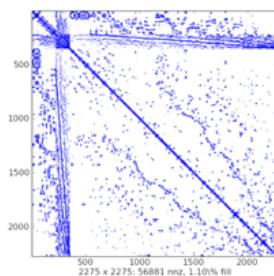
14.1.4 Prerequisites

recent versions of

- numpy
- scipy
- matplotlib (optional)
- ipython (the enhancements come handy)

14.1.5 Sparsity Structure Visualization

- spy() from matplotlib
- example plots:



14.2 Storage Schemes

- seven sparse matrix types in `scipy.sparse`:
 1. `csc_matrix`: Compressed Sparse Column format
 2. `csr_matrix`: Compressed Sparse Row format
 3. `bsr_matrix`: Block Sparse Row format
 4. `lil_matrix`: List of Lists format
 5. `dok_matrix`: Dictionary of Keys format
 6. `coo_matrix`: COOrdinate format (aka IJV, triplet format)
 7. `dia_matrix`: DIAGONAL format
- each suitable for some tasks
- many employ sparsenots C++ module by Nathan Bell
- assume the following is imported:

```
>>> import numpy as np
>>> import scipy.sparse as sps
>>> import matplotlib.pyplot as plt
```

- warning for NumPy users:
 - the multiplication with '*' is the *matrix multiplication* (dot product)
 - **not part of NumPy!**

* passing a sparse matrix object to NumPy functions expecting ndarray/matrix does not work

14.2.1 Common Methods

- all `scipy.sparse` classes are subclasses of `spmatrix`
 - default implementation of arithmetic operations
 - * always converts to CSR
 - * subclasses override for efficiency
 - shape, data type set/get
 - nonzero indices
 - format conversion, interaction with NumPy (`toarray()`, `todense()`)

- ...

- **attributes:**

- `mtx.A` - same as `mtx.toarray()`
- `mtx.T` - transpose (same as `mtx.transpose()`)
- `mtx.H` - Hermitian (conjugate) transpose
- `mtx.real` - real part of complex matrix
- `mtx.imag` - imaginary part of complex matrix
- `mtx.size` - the number of nonzeros (same as `self.getnnz()`)
- `mtx.shape` - the number of rows and columns (tuple)

- data usually stored in NumPy arrays

14.2.2 Sparse Matrix Classes

Diagonal Format (DIA)

- very simple scheme
- **diagonals in dense NumPy array of shape (`n_diag, length`)**
 - fixed length -> waste space a bit when far from main diagonal
 - subclass of `_data_matrix` (sparse matrix classes with `data` attribute)
- **offset for each diagonal**
 - 0 is the main diagonal
 - negative offset = below
 - positive offset = above
- fast matrix * vector (`sparsenorm`)
- **fast and easy item-wise operations**
 - manipulate data array directly (fast NumPy machinery)
- **constructor accepts:**
 - dense matrix (array)
 - sparse matrix
 - shape tuple (create empty matrix)
 - `(data, offsets)` tuple
- no slicing, no individual item access
- **use:**
 - rather specialized
 - solving PDEs by finite differences
 - with an iterative solver

Examples

- create some DIA matrices:

```
>>> data = np.array([[1, 2, 3, 4]]).repeat(3, axis=0)
>>> data
array([[1, 2, 3, 4],
       [1, 2, 3, 4],
       [1, 2, 3, 4]])
>>> offsets = np.array([0, -1, 2])
>>> mtx = sps.dia_matrix((data, offsets), shape=(4, 4))
>>> mtx
<4x4 sparse matrix of type '<type 'numpy.int32'>'>
      with 9 stored elements (3 diagonals) in DIAGONAL format>
>>> mtx.todense()
matrix([[1, 0, 0, 0],
       [1, 2, 0, 4],
       [0, 2, 3, 0],
       [0, 0, 3, 4]])

>>> data = np.arange(12).reshape((3, 4)) + 1
>>> data
array([[ 1,  2,  3,  4],
       [ 5,  6,  7,  8],
       [ 9, 10, 11, 12]])
>>> mtx = sps.dia_matrix((data, offsets), shape=(4, 4))
>>> mtx.data
array([[ 1,  2,  3,  4],
       [ 5,  6,  7,  8],
       [ 9, 10, 11, 12]])
>>> mtx.offsets
array([ 0, -1,  2])
>>> print mtx
(0, 0)      1
(1, 1)      2
(2, 2)      3
(3, 3)      4
(1, 0)      5
(2, 1)      6
(3, 2)      7
(0, 2)     11
(1, 3)     12
>>> mtx.todense()
matrix([[ 1,  0, 11,  0],
       [ 5,  2,  0, 12],
       [ 0,  6,  3,  0],
       [ 0,  0,  7,  4]])
```

- explanation with a scheme:

offset: row	
2: 9	
1: --10-----	
0: 1 . 11 .	
-1: 5 2 . 12	
-2: . 6 3 .	
-3: . . 7 4	
-----8	

- matrix-vector multiplication

```
>>> vec = np.ones((4,))
>>> vec
array([ 1.,  1.,  1.,  1.])
>>> mtx * vec
array([[ 12.,  19.,   9.,  11.])
>>> mtx.toarray() * vec
array([[ 1.,   0.,  11.,   0.],
       [ 5.,   2.,   0.,  12.],
       [ 0.,   6.,   3.,   0.],
       [ 0.,   0.,   7.,   4.]])
```

List of Lists Format (LIL)

- **row-based linked list**
 - each row is a Python list (sorted) of column indices of non-zero elements
 - rows stored in a NumPy array (`dtype=np.object`)
 - non-zero values data stored analogously
- efficient for constructing sparse matrices incrementally
- **constructor accepts:**
 - dense matrix (array)
 - sparse matrix
 - shape tuple (create empty matrix)
- flexible slicing, changing sparsity structure is efficient
- slow arithmetics, slow column slicing due to being row-based
- **use:**
 - when sparsity pattern is not known apriori or changes
 - example: reading a sparse matrix from a text file

Examples

- create an empty LIL matrix:

```
>>> mtx = sps.lil_matrix((4, 5))
```

- prepare random data:

```
>>> from numpy.random import rand
>>> data = np.round(rand(2, 3))
>>> data
array([[ 0.,  0.,  1.],
       [ 0.,  0.,  1.]])
```

- assign the data using fancy indexing:

```
>>> mtx[:2, [1, 2, 3]] = data
>>> mtx
<4x5 sparse matrix of type '<type 'numpy.float64'>'>
      with 2 stored elements in LInked List format>
>>> print mtx
(0, 3)      1.0
(1, 3)      1.0
>>> mtx.todense()
```

```
matrix([[ 0.,  0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.]])
>>> mtx.toarray()
array([[ 0.,  0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.]])
```

- more slicing and indexing:

```
>>> mtx = sps.lil_matrix([[0, 1, 2, 0], [3, 0, 1, 0], [1, 0, 0, 1]])
>>> mtx.todense()
matrix([[0, 1, 2, 0],
       [3, 0, 1, 0],
       [1, 0, 0, 1]])
>>> print mtx
(0, 1)      1
(0, 2)      2
(1, 0)      3
(1, 2)      1
(2, 0)      1
(2, 3)      1
>>> mtx[:2, :]
<2x4 sparse matrix of type '<type 'numpy.int32'>'>
      with 4 stored elements in LInked List format>
>>> mtx[2, :].todense()
matrix([[0, 1, 2, 0],
       [3, 0, 1, 0]])
>>> mtx[1:2, [0,2]].todense()
matrix([[3, 1]])
>>> mtx.todense()
matrix([[0, 1, 2, 0],
       [3, 0, 1, 0],
       [1, 0, 0, 1]])
```

Dictionary of Keys Format (DOK)

- **subclass of Python dict**
 - keys are (row, column) index tuples (no duplicate entries allowed)
 - values are corresponding non-zero values
- efficient for constructing sparse matrices incrementally
- **constructor accepts:**
 - dense matrix (array)
 - sparse matrix
 - shape tuple (create empty matrix)
- efficient O(1) access to individual elements
- flexible slicing, changing sparsity structure is efficient
- can be efficiently converted to a coo_matrix once constructed
- slow arithmetics (for loops with `dict.iteritems()`)
- **use:**
 - when sparsity pattern is not known apriori or changes

Examples

- create a DOK matrix element by element:

```
>>> mtx = sps.dok_matrix((5, 5), dtype=np.float64)
>>> mtx
<5x5 sparse matrix of type '<type 'numpy.float64'>'  
      with 0 stored elements in Dictionary Of Keys format>
>>> for ir in range(5):
>>>     for ic in range(5):
>>>         mtx[ir, ic] = 1.0 * (ir != ic)
>>> mtx
<5x5 sparse matrix of type '<type 'numpy.float64'>'  
      with 25 stored elements in Dictionary Of Keys format>
>>> mtx.todense()
matrix([[ 0.,  1.,  1.,  1.,  1.],
       [ 1.,  0.,  1.,  1.,  1.],
       [ 1.,  1.,  0.,  1.,  1.],
       [ 1.,  1.,  1.,  0.,  1.],
       [ 1.,  1.,  1.,  1.,  0.]])
```

- something is wrong, let's start over:

```
>>> mtx = sps.dok_matrix((5, 5), dtype=np.float64)
>>> for ir in range(5):
>>>     for ic in range(5):
>>>         if (ir != ic): mtx[ir, ic] = 1.0
>>> mtx
<5x5 sparse matrix of type '<type 'numpy.float64'>'  
      with 20 stored elements in Dictionary Of Keys format>
```

- slicing and indexing:

```
>>> mtx[1, 1]
0.0
>>> mtx[1, 1:3]
<1x2 sparse matrix of type '<type 'numpy.float64'>'  
      with 1 stored elements in Dictionary Of Keys format>
>>> mtx[1, 1:3].todense()
matrix([[ 0.,  1.]])
>>> mtx[[2,1], 1:3].todense()
-----
Traceback (most recent call last):
<snip>
NotImplementedError: fancy indexing supported over one axis only
```

Coordinate Format (COO)

- also known as the ‘ijv’ or ‘triplet’ format
 - three NumPy arrays: row, col, data
 - data[i] is value at (row[i], col[i]) position
 - permits duplicate entries
 - subclass of _data_matrix (sparse matrix classes with data attribute)
- fast format for constructing sparse matrices
- constructor accepts:**
 - dense matrix (array)
 - sparse matrix

- shape tuple (create empty matrix)
- (data, ij) tuple
- very fast conversion to and from CSR/CSC formats
- fast matrix * vector (sparsitoools)
- fast and easy item-wise operations**
 - manipulate data array directly (fast NumPy machinery)
- no slicing, no arithmetics (directly)
- use:**
 - facilitates fast conversion among sparse formats
 - when converting to other format (usually CSR or CSC), duplicate entries are summed together
 - * facilitates efficient construction of finite element matrices

Examples

- create empty COO matrix:

```
>>> mtx = sps.coo_matrix((3, 4), dtype=np.int8)
>>> mtx.todense()
matrix([[0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0]], dtype=int8)
```

- create using (data, ij) tuple:

```
>>> row = np.array([0, 3, 1, 0])
>>> col = np.array([0, 3, 1, 2])
>>> data = np.array([4, 5, 7, 9])
>>> mtx = sps.coo_matrix((data, (row, col)), shape=(4, 4))
>>> mtx
<4x4 sparse matrix of type '<type 'numpy.int32'>'  
      with 4 stored elements in COOrdinate format>
>>> mtx.todense()
matrix([[4, 0, 9, 0],
       [0, 7, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 5]])
```

- duplicates entries are summed together:

```
>>> row = np.array([0, 0, 1, 3, 1, 0, 0])
>>> col = np.array([0, 2, 1, 3, 1, 0, 0])
>>> data = np.array([1, 1, 1, 1, 1, 1, 1])
>>> mtx = sps.coo_matrix((data, (row, col)), shape=(4, 4))
>>> mtx.todense()
matrix([[3, 0, 1, 0],
       [0, 2, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 1]])
```

- no slicing...:

```
>>> mtx[2, 3]
-----
Traceback (most recent call last):
File "<ipython console>", line 1, in <module>
TypeError: 'coo_matrix' object is unsubscriptable
```

Compressed Sparse Row Format (CSR)

- **row oriented**
 - three NumPy arrays: `indices`, `indptr`, `data`
 - * `indices` is array of column indices
 - * `data` is array of corresponding nonzero values
 - * `indptr` points to row starts in `indices` and `data`
 - * length is `n_row + 1`, last item = number of values = length of both `indices` and `data`
 - * nonzero values of the `i`-th row are `data[indptr[i]:indptr[i+1]]` with column indices `indices[indptr[i]:indptr[i+1]]`
 - * item (i, j) can be accessed as `data[indptr[i]+k]`, where `k` is position of `j` in `indices[indptr[i]:indptr[i+1]]`
 - subclass of `_cs_matrix` (common CSR/CSC functionality)
 - * subclass of `_data_matrix` (sparse matrix classes with `data` attribute)
- fast matrix vector products and other arithmetics (sparsenorms)
- **constructor accepts:**
 - dense matrix (array)
 - sparse matrix
 - shape tuple (create empty matrix)
 - `(data, ij)` tuple
 - `(data, indices, indptr)` tuple
- efficient row slicing, row-oriented operations
- slow column slicing, expensive changes to the sparsity structure
- **use:**
 - actual computations (most linear solvers support this format)

```
>>> mtx.data
array([1, 2, 3, 4, 5, 6])
>>> mtx.indices
array([0, 2, 2, 0, 1, 2])
>>> mtx.indptr
array([0, 2, 3, 6])
```

- create using `(data, indices, indptr)` tuple:

```
>>> data = np.array([1, 2, 3, 4, 5, 6])
>>> indices = np.array([0, 2, 2, 0, 1, 2])
>>> indptr = np.array([0, 2, 3, 6])
>>> mtx = sps.csr_matrix((data, indices, indptr), shape=(3, 3))
>>> mtx.todense()
matrix([[1, 0, 2],
       [0, 0, 3],
       [4, 5, 6]])
```

Compressed Sparse Column Format (CSC)

- **column oriented**
 - three NumPy arrays: `indices`, `indptr`, `data`
 - * `indices` is array of row indices
 - * `data` is array of corresponding nonzero values
 - * `indptr` points to column starts in `indices` and `data`
 - * length is `n_col + 1`, last item = number of values = length of both `indices` and `data`
 - * nonzero values of the `i`-th column are `data[indptr[i]:indptr[i+1]]` with row indices `indices[indptr[i]:indptr[i+1]]`
 - * item (i, j) can be accessed as `data[indptr[j]+k]`, where `k` is position of `i` in `indices[indptr[j]:indptr[j+1]]`
 - subclass of `_cs_matrix` (common CSR/CSC functionality)
 - * subclass of `_data_matrix` (sparse matrix classes with `data` attribute)
- fast matrix vector products and other arithmetics (sparsenorms)
- **constructor accepts:**
 - dense matrix (array)
 - sparse matrix
 - shape tuple (create empty matrix)
 - `(data, ij)` tuple
 - `(data, indices, indptr)` tuple
- efficient column slicing, column-oriented operations
- slow row slicing, expensive changes to the sparsity structure
- **use:**
 - actual computations (most linear solvers support this format)

Examples

- create empty CSR matrix:

```
>>> mtx = sps.csr_matrix((3, 4), dtype=np.int8)
>>> mtx.todense()
matrix([[0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0]], dtype=int8)
```

- create using `(data, ij)` tuple:

```
>>> row = np.array([0, 0, 1, 2, 2, 2])
>>> col = np.array([0, 2, 2, 0, 1, 2])
>>> data = np.array([1, 2, 3, 4, 5, 6])
>>> mtx = sps.csr_matrix((data, (row, col)), shape=(3, 3))
>>> mtx
<3x3 sparse matrix of type '<type 'numpy.int32'>'>
      with 6 stored elements in Compressed Sparse Row format>
>>> mtx.todense()
matrix([[1, 0, 2],
       [0, 0, 3],
       [4, 5, 6]])
```

Examples

- create empty CSC matrix:

```
>>> mtx = sps.csc_matrix((3, 4), dtype=np.int8)
>>> mtx.todense()
matrix([[0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0]], dtype=int8)
```

- create using (data, ij) tuple:

```
>>> row = np.array([0, 0, 1, 2, 2, 2])
>>> col = np.array([0, 2, 2, 0, 1, 2])
>>> data = np.array([1, 2, 3, 4, 5, 6])
>>> mtx = sps.csc_matrix((data, (row, col)), shape=(3, 3))
>>> mtx
<3x3 sparse matrix of type '<type 'numpy.int32'>'>
      with 6 stored elements in Compressed Sparse Column format
>>> mtx.todense()
matrix([[1, 0, 2],
       [0, 0, 3],
       [4, 5, 6]])
>>> mtx.data
array([1, 4, 5, 2, 3, 6])
>>> mtx.indices
array([0, 2, 2, 0, 1, 2])
>>> mtx.indptr
array([0, 2, 3, 6])
```

- create using (data, indices, indptr) tuple:

```
>>> data = np.array([1, 4, 5, 2, 3, 6])
>>> indices = np.array([0, 2, 2, 0, 1, 2])
>>> indptr = np.array([0, 2, 3, 6])
>>> mtx = sps.csc_matrix((data, indices, indptr), shape=(3, 3))
>>> mtx.todense()
matrix([[1, 0, 2],
       [0, 0, 3],
       [4, 5, 6]])
```

Block Compressed Row Format (BSR)

- basically a CSR with dense sub-matrices of fixed shape instead of scalar items
 - block size (R, C) must evenly divide the shape of the matrix (M, N)
 - three NumPy arrays: **indices**, **indptr**, **data**
 - * indices is array of column indices for each block
 - * data is array of corresponding nonzero values of shape (nnz, R, C)
 - * ...
 - subclass of **_cs_matrix** (common CSR/CSC functionality)
 - * subclass of **_data_matrix** (sparse matrix classes with data attribute)
- fast matrix vector products and other arithmetics (sparse tools)
- constructor accepts:
 - dense matrix (array)
 - sparse matrix

- shape tuple (create empty matrix)
- (data, ij) tuple
- (data, indices, indptr) tuple

- many arithmetic operations considerably more efficient than CSR for sparse matrices with dense sub-matrices

- use:
 - like CSR
 - vector-valued finite element discretizations

Examples

- create empty BSR matrix with (1, 1) block size (like CSR...):

```
>>> mtx = sps.bsr_matrix((3, 4), dtype=np.int8)
>>> mtx
<3x4 sparse matrix of type '<type 'numpy.int8'>'>
      with 0 stored elements (blocksize = 1x1) in Block Sparse Row format
>>> mtx.todense()
matrix([[0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0]], dtype=int8)
```

- create empty BSR matrix with (3, 2) block size:

```
>>> mtx = sps.bsr_matrix((3, 4), blocksize=(3, 2), dtype=np.int8)
>>> mtx
<3x4 sparse matrix of type '<type 'numpy.int8'>'>
      with 0 stored elements (blocksize = 3x2) in Block Sparse Row format
>>> mtx.todense()
matrix([[0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0]], dtype=int8)
```

– a bug?

- create using (data, ij) tuple with (1, 1) block size (like CSR...):

```
>>> row = np.array([0, 0, 1, 2, 2, 2])
>>> col = np.array([0, 2, 2, 0, 1, 2])
>>> data = np.array([1, 2, 3, 4, 5, 6])
>>> mtx = sps.bsr_matrix((data, (row, col)), shape=(3, 3))
>>> mtx
<3x3 sparse matrix of type '<type 'numpy.int32'>'>
      with 6 stored elements (blocksize = 1x1) in Block Sparse Row format
>>> mtx.todense()
matrix([[1, 0, 2],
       [0, 0, 3],
       [4, 5, 6]])
>>> mtx.data
array([[1],
       [[2]],
       [[3]],
       [[4]],
       [[5]],
       [[6]]])
```

```

[[6]])
>>> mtx.indices
array([0, 2, 2, 0, 1, 2])
>>> mtx.indptr
array([0, 2, 3, 6])

```

- create using (data, indices, indptr) tuple with (2, 2) block size:

```

>>> indptr = np.array([0, 2, 3, 6])
>>> indices = np.array([0, 2, 2, 0, 1, 2])
>>> data = np.array([1, 2, 3, 4, 5, 6]).repeat(4).reshape(6, 2, 2)
>>> mtx = sps.bsr_matrix((data, indices, indptr), shape=(6, 6))
>>> mtx.todense()
matrix([[1, 0, 0, 2, 2],
       [1, 0, 0, 2, 2],
       [0, 0, 0, 3, 3],
       [0, 0, 0, 3, 3],
       [4, 4, 5, 6, 6],
       [4, 4, 5, 6, 6]])
>>> data
array([[[1, 1],
       [1, 1],
       [2, 2],
       [2, 2],
       [3, 3],
       [3, 3],
       [4, 4],
       [4, 4],
       [5, 5],
       [5, 5],
       [6, 6],
       [6, 6]]])

```

14.2.3 Summary

Table 14.1: Summary of storage schemes.

format	matrix * vector	get item	fancy get	set item	fancy set	solvers	note
DIA	sparsetools	iterative	has data array, specialized
LIL	via CSR	yes	yes	yes	yes	iterative	arithmetics via CSR, incremental construction
DOK	python	yes	one axis only	yes	yes	iterative	O(1) item access, incremental construction
COO	sparsetools	iterative	has data array, facilitates fast conversion
CSR	sparsetools	yes	yes	slow	.	any	has data array, fast row-wise ops
CSC	sparsetools	yes	yes	slow	.	any	has data array, fast column-wise ops
BSR	sparsetools	specialized	has data array, specialized

14.3 Linear System Solvers

- sparse matrix/eigenvalue problem solvers live in `scipy.sparse.linalg`
- the submodules:

- `dsolve`: direct factorization methods for solving linear systems
- `isolve`: iterative methods for solving linear systems
- `eigen`: sparse eigenvalue problem solvers

- all solvers are accessible from:

```

>>> import scipy.sparse.linalg as spla
>>> spla.__all__
['LinearOperator', 'Tester', 'arpack', 'aslinearoperator', 'bicg',
 'bicgstab', 'cg', 'cgs', 'csc_matrix', 'csr_matrix', 'dsolve',
 'eigen', 'eigen_symmetric', 'factorized', 'gmres', 'interface',
 'isolve', 'iterative', 'lgmres', 'linsolve', 'lobpcg', 'lsqr',
 'minres', 'np', 'qmr', 'speigs', 'spilu', 'splu', 'spsolve', 'svd',
 'test', 'umfpack', 'use_solver', 'utils', 'warnings']

```

14.3.1 Sparse Direct Solvers

- default solver: **SuperLU 4.0**
 - included in SciPy
 - real and complex systems
 - both single and double precision
- optional: **umfpack**
 - real and complex systems
 - double precision only
 - recommended for performance
 - wrappers now live in `scikits.umfpack`
 - check-out the new `scikits.suitesparse` by Nathaniel Smith

Examples

- import the whole module, and see its docstring:

```

>>> import scipy.sparse.linalg.dsolve as dsl
>>> help(dsl)

```

- both superlu and umfpack can be used (if the latter is installed) as follows:

- prepare a linear system:

```

>>> import numpy as np
>>> import scipy.sparse as sps
>>> mtx = sps.spdiags([[1, 2, 3, 4, 5], [6, 5, 8, 9, 10]], [0, 1], 5, 5)
>>> mtx.todense()
matrix([[ 1,  5,  0,  0,  0],
       [ 0,  2,  8,  0,  0],
       [ 0,  0,  3,  9,  0],
       [ 0,  0,  0,  4,  10],
       [ 0,  0,  0,  0,  5]])
>>> rhs = np.array([1, 2, 3, 4, 5])

```

- solve as single precision real:

```
>>> mtx1 = mtx.astype(np.float32)
>>> x = dsl.spsolve(mtx1, rhs, use_umfpack=False)
>>> print x
>>> print "Error: ", mtx1 * x - b
```

- solve as double precision real:

```
>>> mtx2 = mtx.astype(np.float64)
>>> x = dsl.spsolve(mtx2, rhs, use_umfpack=True)
>>> print x
>>> print "Error: ", mtx2 * x - b
```

- solve as single precision complex:

```
>>> mtx1 = mtx.astype(np.complex64)
>>> x = dsl.spsolve(mtx1, rhs, use_umfpack=False)
>>> print x
>>> print "Error: ", mtx1 * x - b
```

- solve as double precision complex:

```
>>> mtx2 = mtx.astype(np.complex128)
>>> x = dsl.spsolve(mtx2, rhs, use_umfpack=True)
>>> print x
>>> print "Error: ", mtx2 * x - b
```

```
"""
Construct a 1000x1000 lil_matrix and add some values to it, convert it
to CSR format and solve A x = b for x:and solve a linear system with a
direct solver.
"""

```

```
import numpy as np
import scipy.sparse as sps
from matplotlib import pyplot as plt
from scipy.sparse.linalg.dsolve import linsolve

rand = np.random.rand

mtx = sps.lil_matrix((1000, 1000), dtype=np.float64)
mtx[0, :100] = rand(100)
mtx[1, 100:200] = mtx[0, :100]
mtx.setdiag(rand(1000))

plt.clf()
plt.spy(mtx, marker='.', markersize=2)
plt.show()

mtx = mtx.tocsr()
rhs = rand(1000)

x = linsolve.spsolve(mtx, rhs)

print 'residual:', np.linalg.norm(mtx * x - rhs)
```

- examples/direct_solve.py

14.3.2 Iterative Solvers

- the `isolve` module contains the following solvers:

- `bicg` (BIConjugate Gradient)

- `bicgstab` (BIConjugate Gradient STABilized)

- `cg` (Conjugate Gradient) - symmetric positive definite matrices only
- `cgs` (Conjugate Gradient Squared)
- `gmres` (Generalized Minimal RESidual)
- `minres` (MINimum RESidual)
- `qmr` (Quasi-Minimal Residual)

Common Parameters

- mandatory:

A [{sparse matrix, dense matrix, LinearOperator}] The N-by-N matrix of the linear system.

b [{array, matrix}] Right hand side of the linear system. Has shape (N,) or (N,1).

- optional:

x0 [{array, matrix}] Starting guess for the solution.

tol [float] Relative tolerance to achieve before terminating.

maxiter [integer] Maximum number of iterations. Iteration will stop after maxiter steps even if the specified tolerance has not been achieved.

M [{sparse matrix, dense matrix, LinearOperator}] Preconditioner for A. The preconditioner should approximate the inverse of A. Effective preconditioning dramatically improves the rate of convergence, which implies that fewer iterations are needed to reach a given error tolerance.

callback [function] User-supplied function to call after each iteration. It is called as callback(xk), where xk is the current solution vector.

LinearOperator Class

```
from scipy.sparse.linalg.interface import LinearOperator
```

- common interface for performing matrix vector products
- useful abstraction that enables using dense and sparse matrices within the solvers, as well as *matrix-free* solutions
- has `shape` and `matvec()` (+ some optional parameters)
- example:

```
>>> import numpy as np
>>> from scipy.sparse.linalg import LinearOperator
>>> def mv(v):
...     return np.array([2*v[0], 3*v[1]])
...
>>> A = LinearOperator((2, 2), matvec=mv)
>>> A
<2x2 LinearOperator with unspecified dtype>
>>> A.matvec(np.ones(2))
array([ 2.,  3.])
>>> A * np.ones(2)
array([ 2.,  3.])
```

A Few Notes on Preconditioning

- problem specific
- often hard to develop
- if not sure, try ILU
 - available in dsolve as spilu()

14.3.3 Eigenvalue Problem Solvers

The eigen module

- arpack * a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems
- lobpcg (Locally Optimal Block Preconditioned Conjugate Gradient Method) * works very well in combination with PyAMG * example by Nathan Bell:

```
"""
Compute eigenvectors and eigenvalues using a preconditioned eigensolver

In this example Smoothed Aggregation (SA) is used to precondition
the LOBPCG eigensolver on a two-dimensional Poisson problem with
Dirichlet boundary conditions.
"""

import scipy
from scipy.sparse.linalg import lobpcg

from pyamg import smoothed_aggregation_solver
from pyamg.gallery import poisson

N = 100
K = 9
A = poisson((N,N), format='csr')

# create the AMG hierarchy
ml = smoothed_aggregation_solver(A)

# initial approximation to the K eigenvectors
X = scipy.rand(A.shape[0], K)

# preconditioner based on ml
M = ml.aspreconditioner()

# compute eigenvalues and eigenvectors with LOBPCG
W,V = lobpcg(A, X, M=M, tol=1e-8, largest=False)

#plot the eigenvectors
import pylab

pylab.figure(figsize=(9,9))

for i in range(K):
    pylab.subplot(3, 3, i+1)
    pylab.title('Eigenvector %d' % i)
    pylab.pcolor(V[:,i].reshape(N,N))
    pylab.axis('equal')
    pylab.axis('off')
pylab.show()
```

- examples/pyamg_with_lobpcg.py

- example by Nils Wagner:
 - examples/lobpcg_sakurai.py
- output:

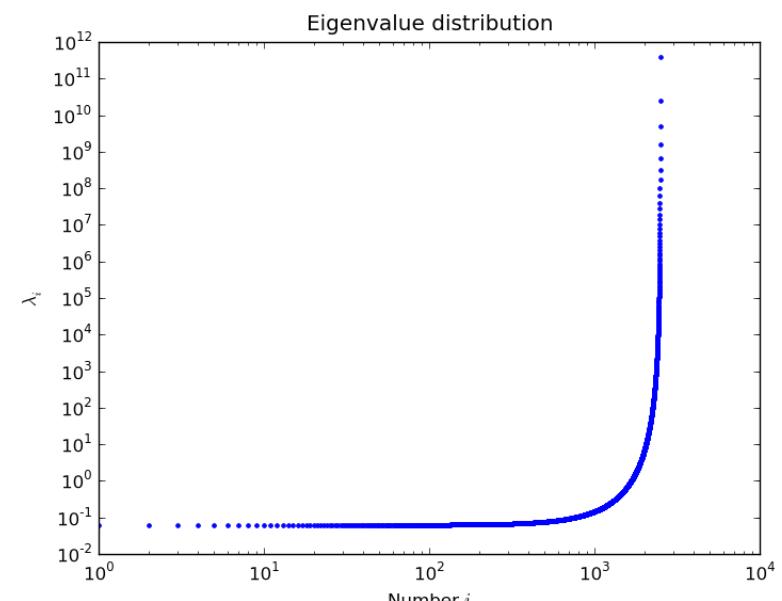
```
$ python examples/lobpcg_sakurai.py
Results by LOBPCG for n=2500

[ 0.06250083  0.06250028  0.06250007]

Exact eigenvalues

[ 0.06250005  0.0625002   0.06250044]

Elapsed time 7.01
```



14.4 Other Interesting Packages

- PyAMG
 - algebraic multigrid solvers
 - <http://code.google.com/p/pyamg>
- Pysparse
 - own sparse matrix classes
 - matrix and eigenvalue problem solvers

– <http://pysparse.sourceforge.net/>

Image manipulation and processing using Numpy and Scipy

authors Emmanuelle Gouillart, Gaël Varoquaux

Image = 2-D numerical array

(or 3-D: CT, MRI, 2D + time; 4-D, ...)

Here, **image == Numpy array** `np.array`

Tools used in this tutorial:

- `numpy`: basic array manipulation
- `scipy`: `scipy.ndimage` submodule dedicated to image processing (n-dimensional images). See <http://docs.scipy.org/doc/scipy/reference/tutorial/ndimage.html>
- a few examples use specialized toolkits working with `np.array`:
 - `Scikit Image`
 - `scikit-learn`

Common tasks in image processing:

- Input/Output, displaying images
- Basic manipulations: cropping, flipping, rotating, ...
- Image filtering: denoising, sharpening
- Image segmentation: labeling pixels corresponding to different objects
- Classification
- ...

More powerful and complete modules:

- `OpenCV` (Python bindings)
- `CellProfiler`
- `ITK` with Python bindings
- many more...

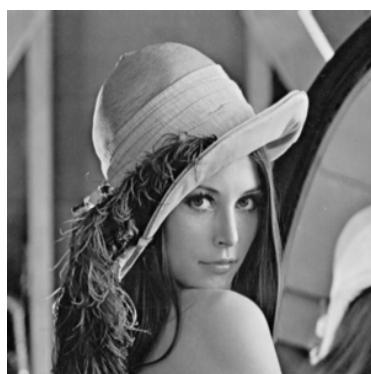
Chapters contents

- Opening and writing to image files (page 237)
- Displaying images (page 238)
- Basic manipulations (page 240)
 - Statistical information (page 241)
 - Geometrical transformations (page 242)
- Image filtering (page 242)
 - Blurring/smoothing (page 243)
 - Sharpening (page 243)
 - Denoising (page 244)
 - Mathematical morphology (page 247)
- Feature extraction (page 251)
 - Edge detection (page 251)
 - Segmentation (page 253)
- Measuring objects properties (page 257)

15.1 Opening and writing to image files

Writing an array to a file

```
>>> import scipy
>>> l = scipy.lena()
>>> from scipy import misc
>>> misc.imsave('lena.png', l) # uses the Image module (PIL)
```



Creating a numpy array from an image file

```
>>> lena = misc.imread('lena.png')
>>> type(lena)
<type 'numpy.ndarray'>
>>> lena.shape, lena.dtype
((512, 512), dtype('uint8'))
```

`dtype` is `uint8` for 8-bit images (0-255)

Opening raw files (camera, 3-D images)

```
>>> l.tofile('lena.raw') # Create raw file
>>> lena_from_raw = np.fromfile('lena.raw', dtype=np.int64)
>>> lena_from_raw.shape
```

```
(262144,
>>> lena_from_raw.shape = (512, 512)
>>> import os
>>> os.remove('lena.raw')
```

Need to know the shape and `dtype` of the image (how to separate data bytes).

For large data, use `np.memmap` for memory mapping:

```
>>> lena_memmap = np.memmap('lena.raw', dtype=np.int64, shape=(512, 512))
```

(data are read from the file, and not loaded into memory)

Working on a list of image files

```
>>> from glob import glob
>>> filelist = glob('pattern*.png')
>>> filelist.sort()
```

15.2 Displaying images

Use `matplotlib` and `imshow` to display an image inside a `matplotlib` figure:

```
>>> l = scipy.lena()
>>> import matplotlib.pyplot as plt
>>> plt.imshow(l, cmap=plt.cm.gray)
<matplotlib.image.AxesImage object at 0x3c7f710>
```

Increase contrast by setting `min` and `max` values:

```
>>> plt.imshow(l, cmap=plt.cm.gray, vmin=30, vmax=200)
<matplotlib.image.AxesImage object at 0x33ef750>
>>> # Remove axes and ticks
>>> plt.axis('off')
(-0.5, 511.5, 511.5, -0.5)
```

Draw contour lines:

```
>>> plt.contour(l, [60, 211])
<matplotlib.contour.ContourSet instance at 0x33f8c20>
```

```
import numpy as np
import scipy
import matplotlib.pyplot as plt

l = scipy.lena()

plt.figure(figsize=(10, 3.6))

plt.subplot(131)
plt.imshow(l, cmap=plt.cm.gray)

plt.subplot(132)
plt.imshow(l, cmap=plt.cm.gray, vmin=30, vmax=200)
plt.axis('off')

plt.subplot(133)
plt.imshow(l, cmap=plt.cm.gray)
plt.contour(l, [60, 211])
plt.axis('off')

plt.subplots_adjust(wspace=0, hspace=0., top=0.99, bottom=0.01, left=0.05, right=0.99)
plt.show()
```



For fine inspection of intensity variations, use `interpolation='nearest'`:

```
>>> plt.imshow(l[200:220, 200:220], cmap=plt.cm.gray)
>>> plt.imshow(l[200:220, 200:220], cmap=plt.cm.gray, interpolation='nearest')
```

```
import numpy as np
import scipy
import matplotlib.pyplot as plt

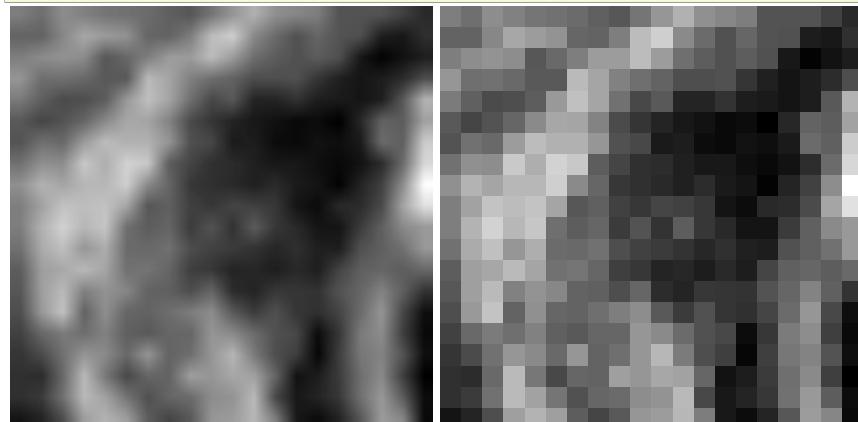
l = scipy.lena()

plt.figure(figsize=(8, 4))

plt.subplot(121)
plt.imshow(l[200:220, 200:220], cmap=plt.cm.gray)
plt.axis('off')

plt.subplot(122)
plt.imshow(l[200:220, 200:220], cmap=plt.cm.gray, interpolation='nearest')
plt.axis('off')

plt.subplots_adjust(wspace=0.02, hspace=0.02, top=1, bottom=0, left=0, right=1)
plt.show()
```



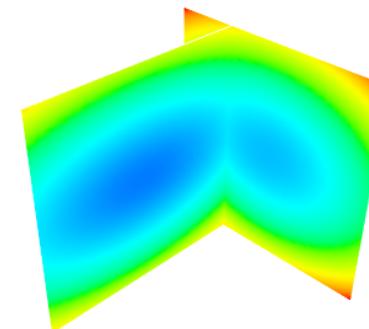
Other packages sometimes use graphical toolkits for visualization (GTK, Qt):

```
>>> import scikits.image.io as im_io
>>> im_io.use_plugin('gtk', 'imshow')
>>> im_io.imshow(l)
```

3-D visualization: Mayavi

See [3D plotting with Mayavi](#) (page 266) and [Volumetric data](#) (page 269).

- Image plane widgets
- Isosurfaces
- ...



15.3 Basic manipulations

Images are arrays: use the whole numpy machinery.



0	1	2
3	4	5
6	7	8

```
>>> lena = scipy.lena()
>>> lena[0, 40]
166
>>> # Slicing
>>> lena[10:13, 20:23]
array([[158, 156, 157],
       [157, 155, 155],
       [157, 157, 158]])
>>> lena[100:120] = 255
>>>
```

```
>>> lx, ly = lena.shape
>>> X, Y = np.ogrid[0:lx, 0:ly]
>>> mask = (X - lx/2)**2 + (Y - ly/2)**2 > lx*ly/4
>>> # Masks
>>> lena[mask] = 0
>>> # Fancy indexing
>>> lena[range(400), range(400)] = 255
```

```
import numpy as np
import scipy
import matplotlib.pyplot as plt

lena = scipy.lena()
lena[10:13, 20:23] = 255
lena[100:120] = 255

lx, ly = lena.shape
X, Y = np.ogrid[0:lx, 0:ly]
mask = (X - lx/2)**2 + (Y - ly/2)**2 > lx*ly/4
lena[mask] = 0
lena[range(400), range(400)] = 255

plt.figure(figsize=(3,3))
plt.axes([0, 0, 1, 1])
plt.imshow(lena, cmap=plt.cm.gray)
plt.axis('off')
```



15.3.1 Statistical information

```
>>> lena = scipy.lena()
>>> lena.mean()
124.04678344726562
>>> lena.max(), lena.min()
(245, 25)
```

`np.histogram`

15.3.2 Geometrical transformations

```
>>> lena = scipy.lena()
>>> lx, ly = lena.shape
>>> # Cropping
>>> crop_lena = lena[lx/4:-lx/4, ly/4:-ly/4]
>>> # up <-> down flip
>>> flip_ud_lena = np.flipud(lena)
>>> # rotation
>>> rotate_lena = ndimage.rotate(lena, 45)
>>> rotate_lena_noreshape = ndimage.rotate(lena, 45, reshape=False)
```

```
import numpy as np
import scipy
from scipy import ndimage
import matplotlib.pyplot as plt

lena = scipy.lena()
lx, ly = lena.shape
# Cropping
crop_lena = lena[lx/4:-lx/4, ly/4:-ly/4]
# up <-> down flip
flip_ud_lena = np.flipud(lena)
# rotation
rotate_lena = ndimage.rotate(lena, 45)
rotate_lena_noreshape = ndimage.rotate(lena, 45, reshape=False)

plt.figure(figsize=(12.5, 2.5))
```

```
plt.subplot(151)
plt.imshow(lena, cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(152)
plt.imshow(crop_lena, cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(153)
plt.imshow(flip_ud_lena, cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(154)
plt.imshow(rotate_lena, cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(155)
plt.imshow(rotate_lena_noreshape, cmap=plt.cm.gray)
plt.axis('off')

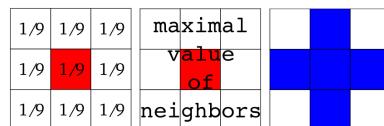
plt.subplots_adjust(wspace=0.02, hspace=0.3, top=1, bottom=0.1, left=0, right=1)
```



15.4 Image filtering

Local filters: replace the value of pixels by a function of the values of neighboring pixels.

Neighbourhood: square (choose size), disk, or more complicated *structuring element*.



15.4.1 Blurring/smoothing

Gaussian filter from `scipy.ndimage`:

```
>>> lena = scipy.lena()
>>> blurred_lena = ndimage.gaussian_filter(lena, sigma=3)
>>> very_blurred = ndimage.gaussian_filter(lena, sigma=5)
```

Uniform filter

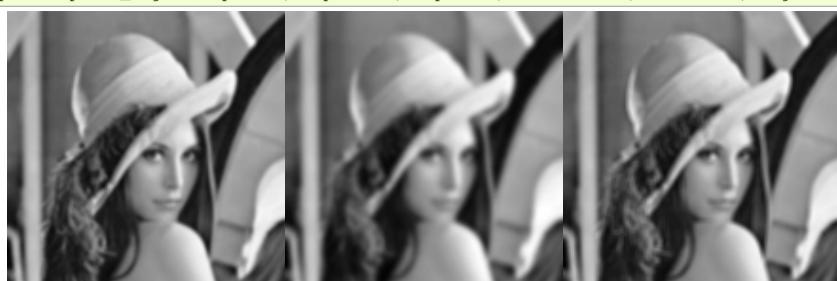
```
>>> local_mean = ndimage.uniform_filter(lena, size=11)
```

```
import numpy as np
import scipy
from scipy import ndimage
import matplotlib.pyplot as plt

lena = scipy.lena()
blurred_lena = ndimage.gaussian_filter(lena, sigma=3)
very_blurred = ndimage.gaussian_filter(lena, sigma=5)
local_mean = ndimage.uniform_filter(lena, size=11)

plt.figure(figsize=(9, 3))
plt.subplot(131)
plt.imshow(blurred_lena, cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(132)
plt.imshow(very_blurred, cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(133)
plt.imshow(local_mean, cmap=plt.cm.gray)
plt.axis('off')

plt.subplots_adjust(wspace=0, hspace=0., top=0.99, bottom=0.01, left=0.01, right=0.99)
```



15.4.2 Sharpening

Sharpen a blurred image:

```
>>> lena = scipy.lena()
>>> blurred_1 = ndimage.gaussian_filter(lena, 3)
```

increase the weight of edges by adding an approximation of the Laplacian:

```
>>> filter_blurred_1 = ndimage.gaussian_filter(blurred_1, 1)
>>> alpha = 30
>>> sharpened = blurred_1 + alpha * (blurred_1 - filter_blurred_1)
```

```
import numpy as np
import scipy
from scipy import ndimage
import matplotlib.pyplot as plt

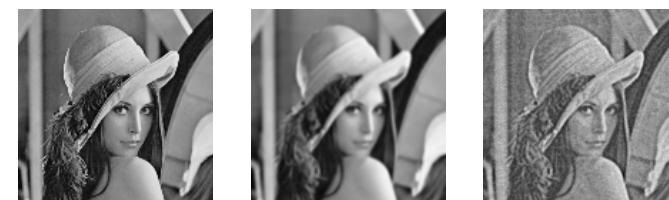
l = scipy.lena()
blurred_1 = ndimage.gaussian_filter(l, 3)

filter_blurred_1 = ndimage.gaussian_filter(blurred_1, 1)

alpha = 30
sharpened = blurred_1 + alpha * (blurred_1 - filter_blurred_1)

plt.figure(figsize=(12, 4))

plt.subplot(131)
plt.imshow(l, cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(132)
plt.imshow(blurred_1, cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(133)
plt.imshow(sharpened, cmap=plt.cm.gray)
plt.axis('off')
```



15.4.3 Denoising

Noisy lena:

```
>>> l = scipy.lena()
>>> l = l[230:310, 210:350]
>>> noisy = l + 0.4*l.std()*np.random.random(l.shape)
```

A **Gaussian filter** smoothes the noise out... and the edges as well:

```
>>> gauss_denoised = ndimage.gaussian_filter(noisy, 2)
```

Most local linear isotropic filters blur the image (`ndimage.uniform_filter`)

A **median filter** preserves better the edges:

```
>>> med_denoised = ndimage.median_filter(noisy, 3)

import numpy as np
import scipy
from scipy import ndimage
import matplotlib.pyplot as plt

l = scipylena()
l = l[230:290, 220:320]

noisy = l + 0.4*l.std()*np.random.random(l.shape)

gauss_denoised = ndimage.gaussian_filter(noisy, 2)
med_denoised = ndimage.median_filter(noisy, 3)

plt.figure(figsize=(12,2.8))

plt.subplot(131)
plt.imshow(noisy, cmap=plt.cm.gray, vmin=40, vmax=220)
plt.axis('off')
plt.title('noisy', fontsize=20)

plt.subplot(132)
plt.imshow(gauss_denoised, cmap=plt.cm.gray, vmin=40, vmax=220)
plt.axis('off')
plt.title('Gaussian filter', fontsize=20)

plt.subplot(133)
plt.imshow(med_denoised, cmap=plt.cm.gray, vmin=40, vmax=220)
plt.axis('off')
plt.title('Median filter', fontsize=20)

plt.subplots_adjust(wspace=0.02, hspace=0.02, top=0.9, bottom=0, left=0, right=1)

noisy          Gaussian filter      Median filter

```

Median filter: better result for straight boundaries (**low curvature**):

```
>>> im = np.zeros((20, 20))
>>> im[5:-5, 5:-5] = 1
>>> im = ndimage.distance_transform_bf(im)
>>> im_noise = im + 0.2*np.random.randn(*im.shape)
>>> im_med = ndimage.median_filter(im_noise, 3)

import numpy as np
import scipy
from scipy import ndimage
import matplotlib.pyplot as plt

im = np.zeros((20, 20))
im[5:-5, 5:-5] = 1
im = ndimage.distance_transform_bf(im)
im_noise = im + 0.2*np.random.randn(*im.shape)

im_med = ndimage.median_filter(im_noise, 3)
```



Other rank filter: `ndimage.maximum_filter`, `ndimage.percentile_filter`

Other local non-linear filters: Wiener (`scipy.signal.wiener`), etc.

Non-local filters

Total-variation (TV) denoising. Find a new image so that the total-variation of the image (integral of the norm L1 of the gradient) is minimized, while being close to the measured image:

```
>>> # from scikits.image.filter import tv_denoise
>>> from tv_denoise import tv_denoise
>>> tv_denoised = tv_denoise(noisy, weight=10)
>>> # More denoising (to the expense of fidelity to data)
>>> tv_denoised = tv_denoise(noisy, weight=50)
```

The total variation filter `tv_denoise` is available in the `scikits.image`, (doc: <http://scikits-image.org/docs/dev/api/scikits.image.filter.html#tv-denoise>), but for convenience we've shipped it as a standalone module with this tutorial.

```
import numpy as np
import scipy
from scipy import ndimage
import matplotlib.pyplot as plt
# from scikits.image.filter import tv_denoise
from tv_denoise import tv_denoise

l = scipylena()
l = l[230:290, 220:320]
```

```

noisy = 1 + 0.4*l.std()*np.random.random(l.shape)

tv_denoised = tv_denoise(noisy, weight=10)

plt.figure(figsize=(12,2.8))

plt.subplot(131)
plt.imshow(noisy, cmap=plt.cm.gray, vmin=40, vmax=220)
plt.axis('off')
plt.title('noisy', fontsize=20)
plt.subplot(132)
plt.imshow(tv_denoised, cmap=plt.cm.gray, vmin=40, vmax=220)
plt.axis('off')
plt.title('TV denoising', fontsize=20)

tv_denoised = tv_denoise(noisy, weight=50)
plt.subplot(133)
plt.imshow(tv_denoised, cmap=plt.cm.gray, vmin=40, vmax=220)
plt.axis('off')
plt.title('(more) TV denoising', fontsize=20)

plt.subplots_adjust(wspace=0.02, hspace=0.02, top=0.9, bottom=0, left=0, right=1)

```



15.4.4 Mathematical morphology

See http://en.wikipedia.org/wiki/Mathematical_morphology

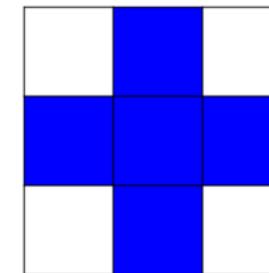
Probe an image with a simple shape (a **structuring element**), and modify this image according to how the shape locally fits or misses the image.

Structuring element:

```

>>> el = ndimage.generate_binary_structure(2, 1)
>>> el
array([[False,  True, False],
       [ True,  True,  True],
       [False,  True, False]], dtype=bool)
>>> el.astype(np.int)
array([[0, 1, 0],
       [1, 1, 1],
       [0, 1, 0]])

```



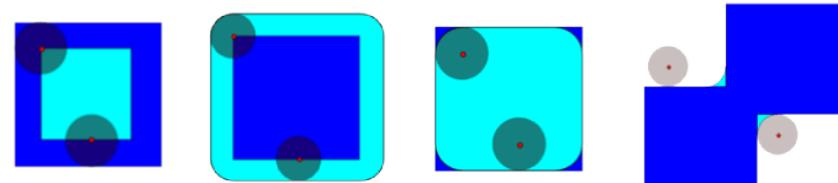
Erosion = minimum filter. Replace the value of a pixel by the minimal value covered by the structuring element.:

```

>>> a = np.zeros((7,7), dtype=np.int)
>>> a[1:6, 2:5] = 1
>>> a
array([[0, 0, 0, 0, 0, 0, 0],
       [0, 0, 1, 1, 0, 0, 0],
       [0, 0, 1, 1, 0, 0, 0],
       [0, 0, 1, 1, 0, 0, 0],
       [0, 0, 1, 1, 0, 0, 0],
       [0, 0, 1, 1, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0]])
>>> ndimage.binary_erosion(a).astype(a.dtype)
array([[0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0]])
>>> #Erosion removes objects smaller than the structure
>>> ndimage.binary_erosion(a, structure=np.ones((5,5))).astype(a.dtype)
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, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0]])

```

Erosion Dilation Opening Closing



Dilation: maximum filter:

```

>>> a = np.zeros((5, 5))
>>> a[2, 2] = 1
>>> a
array([[0., 0., 0., 0., 0.],
       [0., 0., 0., 0., 0.],
       [0., 0., 1., 0., 0.],
       [0., 0., 0., 0., 0.],
       [0., 0., 0., 0., 0.]])

```

```
[ 0.,  0.,  0.,  0.,  0.],
[ 0.,  0.,  1.,  0.,  0.],
[ 0.,  0.,  0.,  0.,  0.],
[ 0.,  0.,  0.,  0.,  0.])
>>> ndimage.binary_dilation(a).astype(a.dtype)
array([[ 0.,  0.,  0.,  0.,  0.],
[ 0.,  0.,  1.,  0.,  0.],
[ 0.,  0.,  1.,  1.,  0.],
[ 0.,  0.,  1.,  0.,  0.],
[ 0.,  0.,  0.,  0.,  0.]])
```

Also works for grey-valued images:

```
>>> np.random.seed(2)
>>> x, y = (63*np.random((2, 8))).astype(np.int)
>>> im[x, y] = np.arange(8)
>>>
>>> bigger_points = ndimage.grey_dilation(im, size=(5, 5), structure=np.ones((5, 5)))
>>>
>>> square = np.zeros((16, 16))
>>> square[4:-4, 4:-4] = 1
>>> dist = ndimage.distance_transform_bf(square)
>>> dilate_dist = ndimage.grey_dilation(dist, size=(3, 3), \
...     structure=np.ones((3, 3)))
```

```
import numpy as np
from scipy import ndimage
import matplotlib.pyplot as plt

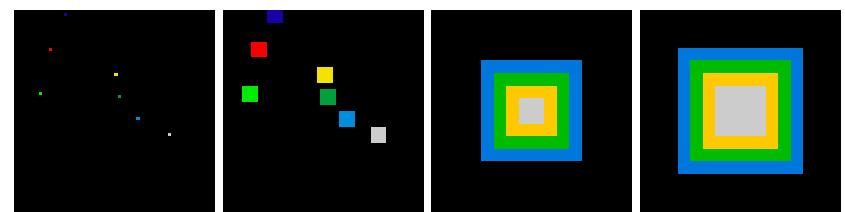
im = np.zeros((64, 64))
np.random.seed(2)
x, y = (63*np.random((2, 8))).astype(np.int)
im[x, y] = np.arange(8)

bigger_points = ndimage.grey_dilation(im, size=(5, 5), structure=np.ones((5, 5)))

square = np.zeros((16, 16))
square[4:-4, 4:-4] = 1
dist = ndimage.distance_transform_bf(square)
dilate_dist = ndimage.grey_dilation(dist, size=(3, 3), \
    structure=np.ones((3, 3)))

plt.figure(figsize=(12.5, 3))
plt.subplot(141)
plt.imshow(im, interpolation='nearest', cmap=plt.cm.spectral)
plt.axis('off')
plt.subplot(142)
plt.imshow(bigger_points, interpolation='nearest', cmap=plt.cm.spectral)
plt.axis('off')
plt.subplot(143)
plt.imshow(dist, interpolation='nearest', cmap=plt.cm.spectral)
plt.axis('off')
plt.subplot(144)
plt.imshow(dilate_dist, interpolation='nearest', cmap=plt.cm.spectral)
plt.axis('off')

plt.subplots_adjust(wspace=0, hspace=0.02, top=0.99, bottom=0.01, left=0.01, right=0.99)
```



Opening: erosion + dilation:

```
>>> a = np.zeros((5,5), dtype=np.int)
>>> a[1:4, 1:4] = 1; a[4, 4] = 1
>>> a
array([[ 0,  0,  0,  0,  0],
[ 0,  1,  1,  1,  0],
[ 0,  1,  1,  1,  0],
[ 0,  1,  1,  1,  0],
[ 0,  0,  0,  0,  1]])
>>> # Opening removes small objects
>>> ndimage.binary_opening(a, structure=np.ones((3,3))).astype(np.int)
array([[ 0,  0,  0,  0,  0],
[ 0,  1,  1,  1,  0],
[ 0,  1,  1,  1,  0],
[ 0,  1,  1,  1,  0],
[ 0,  0,  0,  0,  0]])
>>> # Opening can also smooth corners
>>> ndimage.binary_opening(a).astype(np.int)
array([[ 0,  0,  0,  0,  0],
[ 0,  0,  1,  0,  0],
[ 0,  1,  1,  1,  0],
[ 0,  0,  1,  0,  0],
[ 0,  0,  0,  0,  0]])
```

Application: remove noise:

```
>>> square = np.zeros((32, 32))
>>> square[10:-10, 10:-10] = 1
>>> np.random.seed(2)
>>> x, y = (32*np.random((2, 20))).astype(np.int)
>>> square[x, y] = 1
>>>
>>> open_square = ndimage.binary_opening(square)
>>>
>>> eroded_square = ndimage.binary_erosion(square)
>>> reconstruction = ndimage.binary_propagation(eroded_square, mask=square)
```

```
import numpy as np
from scipy import ndimage
import matplotlib.pyplot as plt

square = np.zeros((32, 32))
square[10:-10, 10:-10] = 1
np.random.seed(2)
x, y = (32*np.random((2, 20))).astype(np.int)
square[x, y] = 1

open_square = ndimage.binary_opening(square)

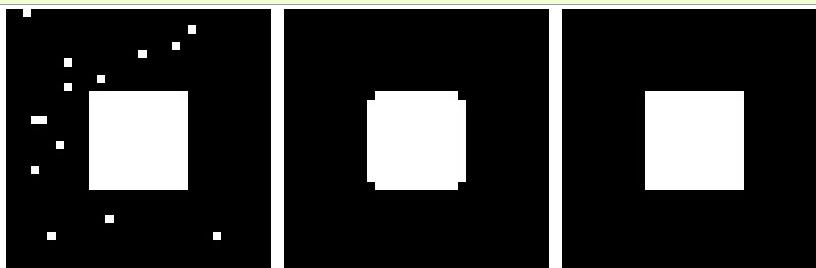
eroded_square = ndimage.binary_erosion(square)
reconstruction = ndimage.binary_propagation(eroded_square, mask=square)
```

```

plt.figure(figsize=(9.5, 3))
plt.subplot(131)
plt.imshow(square, cmap=plt.cm.gray, interpolation='nearest')
plt.axis('off')
plt.subplot(132)
plt.imshow(open_square, cmap=plt.cm.gray, interpolation='nearest')
plt.axis('off')
plt.subplot(133)
plt.imshow(reconstruction, cmap=plt.cm.gray, interpolation='nearest')
plt.axis('off')

plt.subplots_adjust(wspace=0, hspace=0.02, top=0.99, bottom=0.01, left=0.01, right=0.99)

```



Closing: dilation + erosion

Many other mathematical morphology operations: hit and miss transform, tophat, etc.

15.5 Feature extraction

15.5.1 Edge detection

Synthetic data:

```

>>> im = np.zeros((256, 256))
>>> im[64:-64, 64:-64] = 1
>>>
>>> im = ndimage.rotate(im, 15, mode='constant')
>>> im = ndimage.gaussian_filter(im, 8)

```

Use a **gradient operator (Sobel)** to find high intensity variations:

```

>>> sx = ndimage.sobel(im, axis=0, mode='constant')
>>> sy = ndimage.sobel(im, axis=1, mode='constant')
>>> sob = np.hypot(sx, sy)

```

```

import numpy as np
from scipy import ndimage
import matplotlib.pyplot as plt

im = np.zeros((256, 256))
im[64:-64, 64:-64] = 1

im = ndimage.rotate(im, 15, mode='constant')
im = ndimage.gaussian_filter(im, 8)

sx = ndimage.sobel(im, axis=0, mode='constant')
sy = ndimage.sobel(im, axis=1, mode='constant')
sob = np.hypot(sx, sy)

```

```

plt.figure(figsize=(16, 5))
plt.subplot(141)
plt.imshow(im, cmap=plt.cm.gray)
plt.axis('off')
plt.title('square', fontsize=20)
plt.subplot(142)
plt.imshow(sx)
plt.axis('off')
plt.title('Sobel (x direction)', fontsize=20)
plt.subplot(143)
plt.imshow(sob)
plt.axis('off')
plt.title('Sobel filter', fontsize=20)

```

```

im += 0.07*np.random.random(im.shape)

sx = ndimage.sobel(im, axis=0, mode='constant')
sy = ndimage.sobel(im, axis=1, mode='constant')
sob = np.hypot(sx, sy)

```

```

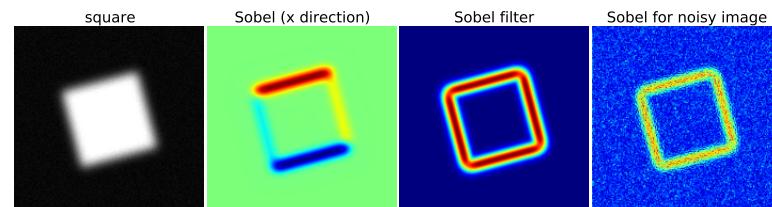
plt.subplot(144)
plt.imshow(sob)
plt.axis('off')
plt.title('Sobel for noisy image', fontsize=20)

```

```

plt.subplots_adjust(wspace=0.02, hspace=0.02, top=1, bottom=0, left=0, right=0.9)

```



Canny filter:

The Canny filter is available in the scikits.image, (doc: <http://scikits-image.org/docs/dev/api/scikits.image.filter.html#canny>), but for convenience we've shipped it as a standalone module with this tutorial.

```

>>> #from scikits.image.filter import canny
>>> #or use module shipped with tutorial
>>> im += 0.1*np.random.random(im.shape)
>>> edges = canny(im, 1, 0.4, 0.2) # not enough smoothing
>>> edges = canny(im, 3, 0.3, 0.2) # better parameters

```

```

import numpy as np
from scipy import ndimage
import matplotlib.pyplot as plt
#from scikits.image.filter import canny
#from image_source_canny import canny

```

```

im = np.zeros((256, 256))
im[64:-64, 64:-64] = 1

```

```

im = ndimage.rotate(im, 15, mode='constant')
im = ndimage.gaussian_filter(im, 8)

im += 0.1*np.random.random(im.shape)

edges = canny(im, 1, 0.4, 0.2)

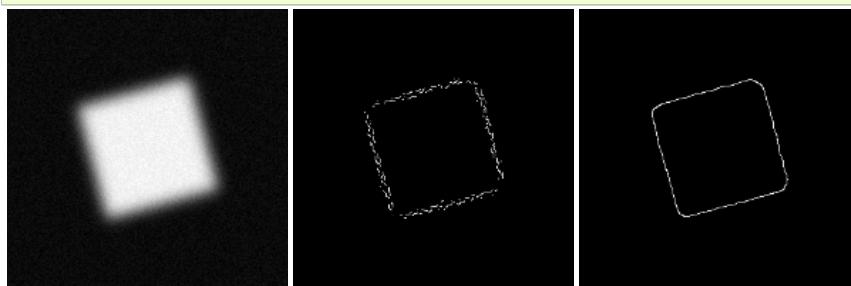
plt.figure(figsize=(12, 4))

plt.subplot(131)
plt.imshow(im, cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(132)
plt.imshow(edges, cmap=plt.cm.gray)
plt.axis('off')

edges = canny(im, 3, 0.3, 0.2)
plt.subplot(133)
plt.imshow(edges, cmap=plt.cm.gray)
plt.axis('off')

plt.subplots_adjust(wspace=0.02, hspace=0.02, top=1, bottom=0, left=0, right=1)

```



Several parameters need to be adjusted... risk of overfitting

15.5.2 Segmentation

- Histogram-based segmentation (no spatial information)

```

>>> n = 10
>>> l = 256
>>> im = np.zeros((l, l))
>>> np.random.seed(1)
>>> points = l*np.random.random((2, n**2))
>>> im[(points[0]).astype(np.int), (points[1]).astype(np.int)] = 1
>>> im = ndimage.gaussian_filter(im, sigma=1/(4.*n))
>>> #
>>> mask = (im > im.mean()).astype(np.float)
>>> #
>>> mask += 0.1 * im
>>> #
>>> img = mask + 0.2*np.random.randn(*mask.shape)
>>> #
>>> hist, bin_edges = np.histogram(img, bins=60)
>>> bin_centers = 0.5*(bin_edges[:-1] + bin_edges[1:])
>>> #
>>> binary_img = img > 0.5

```

```

import numpy as np
from scipy import ndimage
import matplotlib.pyplot as plt

np.random.seed(1)
n = 10
l = 256
im = np.zeros((l, l))
points = l*np.random.random((2, n**2))
im[(points[0]).astype(np.int), (points[1]).astype(np.int)] = 1
im = ndimage.gaussian_filter(im, sigma=1/(4.*n))

mask = (im > im.mean()).astype(np.float)
mask += 0.1 * im

img = mask + 0.2*np.random.randn(*mask.shape)

hist, bin_edges = np.histogram(img, bins=60)
bin_centers = 0.5*(bin_edges[:-1] + bin_edges[1:])

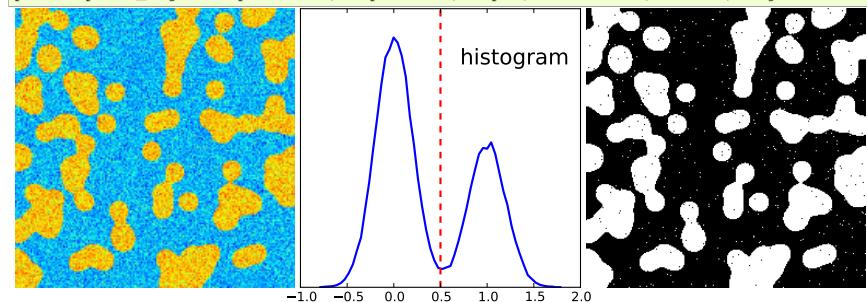
binary_img = img > 0.5

plt.figure(figsize=(11,4))

plt.subplot(131)
plt.imshow(img)
plt.axis('off')
plt.subplot(132)
plt.plot(bin_centers, hist, lw=2)
plt.axvline(0.5, color='r', ls='--', lw=2)
plt.text(0.57, 0.8, 'histogram', fontsize=20, transform = plt.gca().transAxes)
plt.yticks([])
plt.subplot(133)
plt.imshow(binary_img, cmap=plt.cm.gray, interpolation='nearest')
plt.axis('off')

plt.subplots_adjust(wspace=0.02, hspace=0.3, top=1, bottom=0.1, left=0, right=1)

```



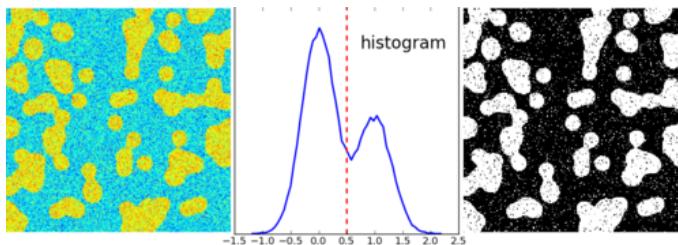
Automatic thresholding: use Gaussian mixture model:

```

>>> mask = (im > im.mean()).astype(np.float)
>>>
>>> mask += 0.1 * im
>>>
>>> img = mask + 0.3*np.random.randn(*mask.shape)
>>>
>>> from scikits.learn.mixture import GMM

```

```
>>> classif = GMM(n_components=2, cvtype='full')
>>> classif.fit(img.reshape((img.size, 1)))
GMM(cvtype='full', n_components=2)
>>>
>>> classif.means
array([[ 0.9353155 ],
[-0.02966039]])
>>> np.sqrt(classif.covars).ravel()
array([ 0.35074631,  0.28225327])
>>> classif.weights
array([ 0.40989799,  0.59010201])
>>> threshold = np.mean(classif.means)
>>> binary_img = img > threshold
```



Use mathematical morphology to clean up the result:

```
>>> # Remove small white regions
>>> open_img = ndimage.binary_opening(binary_img)
>>> # Remove small black hole
>>> close_img = ndimage.binary_closing(open_img)
```

```
import numpy as np
from scipy import ndimage
import matplotlib.pyplot as plt
from scikits.learn.mixture import GMM

np.random.seed(1)
n = 10
l = 256
im = np.zeros((l, l))
points = 1*np.random.randint((2, n**2))
im[(points[0]).astype(np.int), (points[1]).astype(np.int)] = 1
im = ndimage.gaussian_filter(im, sigma=1/(4.*n))

mask = (im > im.mean()).astype(np.float)

img = mask + 0.3*np.random.randn(*mask.shape)

binary_img = img > 0.5

# Remove small white regions
open_img = ndimage.binary_opening(binary_img)
# Remove small black hole
close_img = ndimage.binary_closing(open_img)

plt.figure(figsize=(12, 3))

l = 128
```

```
plt.subplot(141)
plt.imshow(binary_img[:, :], cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(142)
plt.imshow(open_img[:, :], cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(143)
plt.imshow(close_img[:, :], cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(144)
plt.imshow(mask[:, :], cmap=plt.cm.gray)
plt.contour(close_img[:, :], [0.5], linewidths=2, colors='r')
plt.axis('off')

plt.subplots_adjust(wspace=0.02, hspace=0.3, top=1, bottom=0.1, left=0, right=1)

# Better than opening and closing: use reconstruction
eroded_img = ndimage.binary_erosion(binary_img)
reconstruct_img = ndimage.binary_propagation(eroded_img, mask=binary_img)
tmp = np.logical_not(reconstruct_img)
eroded_tmp = ndimage.binary_erosion(tmp)
reconstruct_final = np.logical_not(ndimage.binary_propagation(eroded_tmp, mask=tmp))

#####
plt.subplot(141)
plt.imshow(binary_img[:, :], cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(142)
plt.imshow(eroded_img[:, :], cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(143)
plt.imshow(reconstruct_img[:, :], cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(144)
plt.imshow(mask[:, :], cmap=plt.cm.gray)
plt.contour(reconstruct_final[:, :], [0.5], lw=4)
plt.axis('off')
#####

# Check that reconstruction operations (erosion + propagation) produce a better result than opening/closing:
```

Exercise

Check that reconstruction operations (erosion + propagation) produce a better result than opening/closing:

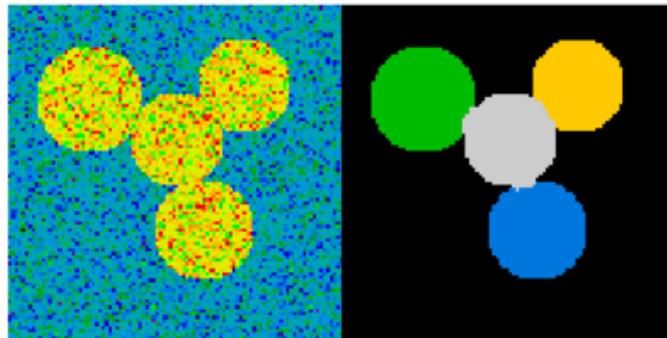
```
>>> eroded_img = ndimage.binary_erosion(binary_img)
>>> reconstruct_img = ndimage.binary_propagation(eroded_img,
>>> mask=binary_img)
>>> tmp = np.logical_not(reconstruct_img)
>>> eroded_tmp = ndimage.binary_erosion(tmp)
>>> reconstruct_final =
>>> np.logical_not(ndimage.binary_propagation(eroded_tmp, mask=tmp))
>>> np.abs(mask - close_img).mean()
0.014678955078125
>>> np.abs(mask - reconstruct_final).mean()
0.004257201484375
```

Exercise

Check how a first denoising step (median filter, total variation) modifies the histogram, and check that the resulting histogram-based segmentation is more accurate.

- Graph-based segmentation: use spatial information.

```
>>> from scikits.learn.feature_extraction import image
>>> from scikits.learn.cluster import spectral_clustering
>>>
>>> l = 100
>>> x, y = np.indices((l, l))
>>>
>>> center1 = (28, 24)
>>> center2 = (40, 50)
>>> center3 = (67, 58)
>>> center4 = (24, 70)
>>>
>>> radius1, radius2, radius3, radius4 = 16, 14, 15, 14
>>>
>>> circle1 = (x - center1[0])**2 + (y - center1[1])**2 < radius1**2
>>> circle2 = (x - center2[0])**2 + (y - center2[1])**2 < radius2**2
>>> circle3 = (x - center3[0])**2 + (y - center3[1])**2 < radius3**2
>>> circle4 = (x - center4[0])**2 + (y - center4[1])**2 < radius4**2
>>>
>>> # 4 circles
>>> img = circle1 + circle2 + circle3 + circle4
>>> mask = img.astype(bool)
>>> img = img.astype(float)
>>>
>>> img += 1 + 0.2*np.random.randn(*img.shape)
>>> # Convert the image into a graph with the value of the gradient on
>>> the
>>> # edges.
>>> graph = image.img_to_graph(img, mask=mask)
>>>
>>> # Take a decreasing function of the gradient: we take it weakly
>>> # dependant from the gradient the segmentation is close to a voronoi
>>> graph.data = np.exp(-graph.data/graph.data.std())
>>>
>>> labels = spectral_clustering(graph, k=4, mode='arpack')
>>> label_im = -np.ones(mask.shape)
>>> label_im[mask] = labels
```



15.6 Measuring objects properties

ndimage.measurements

Synthetic data:

```
>>> n = 10
>>> l = 256
>>> im = np.zeros((l, l))
>>> points = l*np.random.random((2, n**2))
>>> im[(points[0]).astype(np.int), (points[1]).astype(np.int)] = 1
>>> im = ndimage.gaussian_filter(im, sigma=1/(4.*n))
>>> mask = im > im.mean()
```

- Analysis of connected components

Label connected components: ndimage.label:

```
>>> label_im, nb_labels = ndimage.label(mask)
>>> nb_labels # how many regions?
23
>>> plt.imshow(label_im)
<matplotlib.image.AxesImage object at 0x6624d50>
```

```
import numpy as np
from scipy import ndimage
import matplotlib.pyplot as plt

np.random.seed(1)
n = 10
l = 256
im = np.zeros((l, l))
points = l*np.random.random((2, n**2))
im[(points[0]).astype(np.int), (points[1]).astype(np.int)] = 1
im = ndimage.gaussian_filter(im, sigma=1/(4.*n))

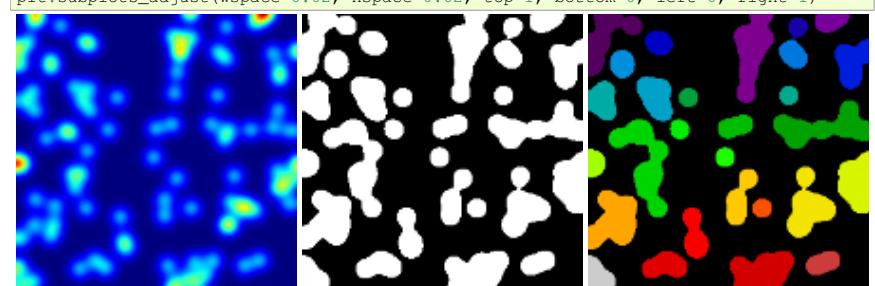
mask = im > im.mean()

label_im, nb_labels = ndimage.label(mask)

plt.figure(figsize=(9,3))

plt.subplot(131)
plt.imshow(im)
plt.axis('off')
plt.subplot(132)
plt.imshow(mask, cmap=plt.cm.gray)
plt.axis('off')
plt.subplot(133)
plt.imshow(label_im, cmap=plt.cm.spectral)
plt.axis('off')

plt.subplots_adjust(wspace=0.02, hspace=0.02, top=1, bottom=0, left=0, right=1)
```



Compute size, mean_value, etc. of each region:

```
>>> sizes = ndimage.sum(mask, label_im, range(nb_labels + 1))
>>> mean_vals = ndimage.sum(im, label_im, range(1, nb_labels + 1))
```

Clean up small connect components:

```
>>> mask_size = sizes < 1000
>>> remove_pixel = mask_size[label_im]
>>> remove_pixel.shape
(256, 256)
>>> label_im[remove_pixel] = 0
>>> plt.imshow(label_im)
```

Now reassign labels with np.searchsorted:

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

```
import numpy as np
from scipy import ndimage
import matplotlib.pyplot as plt

np.random.seed(1)
n = 10
l = 256
im = np.zeros((l, l))
points = 1*np.random.random((2, n**2))
im[(points[0]).astype(np.int), (points[1]).astype(np.int)] = 1
im = ndimage.gaussian_filter(im, sigma=1/(4.*n))

mask = im > im.mean()

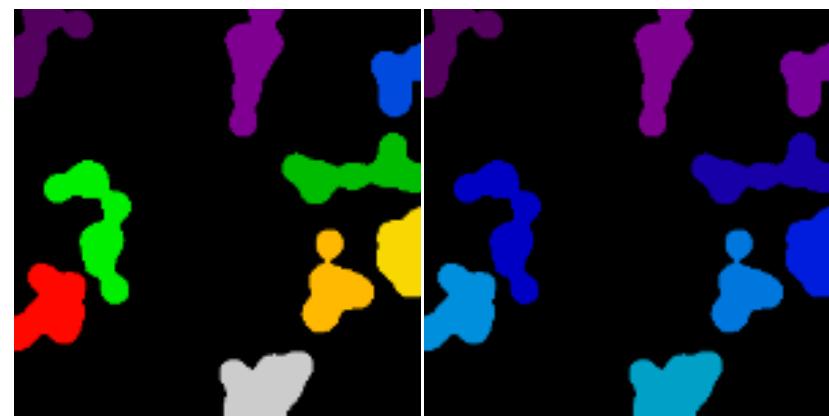
label_im, nb_labels = ndimage.label(mask)

sizes = ndimage.sum(mask, label_im, range(nb_labels + 1))
mask_size = sizes < 1000
remove_pixel = mask_size[label_im]
label_im[remove_pixel] = 0
labels = np.unique(label_im)
label_clean = np.searchsorted(labels, label_im)

plt.figure(figsize=(6 ,3))

plt.subplot(121)
plt.imshow(label_im, cmap=plt.cm.spectral)
plt.axis('off')
plt.subplot(122)
plt.imshow(label_clean, vmax=nb_labels, cmap=plt.cm.spectral)
plt.axis('off')

plt.subplots_adjust(wspace=0.01, hspace=0.01, top=1, bottom=0, left=0, right=1)
```



Find region of interest enclosing object:

```
>>> slice_x, slice_y = ndimage.find_objects(label_im==4)[0]
>>> roi = im[slice_x, slice_y]
>>> plt.imshow(roi)
```

```
import numpy as np
from scipy import ndimage
import matplotlib.pyplot as plt

np.random.seed(1)
n = 10
l = 256
im = np.zeros((l, l))
points = 1*np.random.random((2, n**2))
im[(points[0]).astype(np.int), (points[1]).astype(np.int)] = 1
im = ndimage.gaussian_filter(im, sigma=1/(4.*n))

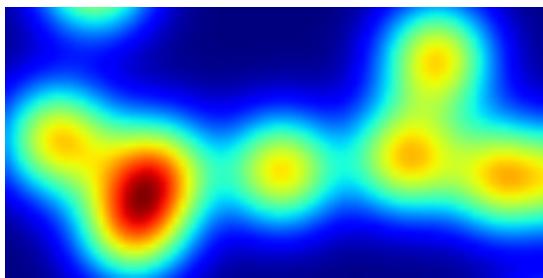
mask = im > im.mean()

label_im, nb_labels = ndimage.label(mask)

sizes = ndimage.sum(mask, label_im, range(nb_labels + 1))
mask_size = sizes < 1000
remove_pixel = mask_size[label_im]
label_im[remove_pixel] = 0
labels = np.unique(label_im)
label_im = np.searchsorted(labels, label_im)

slice_x, slice_y = ndimage.find_objects(label_im==4)[0]
roi = im[slice_x, slice_y]

plt.figure(figsize=(4, 2))
plt.axes([0, 0, 1, 1])
plt.imshow(roi)
plt.axis('off')
```



Other spatial measures: `ndimage.center_of_mass`, `ndimage.maximum_position`, etc.

Can be used outside the limited scope of segmentation applications.

Example: block mean:

```
>>> l = scipylena()
>>> sx, sy = l.shape
>>> X, Y = np.ogrid[0:sx, 0:sy]
>>> regions = sy/6 * (X/4) + Y/6 # note that we use broadcasting
>>> block_mean = ndimage.mean(l, labels=regions, index=np.arange(1,
>>> regions.max() +1))
>>> block_mean.shape = (sx/4, sy/6)
```

```
import numpy as np
import scipy
from scipy import ndimage
import matplotlib.pyplot as plt

l = scipylena()
sx, sy = l.shape
X, Y = np.ogrid[0:sx, 0:sy]

regions = sy/6 * (X/4) + Y/6
block_mean = ndimage.mean(l, labels=regions, index=np.arange(1, regions.max() +1))
block_mean.shape = (sx/4, sy/6)

plt.figure(figsize=(5,5))
plt.imshow(block_mean, cmap=plt.cm.gray)
plt.axis('off')
```



When regions are regular blocks, it is more efficient to use stride tricks (*Example: fake dimensions with strides* (page 175)).

Non-regularly-spaced blocks: radial mean:

```
>>> rbin = (20* r/r.max()).astype(np.int)
>>> radial_mean = ndimage.mean(l, labels=rbin, index=np.arange(1, rbin.max() +1))
```

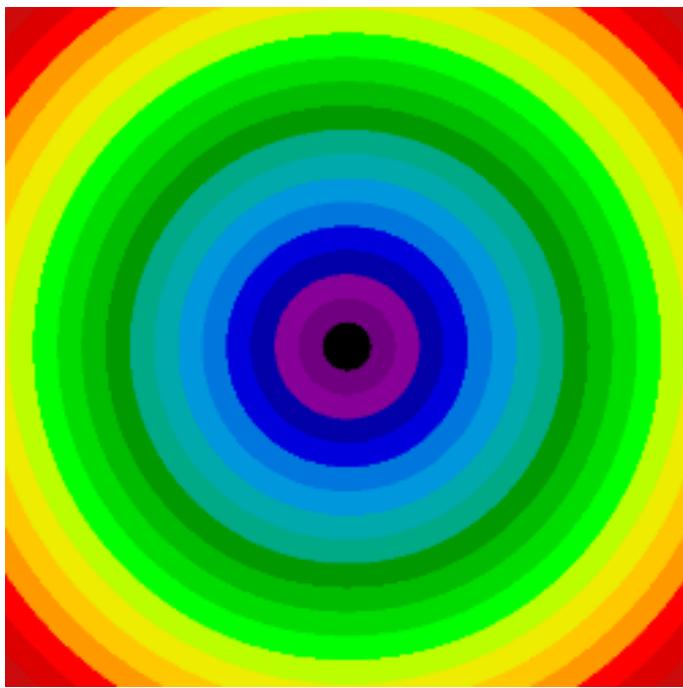
```
import numpy as np
import scipy
from scipy import ndimage
import matplotlib.pyplot as plt

l = scipylena()
sx, sy = l.shape
X, Y = np.ogrid[0:sx, 0:sy]

r = np.hypot(X - sx/2, Y - sy/2)

rbin = (20* r/r.max()).astype(np.int)
radial_mean = ndimage.mean(l, labels=rbin, index=np.arange(1, rbin.max() +1))

plt.figure(figsize=(5,5))
plt.axes([0, 0, 1, 1])
plt.imshow(rbin, cmap=plt.cm.spectral)
plt.axis('off')
```



- Other measures

Correlation function, Fourier/wavelet spectrum, etc.

One example with mathematical morphology: **granulometry** (http://en.wikipedia.org/wiki/Granulometry_%28morphology%29)

```
>>> def disk_structure(n):
...     struct = np.zeros((2 * n + 1, 2 * n + 1))
...     x, y = np.indices((2 * n + 1, 2 * n + 1))
...     mask = (x - n)**2 + (y - n)**2 <= n**2
...     struct[mask] = 1
...     return struct.astype(np.bool)
...
>>>
>>> def granulometry(data, sizes=None):
...     s = max(data.shape)
...     if sizes == None:
...         sizes = range(1, s/2, 2)
...     granulo = [ndimage.binary_opening(data, \
...         structure=disk_structure(n)).sum() for n in sizes]
...     return granulo
...
>>>
>>> np.random.seed(1)
>>> n = 10
>>> l = 256
>>> im = np.zeros((l, l))
>>> points = l*np.random.random((2, n**2))
>>> im[(points[0]).astype(np.int), (points[1]).astype(np.int)] = 1
>>> im = ndimage.gaussian_filter(im, sigma=1/(4.*n))
>>>
```

```
>>> mask = im > im.mean()
>>>
>>> granulo = granulometry(mask, sizes=np.arange(2, 19, 4))

import numpy as np
from scipy import ndimage
import matplotlib.pyplot as plt

def disk_structure(n):
    struct = np.zeros((2 * n + 1, 2 * n + 1))
    x, y = np.indices((2 * n + 1, 2 * n + 1))
    mask = (x - n)**2 + (y - n)**2 <= n**2
    struct[mask] = 1
    return struct.astype(np.bool)

def granulometry(data, sizes=None):
    s = max(data.shape)
    if sizes == None:
        sizes = range(1, s/2, 2)
    granulo = [ndimage.binary_opening(data, \
        structure=disk_structure(n)).sum() for n in sizes]
    return granulo

np.random.seed(1)
n = 10
l = 256
im = np.zeros((l, l))
points = l*np.random.random((2, n**2))
im[(points[0]).astype(np.int), (points[1]).astype(np.int)] = 1
im = ndimage.gaussian_filter(im, sigma=1/(4.*n))

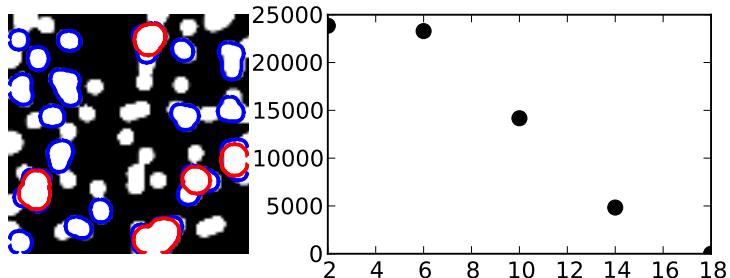
mask = im > im.mean()

granulo = granulometry(mask, sizes=np.arange(2, 19, 4))

plt.figure(figsize=(6, 2.2))

plt.subplot(121)
plt.imshow(mask, cmap=plt.cm.gray)
opened = ndimage.binary_opening(mask, structure=disk_structure(10))
opened_more = ndimage.binary_opening(mask, structure=disk_structure(14))
plt.contour(opened, [0.5], colors='b', linewidths=2)
plt.contour(opened_more, [0.5], colors='r', linewidths=2)
plt.axis('off')
plt.subplot(122)
plt.plot(np.arange(2, 19, 4), granulo, 'ok', ms=8)

plt.subplots_adjust(wspace=0.02, hspace=0.15, top=0.95, bottom=0.15, left=0, right=0.95)
```



3D plotting with Mayavi

author Gaël Varoquaux

16.1 A simple example

Warning: Start `ipython -wthread`

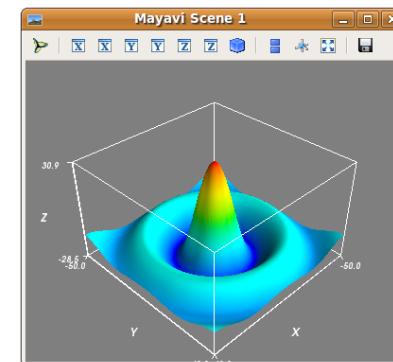
```
import numpy as np

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()
```

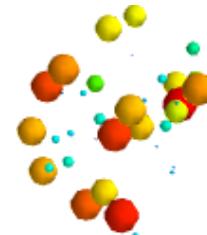
`np.mgrid[-10:10:100j, -10:10:100j]` creates an x,y grid, going from -10 to 10, with 100 steps in each directions.



16.2 3D plotting functions

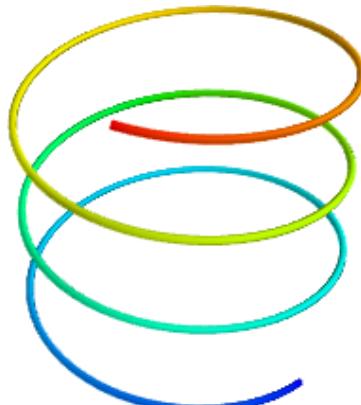
16.2.1 Points

```
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>
```



16.2.2 Lines

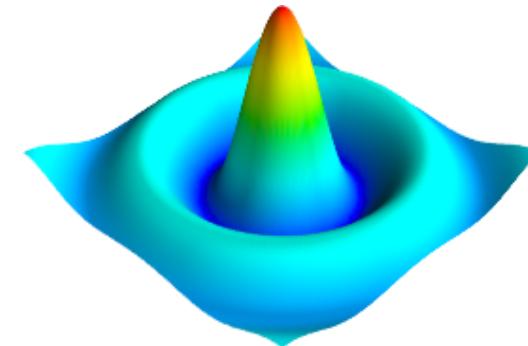
```
In [5]: mlab.clf()
In [6]: t = np.linspace(0, 20, 200)
In [7]: mlab.plot3d(np.sin(t), np.cos(t), 0.1*t, t)
Out[7]: <enthought.mayavi.modules.surface.Surface object at 0xcc3e1dc>
```



16.2.3 Elevation surface

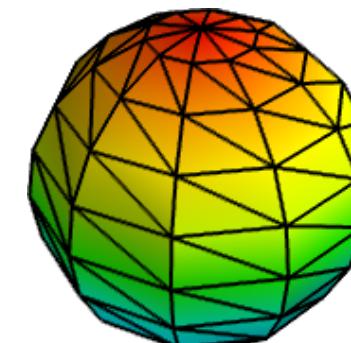
```
In [8]: mlab.clf()
```

```
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 0xcd98fc>
```



16.2.4 Arbitrary regular mesh

```
In [13]: mlab.clf()
In [14]: phi, theta = np.mgrid[0:np.pi:11j, 0:2*np.pi:11j]
In [15]: x = np.sin(phi) * np.cos(theta)
In [16]: y = np.sin(phi) * np.sin(theta)
In [17]: z = np.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 polygons. In *mlab.func* and *mlab.mesh*, the

connectivity is implicitly 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

16.2.5 Volumetric data

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

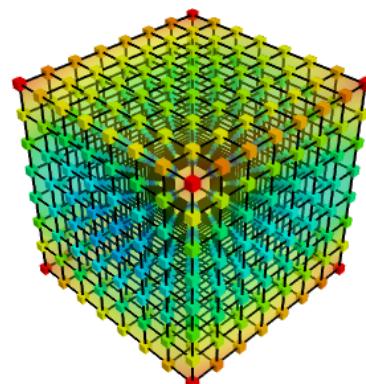
In [21]: x, y, z = np.mgrid[-5:5:64j, -5:5:64j, -5:5:64j]

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>
```



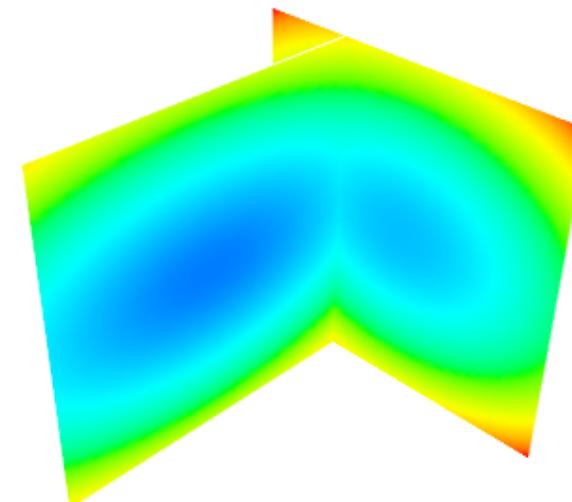
This function works with a regular orthogonal grid:



```
In [25]: s = mlab.pipeline.scalar_field(values)
```

```
In [26]: ipw_x = mlab.pipeline.image_plane_widget(s, plane_orientation='x_axes')
```

```
In [27]: ipw_y = mlab.pipeline.image_plane_widget(s,
plane_orientation='y_axes')
```



Interactive image plane widgets: drag to change the visualized plane.

16.3 Figures and decorations

16.3.1 Figure management

Here is a list of functions useful to control the current figure

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

16.3.2 Changing plot properties

In general, many properties of the various objects on the figure can be changed. If these visualizations are created via `mlab` functions, the easiest way to change them is to use the keyword arguments of these functions, as described in the docstrings.

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. Overrides 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 width 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 useful to reduce the number of points displayed on large datasets

Must be an integer or None.

`mode` the mode of the glyphs. Must be ‘2darrows’ or ‘2dcircles’ 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.

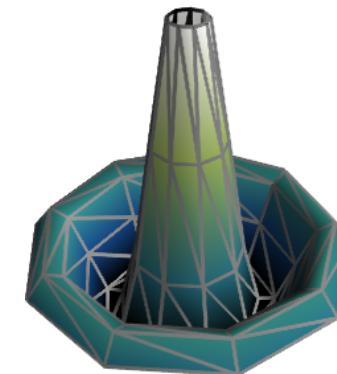
`tube_radius` radius of the tubes used to represent the lines, in mesh mode. If None, simple lines are used.

`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

```
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>
```

**16.3.3 Decorations**

Different items can be added to the figure to carry extra information, such as a colorbar or a title.

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

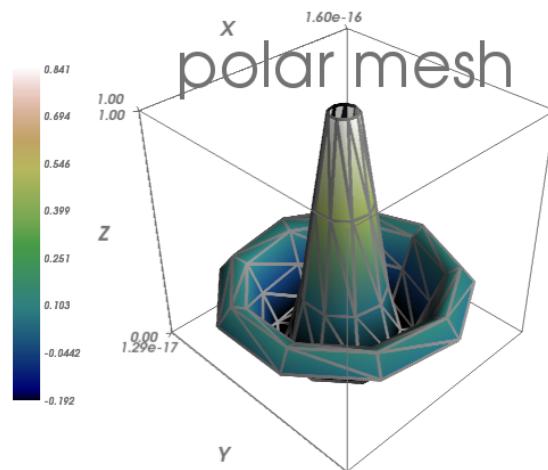
```
In [10]: mlab.title('polar mesh')
Out[10]: <enthought.mayavi.modules.text.Text object at 0xd8ed38c>
```

```
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>
```

Example:

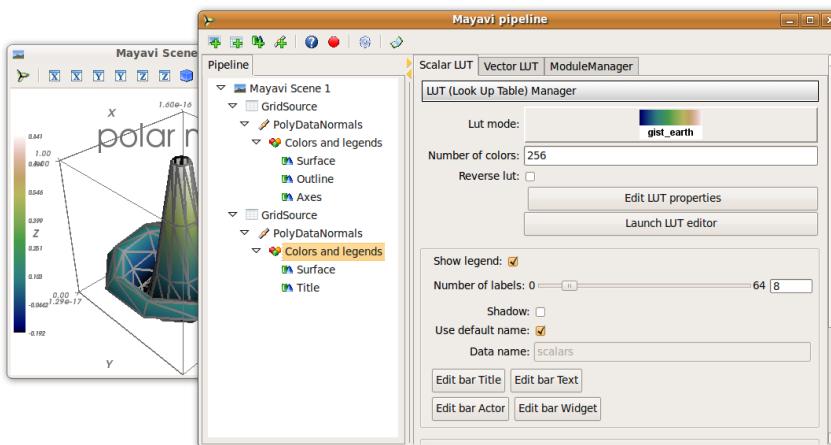
```
In [1]: import numpy as np
In [2]: r, theta = np.mgrid[0:10, -np.pi:np.pi:10j]
In [3]: x = r*np.cos(theta)
In [4]: y = r*np.sin(theta)
In [5]: z = np.sin(r)/r
In [6]: from enthought.mayavi import mlab
In [7]: mlab.mesh(x, y, z, colormap='gist_earth', extent=[0, 1, 0, 1, 0, 1])
Out[7]: <enthought.mayavi.modules.surface.Surface object at 0xde6f08c>
```



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

16.4 Interaction

The quickest way to create beautiful visualization with Mayavi is probably to interactively tweak the various settings. Click on the ‘Mayavi’ button in the scene, and you can control properties of objects with dialogs.



To find out what code can be used to program these changes, click on the red button as you modify those properties, and it will generate the corresponding lines of code.

Sympy : Symbolic Mathematics in Python

author Fabian Pedregosa

Objectives

1. Evaluate expressions with arbitrary precision.
2. Perform algebraic manipulations on symbolic expressions.
3. **Perform basic calculus tasks (limits, differentiation and integration)** with symbolic expressions.
4. Solve polynomial and transcendental equations.
5. Solve some differential equations.

What is SymPy? SymPy is a Python library for symbolic mathematics. It aims to become a full featured computer algebra system that can compete directly with commercial alternatives (Mathematica, Maple) while keeping the code as simple as possible in order to be comprehensible and easily extensible. SymPy is written entirely in Python and does not require any external libraries.

Sympy documentation and packages for installation can be found on <http://sympy.org/>

Chapters contents

- First Steps with SymPy (page 275)
 - Using SymPy as a calculator (page 275)
 - Exercises (page 276)
 - Symbols (page 276)
- Algebraic manipulations (page 276)
 - Expand (page 276)
 - Simplify (page 276)
 - Exercises (page 277)
- Calculus (page 277)
 - Limits (page 277)
 - Differentiation (page 277)
 - Series expansion (page 278)
 - Exercises (page 278)
 - Integration (page 278)
 - Exercises (page 278)
- Equation solving (page 278)
 - Exercises (page 279)
- Linear Algebra (page 279)
 - Matrices (page 279)
 - Differential Equations (page 280)
 - Exercises (page 280)

17.1 First Steps with SymPy

17.1.1 Using SymPy as a calculator

SymPy defines three numerical types: Real, Rational and Integer.

The Rational class represents a rational number as a pair of two Integers: the numerator and the denominator, so Rational(1,2) represents 1/2, Rational(5,2) 5/2 and so on:

```
>>> from sympy import *
>>> a = Rational(1,2)

>>> a
1/2

>>> a**2
1
```

SymPy uses mpmath in the background, which makes it possible to perform computations using arbitrary-precision arithmetic. That way, some special constants, like e, pi, oo (Infinity), are treated as symbols and can be evaluated with arbitrary precision:

```
>>> pi**2
pi**2

>>> pi.evalf()
3.14159265358979

>>> (pi+exp(1)).evalf()
5.85987448204884
```

as you see, evalf evaluates the expression to a floating-point number.

There is also a class representing mathematical infinity, called oo:

```
>>> oo > 99999
True
>>> oo + 1
oo
```

17.1.2 Exercises

1. Calculate $\sqrt{2}$ with 100 decimals.
2. Calculate $1/2 + 1/3$ in rational arithmetic.

17.1.3 Symbols

In contrast to other Computer Algebra Systems, in SymPy you have to declare symbolic variables explicitly:

```
>>> from sympy import *
>>> x = Symbol('x')
>>> y = Symbol('y')
```

Then you can manipulate them:

```
>>> x+y+x-y
2*x

>>> (x+y)**2
(x + y)**2
```

Symbols can now be manipulated using some of python operators: +, -, *, ** (arithmetic), &, |, ~ , >>, << (boolean).

17.2 Algebraic manipulations

SymPy is capable of performing powerful algebraic manipulations. We'll take a look into some of the most frequently used: expand and simplify.

17.2.1 Expand

Use this to expand an algebraic expression. It will try to denest powers and multiplications:

```
In [23]: expand((x+y)**3)
Out[23]: 3*x*y**2 + 3*y*x**2 + x**3 + y**3
```

Further options can be given in form on keywords:

```
In [28]: expand(x+y, complex=True)
Out[28]: I*im(x) + I*im(y) + re(x) + re(y)

In [30]: expand(cos(x+y), trig=True)
Out[30]: cos(x)*cos(y) - sin(x)*sin(y)
```

17.2.2 Simplify

Use simplify if you would like to transform an expression into a simpler form:

```
In [19]: simplify((x+x*y)/x)
Out[19]: 1 + y
```

17.2. Algebraic manipulations

Simplification is a somewhat vague term, and more precises alternatives to simplify exists: powsimp (simplification of exponents), trigsimp (for trigonometric expressions), logcombine, radsimp, together.

17.2.3 Exercises

1. Calculate the expanded form of $(x + y)^6$.
2. Simplify the trigonometric expression $\sin(x) / \cos(x)$

17.3 Calculus

17.3.1 Limits

Limits are easy to use in SymPy, they follow the syntax `limit(function, variable, point)`, so to compute the limit of $f(x)$ as $x \rightarrow 0$, you would issue `limit(f, x, 0)`:

```
>>> limit(sin(x)/x, x, 0)
1
```

you can also calculate the limit at infinity:

```
>>> limit(x, x, oo)
oo

>>> limit(1/x, x, oo)
0

>>> limit(x**x, x, 0)
1
```

17.3.2 Differentiation

You can differentiate any SymPy expression using `diff(func, var)`. Examples:

```
>>> diff(sin(x), x)
cos(x)

>>> diff(sin(2*x), x)
2*cos(2*x)

>>> diff(tan(x), x)
1 + tan(x)**2
```

You can check, that it is correct by:

```
>>> limit((tan(x+y)-tan(x))/y, y, 0)
1 + tan(x)**2
```

Higher derivatives can be calculated using the `diff(func, var, n)` method:

```
>>> diff(sin(2*x), x, 1)
2*cos(2*x)

>>> diff(sin(2*x), x, 2)
-4*sin(2*x)

>>> diff(sin(2*x), x, 3)
-8*cos(2*x)
```

17.3.3 Series expansion

SymPy also knows how to compute the Taylor series of an expression at a point. Use `series(expr, var)`:

```
>>> series(cos(x), x)
1 - x**2/2 + x**4/24 + O(x**6)

>>> series(1/cos(x), x)
1 + x**2/2 + 5*x**4/24 + O(x**6)
```

17.3.4 Exercises

1. Calculate $\lim_{x \rightarrow 0} \sin(x)/x$
2. Calculate the derivative of $\log(x)$ for x .

17.3.5 Integration

SymPy has support for indefinite and definite integration of transcendental elementary and special functions via `integrate()` facility, which uses powerful extended Risch-Norman algorithm and some heuristics and pattern matching. You can integrate elementary functions:

```
>>> integrate(6*x**5, x)
x**6
>>> integrate(sin(x), x)
-cos(x)
>>> integrate(log(x), x)
-x + x*log(x)
>>> integrate(2*x + sinh(x), x)
cosh(x) + x**2
```

Also special functions are handled easily:

```
>>> integrate(exp(-x**2)*erf(x), x)
pi**(1/2)*erf(x)**2/4
```

It is possible to compute definite integral:

```
>>> integrate(x**3, (x, -1, 1))
0
>>> integrate(sin(x), (x, 0, pi/2))
1
>>> integrate(cos(x), (x, -pi/2, pi/2))
2
```

Also improper integrals are supported as well:

```
>>> integrate(exp(-x), (x, 0, oo))
1
>>> integrate(exp(-x**2), (x, -oo, oo))
pi***(1/2)
```

17.3.6 Exercises

17.4 Equation solving

SymPy is able to solve algebraic equations, in one and several variables:

```
In [7]: solve(x**4 - 1, x)
Out[7]: [1, -1, -I, I]
```

As you can see it takes as first argument an expression that is supposed to be equaled to 0. It is able to solve a large part of polynomial equations, and is also capable of solving multiple equations with respect to multiple variables giving a tuple as second argument:

```
In [8]: solve([x + 5*y - 2, -3*x + 6*y - 15], [x, y])
Out[8]: {y: 1, x: -3}
```

It also has (limited) support for trascendental equations:

```
In [9]: solve(exp(x) + 1, x)
Out[9]: [pi*I]
```

Another alternative in the case of polynomial equations is `factor`. `factor` returns the polynomial factorized into irreducible terms, and is capable of computing the factorization over various domains:

```
In [10]: f = x**4 - 3*x**2 + 1
In [11]: factor(f)
Out[11]: (1 + x - x**2)*(1 - x - x**2)

In [12]: factor(f, modulus=5)
Out[12]: (2 + x)**2*(2 - x)**2
```

Sympy is also able to solve boolean equations, that is, to decide if a certain boolean expression is satisfiable or not. For this, we use the function `satisfiable`:

```
In [13]: satisfiable(x & y)
Out[13]: {x: True, y: True}
```

This tells us that $(x \& y)$ is True whenever x and y are both True. If an expression cannot be true, i.e. no values of its arguments can make the expression True, it will return False:

```
In [14]: satisfiable(x & ~x)
Out[14]: False
```

17.4.1 Exercises

1. Solve the system of equations $x + y = 2$, $2 \cdot x + y = 0$
2. Are there boolean values x, y that make $(\sim x \mid y) \& (\sim y \mid x)$ true?

17.5 Linear Algebra

17.5.1 Matrices

Matrices are created as instances from the `Matrix` class:

```
>>> from sympy import Matrix
>>> Matrix([[1,0], [0,1]])
[1, 0]
[0, 1]
```

unlike a NumPy array, you can also put Symbols in it:

```
>>> x = Symbol('x')
>>> y = Symbol('y')
>>> A = Matrix([[1,x], [y,1]])
>>> A
[1, x]
[y, 1]
>>> A**2
```

```
[1 + x*y, 2*x]
[2*y, 1 + x*y]
```

17.5.2 Differential Equations

Sympy is capable of solving (some) Ordinary Differential Equations. `sympy.ode.dsolve` works like this:

```
In [4]: f(x).diff(x, x) + f(x)
Out[4]:
      2
      d
      -----(f(x)) + f(x)
      dx dx
```

```
In [5]: dsolve(f(x).diff(x, x) + f(x), f(x))
Out[5]: C1*sin(x) + C2*cos(x)
```

Keyword arguments can be given to this function in order to help if find the best possible resolution system. For example, if you know that it is a separable equations, you can use keyword `hint='separable'` to force `dsolve` to resolve it as a separable equation.

```
In [6]: dsolve(sin(x)*cos(f(x)) + cos(x)*sin(f(x))*f(x).diff(x), f(x), hint='separable')
Out[6]: -log(1 - sin(f(x))**2)/2 == C1 + log(1 - sin(x)**2)/2
```

17.5.3 Exercises

1. Solve the Bernoulli differential equation $x*f(x).diff(x) + f(x) - f(x)**2$

Warning: TODO: correct this equation and convert to math directive!

2. Solve the same equation using `hint='Bernoulli'`. What do you observe ?

CHAPTER 18

scikit-learn: machine learning in Python

author Fabian Pedregosa

Machine learning is a rapidly-growing field with several machine learning frameworks available for Python:



Prerequisites

- Numpy, Scipy
- IPython
- matplotlib
- scikit-learn (<http://scikit-learn.sourceforge.net>)

Chapters contents

- Loading an example dataset (page 282)
 - Learning and Predicting (page 283)
- Supervised learning (page 283)
 - k-Nearest neighbors classifier (page 283)
 - Support vector machines (SVMs) for classification (page 284)
- Clustering: grouping observations together (page 285)
 - K-means clustering (page 285)
 - Dimension Reduction with Principal Component Analysis (page 286)
- Putting it all together : face recognition with Support Vector Machines (page 287)

18.1 Loading an example dataset



First we will load some data to play with. The data we will use is a very simple flower database known as the Iris dataset.

We have 150 observations of the iris flower specifying some of its characteristics: sepal length, sepal width, petal length and petal width together with its subtype: Iris Setosa, Iris Versicolour, Iris Virginica.

To load the dataset into a Python object:

```
>>> from scikits.learn import datasets
>>> iris = datasets.load_iris()
```

This data is stored in the `.data` member, which is a `(n_samples, n_features)` array.

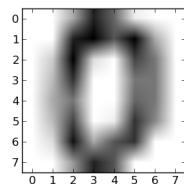
```
>>> iris.data.shape
(150, 4)
```

It is made of 150 observations of irises, each described by the 4 features mentioned earlier.

The information about the class of each observation is stored in the `target` attribute of the dataset. This is an integer ID array of length `n_samples`:

```
>>> iris.target.shape
(150,)
>>> import numpy as np
>>> np.unique(iris.target)
[0, 1, 2]
```

An example of reshaping data: the digits dataset



The digits dataset is made of 1797 images, where each one is a 8x8 pixel image representing a hand-written digits

```
>>> digits = datasets.load_digits()
>>> digits.images.shape
(1797, 8, 8)
>>> import pylab as pl
>>> pl.imshow(digits.images[0], cmap=pl.cm.gray_r)
<matplotlib.image.AxesImage object at ...>
```

To use this dataset with the scikit, we transform each 8x8 image in a feature vector of length 64

```
>>> data = digits.images.reshape((digits.images.shape[0], -1))
```

18.1.1 Learning and Predicting

Now that we've got some data, we would like to learn from the data and predict on new one. In scikit-learn, we learn from existing data by creating an estimator and calling its `fit(X, Y)` method.

```
>>> from scikits.learn import svm
>>> clf = svm.LinearSVC()
>>> clf.fit(iris.data, iris.target) # learn form the data
```

Once we have learned from the data, we can access the parameters of the model:

```
>>> clf.coef_
...
```

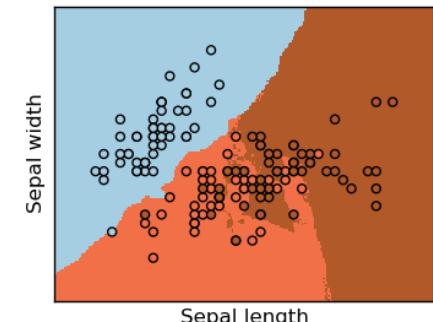
And it can be used to predict the most likely outcome on unseen data:

```
>>> clf.predict([[ 5.0,  3.6,  1.3,  0.25]])
array([0], dtype=int32)
```

18.2 Supervised learning

18.2.1 k-Nearest neighbors classifier

The simplest possible classifier is the nearest neighbor: given a new observation, take the label of the closest learned observation.



KNN (k nearest neighbors) classification example:

```
>>> # Create and fit a nearest-neighbor classifier
>>> from scikits.learn import neighbors
>>> knn = neighbors.NeighborsClassifier()
>>> knn.fit(iris.data, iris.target)
NeighborsClassifier(n_neighbors=5, leaf_size=20, algorithm='auto')
>>> knn.predict([[0.1, 0.2, 0.3, 0.4]])
array([0])
```

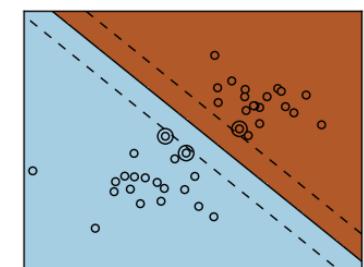
Training set and testing set

When experimenting with learning algorithm, it is important not to test the prediction of an estimator on the data used to fit the estimator.

18.2.2 Support vector machines (SVMs) for classification

Linear Support Vector Machines

SVMs try to build a plane maximizing the margin between the two classes. It selects a subset of the input, called the support vectors, which are the observations closest to the separating plane.



```
>>> from scikits.learn import svm
>>> svc = svm.SVC(kernel='linear')
>>> svc.fit(iris.data, iris.target)
```

18.2. Supervised learning

```
SVC(kernel='linear', C=1.0, probability=False, degree=3, coef0=0.0, tol=0.001,
     shrinking=True, gamma=0.0)
```

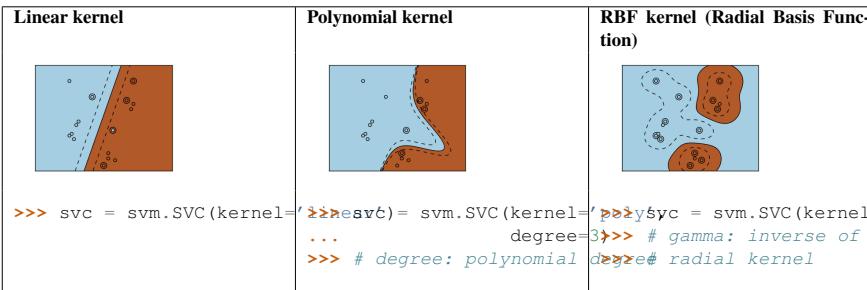
There are several support vector machine implementations in scikit-learn. The most used ones are `svm.SVC`, `svm.NuSVC` and `svm.LinearSVC`.

Excercise

Try classifying the digits dataset with `svm.SVC`. Leave out the last 10% and test prediction performance on these observations.

Using kernels

Classes are not always separable by a hyper-plane, thus it would be desirable to build a decision function that is not linear but that may be for instance polynomial or exponential:



Exercise

Which of the kernels noted above has a better prediction performance on the digits dataset ?

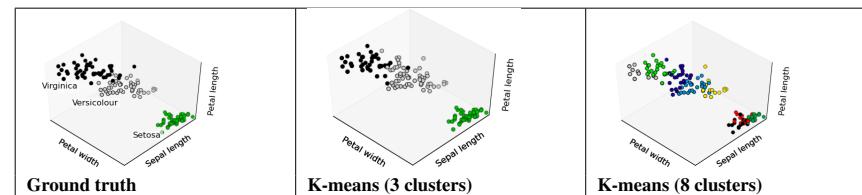
18.3 Clustering: grouping observations together

Given the iris dataset, if we knew that there were 3 types of Iris, but did not have access to their labels: we could try a **clustering task**: split the observations into groups called *clusters*.

18.3.1 K-means clustering

The simplest clustering algorithm is the k-means.

```
>>> from scikits.learn import cluster, datasets
>>> iris = datasets.load_iris()
>>> k_means = cluster.KMeans(k=3)
>>> k_means.fit(iris.data)
KMeans(verbose=0, k=3, max_iter=300, init='k-means++',...
>>> print k_means.labels_[:10]
[1 1 1 1 0 0 0 0 2 2 2 2 2]
>>> print iris.target[:10]
[0 0 0 0 1 1 1 1 2 2 2 2]
```



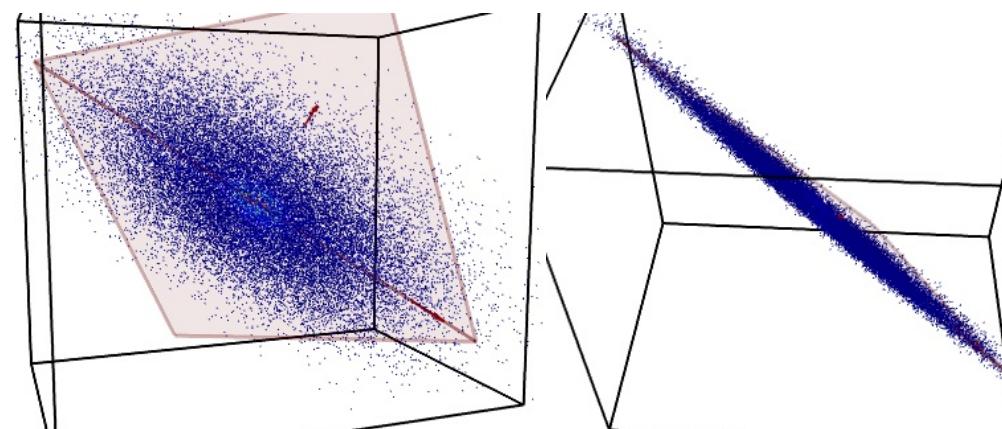
Application to Image Compression

Clustering can be seen as a way of choosing a small number of observations from the information. For instance, this can be used to posterize an image (conversion of a continuous gradation of tone to several regions of fewer tones):

```
>>> import scipy as sp
>>> lena = sp.lena()
>>> X = lena.reshape((-1, 1)) # We need an (n_sample, n_feature) array
>>> k_means = cluster.KMeans(k=5)
>>> k_means.fit(X)
>>> values = k_means.cluster_centers_.squeeze()
>>> labels = k_means.labels_
>>> lena_compressed = np.choose(labels, values)
>>> lena_compressed.shape = lena.shape
```



18.3.2 Dimension Reduction with Principal Component Analysis



The cloud of points spanned by the observations above is very flat in one direction, so that one feature can almost be exactly computed using the other. PCA finds the directions in which the data is not flat

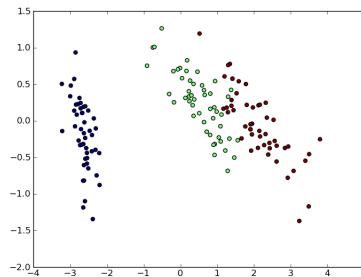
When used to *transform* data, PCA can reduce the dimensionality of the data by projecting on a principal subspace.

Warning: Depending on your version of scikit-learn PCA will be in module `decomposition` or `pca`.

```
>>> from scikits.learn import decomposition
>>> pca = decomposition.PCA(n_components=2)
>>> pca.fit(iris.data)
PCA(copy=True, n_components=2, whiten=False)
>>> X = pca.transform(iris.data)
```

Now we can visualize the (transformed) iris dataset!

```
>>> import pylab as pl
>>> pl.scatter(X[:, 0], X[:, 1], c=iris.target)
>>> pl.show()
```



PCA is not just useful for visualization of high dimensional datasets. It can also be used as a preprocessing step to help speed up supervised methods that are not computationally efficient with high dimensions.

18.4 Putting it all together : face recognition with Support Vector Machines

An example showcasing face recognition using Principal Component Analysis for dimension reduction and Support Vector Machines for classification.



```
"""
Stripped-down version of the face recognition example by Olivier Grisel

http://scikit-learn.sourceforge.net/dev/auto_examples/applications/face_recognition.html

## original shape of images: 50, 37
"""

import numpy as np
from scikits.learn import cross_val, datasets, decomposition, svm

# ..
# .. load data ..
lfw_people = datasets.fetch_lfw_people(min_faces_per_person=70, resize=0.4)
faces = np.reshape(lfw_people.data, (lfw_people.target.shape[0], -1))
train, test = iter(cross_val.StratifiedKFold(lfw_people.target, k=4)).next()
X_train, X_test = faces[train], faces[test]
y_train, y_test = lfw_people.target[train], lfw_people.target[test]

# ..
# .. dimension reduction ..
pca = decomposition.RandomizedPCA(n_components=150, whiten=True)
pca.fit(X_train)
X_train_pca = pca.transform(X_train)
X_test_pca = pca.transform(X_test)

# ..
# .. classification ..
clf = svm.SVC(C=5., gamma=0.001)
clf.fit(X_train_pca, y_train)

# ..
# .. predict on new images ..
for i in range(1, 10):
    print lfw_people.target_names[clf.predict(X_test_pca[i])[0]]
    _ = pl.imshow(X_test[i].reshape(50, 37), cmap=pl.cm.gray)
    _ = raw_input()
```

Full code: `faces.py`

Bibliography

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D

diff, 277, 280
differentiation, 277
dsolve, 280

E

equations
algebraic, 278
differential, 280

I

integration, 278

M

Matrix, 279

P

Python Enhancement Proposals
PEP 255, 153
PEP 3118, 188
PEP 3129, 163
PEP 318, 155, 163
PEP 342, 153
PEP 343, 163
PEP 380, 155
PEP 8, 158

S

solve, 278