Python Scientific lecture notes

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EuroScipy tutorial team

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Part I

Getting started with Python for science

Scientific computing with tools and workflow

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1.1 Why Python?

1.1.1 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.

1.1.2 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.

1.1.3 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.

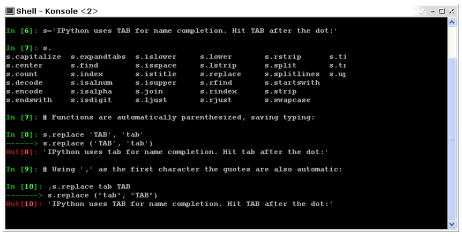
What about Python?

- 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.

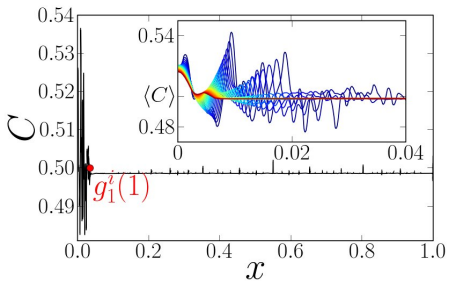
1.2 Scientific Python building blocks

Unlike Matlab, scilab or R, Python does not come with a pre-bundled set of modules for scientific computing. Below are the basic building blocks that can be combined to optain a scientific-computing environment:

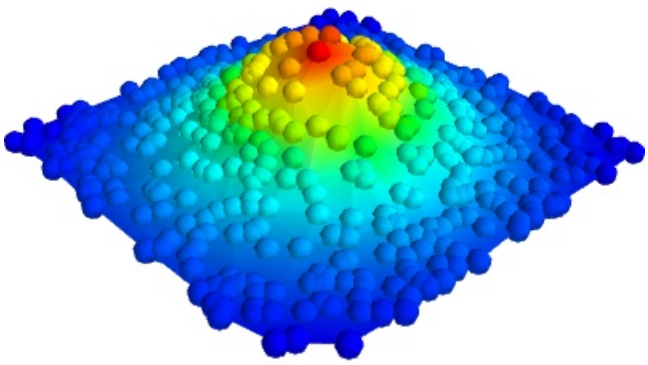
- **Python**, a generic and modern computing language
  - Python language: data types (`string`, `int`), flow control, data collections (lists, dictionaries), patterns, etc.
  - Modules of the standard library.
  - A large number of specialized modules or applications written in Python: web protocols,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



- **IPython**, an advanced **Python shell** http://ipython.scipy.org/moin/
- **Numpy** : provides powerful **numerical arrays** objects, and routines to manipulate them. http://www.numpy.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/

1.3 The interactive workflow: IPython and a text editor

Interactive work to test and understand algorithm: In this section, we describe an interactive workflow with IPython that is handy to explore and understand algorithms.

Python is a general-purpose language. As such, there is not one blessed environement to work into, and not only one way of using it. Although this makes it harder for beginners to find their way, it makes it possible for Python to be used to write programs, in web servers, or embedded devices.

Note: Reference document for this section:

IPython user manual: http://ipython.org/ipython-doc/dev/index.html

---

1.3.1 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.
```

1.3.2 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, We 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

While it is tempting to work only with scripts, that is a file full of instructions following each other, do plan to progressively evolve the script to a set of functions:

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

CHAPTER 2

The Python language

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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.

2.1 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 an 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.

2.2 Basic types

2.2.1 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
```

- 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
```

2.2.2 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 perfomed 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,                  # tripling the quotes allows the
       how are you'''          # 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                                 Traceback (most recent call
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
```

2.3 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.

2.4 Control Flow

Controls the order in which the code is executed.

2.4.1 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.

2.4.2 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
```

2.4.3 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
```

2.4.4 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 else [1]

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

- `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`.

2.4.5 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():
...     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
```

2.4.6 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:

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

2.5 Defining functions

2.5.1 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.

2.5.2 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]: 7.0649999999999995
```

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.

2.5.3 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.

2.5.4 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*.

2.5.5 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
```

2.5.6 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}
```

2.5.7 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 0xeaa0f0>
Namespace:  Interactive
File:               /Users/cburns/src/scipy2009/.../<ipython console>
Definition: funcname(params)
Docstring:
    Concise one-line sentence describing the function.

    Extended summary which can contain multiple paragraphs.
```

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

2.5.8 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}
```

2.5.9 Methods

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

2.5.10 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`

2.6 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)).

2.6.1 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 interpeter'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`.

2.6.2 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 vise-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.

2.6.3 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)
```

2.6.4 '__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
```

2.6.5 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/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.

2.6.6 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/      setupscons.py@  THANKS.txt@
fftpack/        linsolve/    setupscons.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
setupscons.py@
filters.py@  info.pyc      measurements.py@   _ni_support.py@
setupscons.pyc
filters.pyc  __init__.py@  measurements.pyc   _ni_support.pyc  tests/
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.
```

2.6.7 Good practices

Note: Good practices

- **Indentation: no choice!**

Indenting is compulsory in Python. Every commands 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**

2.7 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

2.7.1 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.

2.8 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

---

2.8.1 `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.swo',
 '.python_language.rst.swp',
 '.view_array.py.swp',
 '_static',
 '_templates',
 'basic_types.rst',
 'conf.py',
 'control_flow.rst',
 'debugging.rst',
 ...
```

Make a directory:

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

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

Rename the directory:

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

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

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

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

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

Delete a file:

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

In [45]: fp.close()

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

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

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

os.path: path manipulations

os.path provides common operations on pathnames.

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

In [71]: fp.close()

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

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

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

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

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

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

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

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

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

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

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

Running an external command

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

Walking a directory

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

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

```
/Users/cburns/src/scipy2009/scipy_2009_tutorial/source/control_flow.rst
...
```

Environment variables:

```
In [9]: import os

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

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

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

2.8.2 `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.

2.8.3 `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']
```

2.8.4 `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',
 ...
```

2.8.5 `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

2.9 Exception 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.

2.9.1 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.

2.9.2 Catching exceptions

try/except

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

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

try/finally

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

```
---------------------------------------------------------------------------
ValueError: invalid literal for int() with base 10: 'a'
```

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

Easier to ask for forgiveness than for permission

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

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

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

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

2.9.3 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\xabl'

    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)

2.10 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.

CHAPTER 3

NumPy: creating and manipulating numerical data

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

This chapter gives an overview of Numpy, the core tool for performant numerical computing with Python.

3.1 The numpy array object

Section contents

- What are Numpy and numpy arrays (page 40)
- Reference documentation (page 41)
- Creating arrays (page 41)
- Basic data types (page 43)
- Basic visualization (page 44)
- Indexing and slicing (page 47)
- Copies and views (page 48)
- Fancy indexing (page 50)

3.1.1 What are Numpy and numpy arrays

Python has built-in:

- containers: lists (costless insertion and append), dictionnaries (fast lookup)
- high-level number objects: integers, floating point

Numpy is:

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

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

For example:

An array containing:

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

Why it is useful: Memory-efficient and fast container for numerical operations.

```
In [1]: l = range(1000)

In [2]: %timeit [i**2 for i in l]
1000 loops, best of 3: 403 us per loop

In [3]: a = np.arange(1000)

In [4]: %timeit a**2
100000 loops, best of 3: 12.7 us per loop
```

3.1.2 Reference documentation

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

```
>>> help(np.array)
Help on built-in function array in module numpy.core.multiarray:

array(...)
    array(object, dtype=None, copy=True, order=None, subok=False, ...
...
```

- 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.
...
```

3.1.3 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
```

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

>>> c = np.array([[[1], [2]], [[3], [4]]])
>>> c
array([[[1],
        [2]],

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

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 (exlusive), step
>>> b
array([1, 3, 5, 7])
```

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])
```

- 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]))
>>> d
array([[1, 0, 0, 0],
       [0, 2, 0, 0],
       [0, 0, 3, 0],
       [0, 0, 0, 4]])
```

- `np.random`: random numbers (Mersenne Twister PRNG):

```
>>> a = np.random.rand(4)        # uniform in [0, 1]
>>> a
array([ 0.95799151,  0.14222247,  0.08777354,  0.51887998])

>>> b = np.random.randn(4)       # Gaussian
>>> b
array([ 0.37544699, -0.11425369, -0.47616538,  1.79664113])

>>> np.random.seed(1234)         # Setting the random seed
```

Exercise: Array creation

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

Exercise: Tiling for array creation

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]]
```

3.1.4 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')
```

There are also other types:

Complex

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

Bool

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

Strings

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

Much more int32/int64...

3.1.5 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:

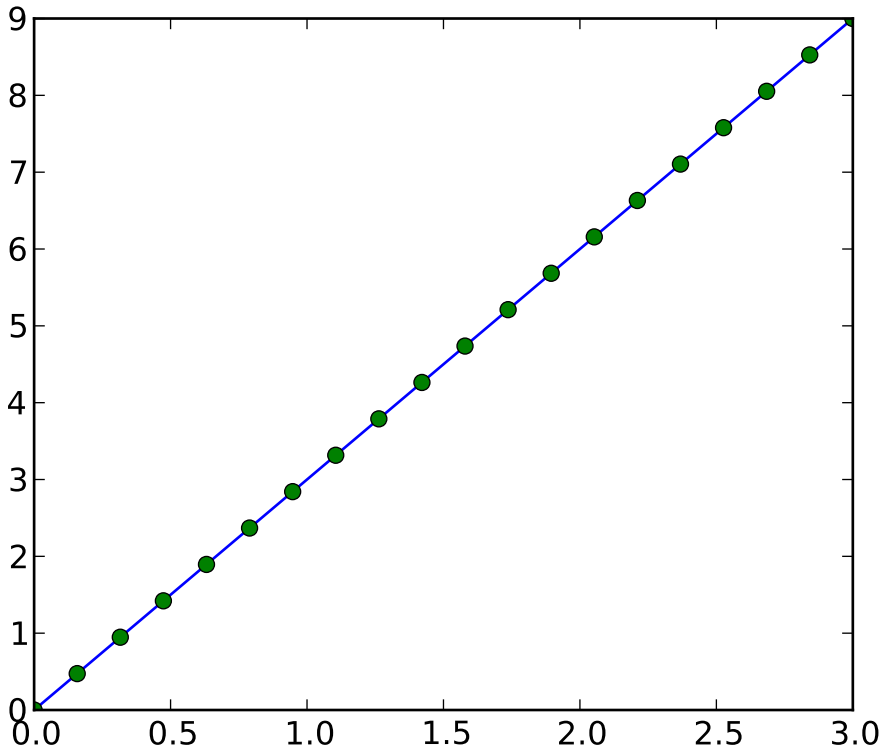
```
>>> import matplotlib.pyplot as plt  # the tidy way
```

The recommended way of working is use `IPython`, started in `pylab` mode:

```
$ ipython -pylab
```

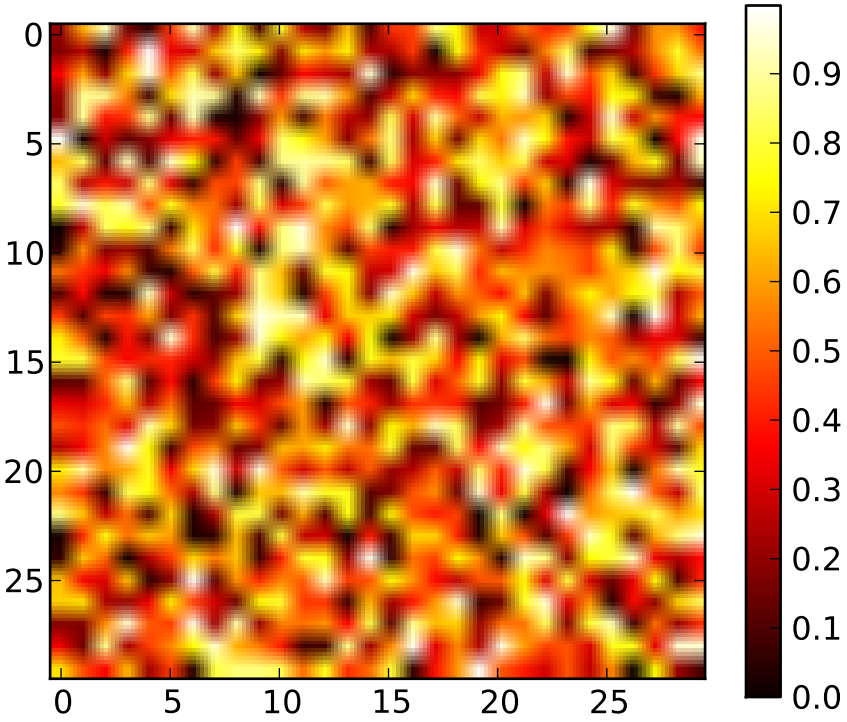
1D plotting

```
>>> x = np.linspace(0, 3, 20)
>>> y = np.linspace(0, 9, 20)
>>> plt.plot(x, y)       # line plot
[<matplotlib.lines.Line2D object at ...>]
>>> plt.plot(x, y, 'o')  # dot plot
[<matplotlib.lines.Line2D object at ...>]
>>> plt.show()           # <-- shows the plot (not needed with Ipython)
```



2D arrays (such as images)

```
>>> image = np.random.rand(30, 30)
>>> plt.imshow(image, cmap=plt.cm.gray)
<matplotlib.image.AxesImage object at ...>
>>> plt.colorbar()
<matplotlib.colorbar.Colorbar instance at ...>
>>> plt.show()
```

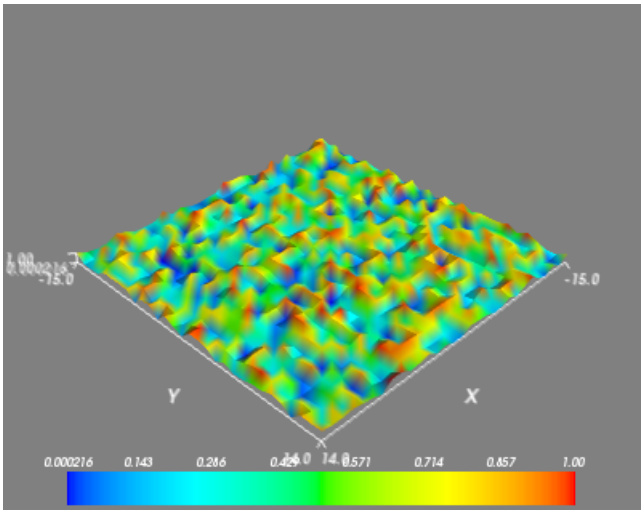


See Also:

More in the *matplotlib chapter* (page 88)

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()
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://github.enthought.com/mayavi/mayavi

See Also:

More in the *Mayavi chapter* (page 254)

3.1.6 Indexing and slicing

The items of an array can be accessed and assigned to the same way as other Python sequences (e.g. lists)

```
>>> 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(3))
>>> a
array([[0, 0, 0],
       [0, 1, 0],
       [0, 0, 2]])
>>> a[1, 1]
1
>>> a[2, 1] = 10 # third line, second column
>>> a
array([[ 0,  0,  0],
       [ 0,  1,  0],
       [ 0, 10,  2]])
>>> a[1]
array([0, 1, 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])
```

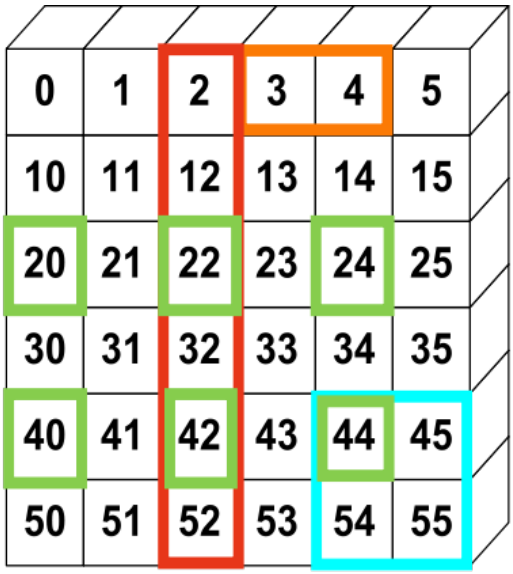
All three slice components are not required: by default, `start` is 0, `end` is the last and `step` is 1:

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

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

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]])
```



3.1.7 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:

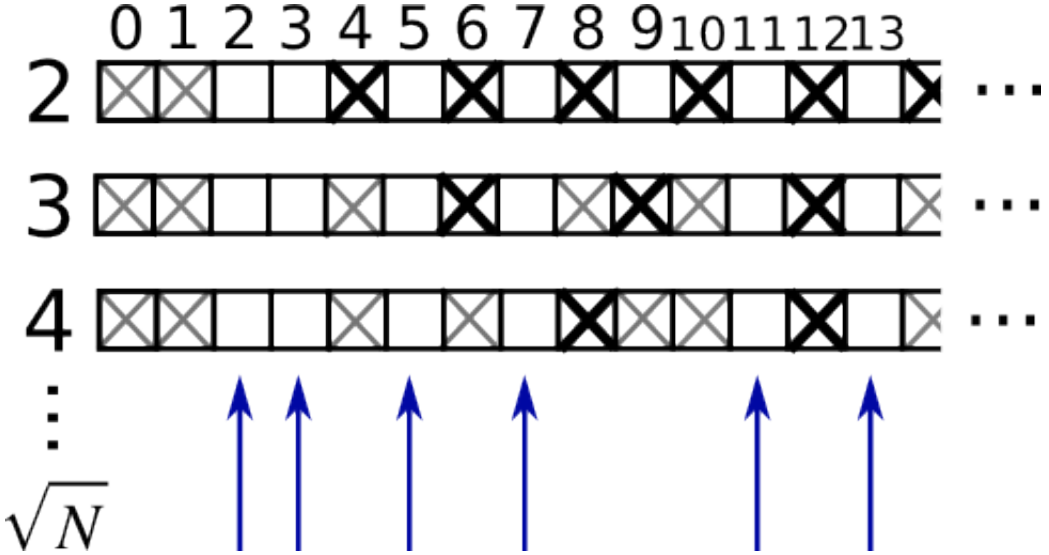
```
>>> a = np.arange(10)
>>> a
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> b = a[::2]; b
array([0, 2, 4, 6, 8])
>>> b[0] = 12
>>> b
array([12,  2,  4,  6,  8])
>>> a   # (!)
array([12,  1,  2,  3,  4,  5,  6,  7,  8,  9])

>>> 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.

Warning: The transpose is a view
As a result, a matrix cannot be made symmetric in-place:

```
>>> a = np.ones((100, 100))
>>> a += a.T
>>> a
array([[ 2.,  2.,  2., ...,  2.,  2.,  2.],
       [ 2.,  2.,  2., ...,  2.,  2.,  2.],
       [ 2.,  2.,  2., ...,  2.,  2.,  2.],
       ...,
       [ 3.,  3.,  3., ...,  2.,  2.,  2.],
       [ 3.,  3.,  3., ...,  2.,  2.,  2.],
       [ 3.,  3.,  3., ...,  2.,  2.,  2.]])
```

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

3.1.8 Fancy indexing

Numpy arrays can be indexed with slices, but also with boolean or integer arrays (**masks**). This method is called *fancy indexing*. It creates **copies not view**.

Using boolean masks

```
>>> np.random.seed(3)
>>> a = np.random.random_integers(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, 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])
```

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

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([2, 3, 2, 4, 2])
```

New values can be assigned with this kind of indexing:

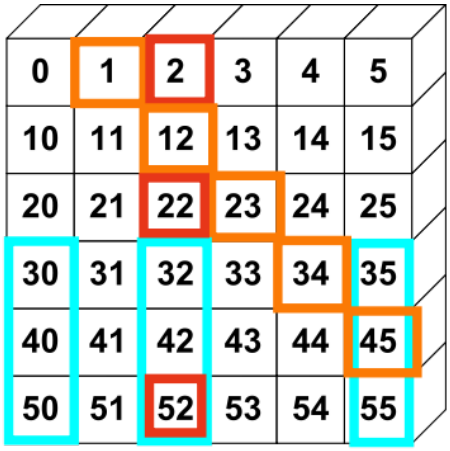
```
>>> a[[9, 7]] = -10
>>> a
array([  0,   1,   2,   3,   4,   5,   6, -10,   8, -10])
```

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)
```

The image below illustrates various fancy indexing applications

```
>>> 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]])
```

3.2 Numerical operations on arrays

Section contents

- Elementwise operations (page 51)
- Basic reductions (page 53)
- Broadcasting (page 57)
- Array shape manipulation (page 60)
- Sorting data (page 63)
- Some exercices (page 64)
- Summary (page 69)

3.2.1 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 + 1) - j
array([ 2,  3,  6, 13, 28])
```

Warning: Array multiplication is not matrix multiplication:

```
>>> c = np.ones((3, 3))
>>> c * c                   # NOT matrix multiplication!
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)
>>> np.logical_or(a, b)
array([ True,  True,  True, False], dtype=bool)
>>> np.logical_and(a, b)
array([ True, False, False, False], dtype=bool)
```

Note: For arrays: "`np.logical_and`" and "`np.logical_or`" for logical operations, not "`and`" and "`or`".

Shape mismatches:

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

Transposition:

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

```
       [ 1.,  0.,  0.],
       [ 1.,  1.,  0.]])
```

Note: Linear algebra

The sub-module `np.linalg` implements basic linear algebra, such as eigenvalue decomposition, solving linear systems... However, it is not garantied to be compiled using efficient routines, and thus we recommend to use `scipy.linalg`, as detailed in section *Linear algebra operations: scipy.linalg* (page 109)

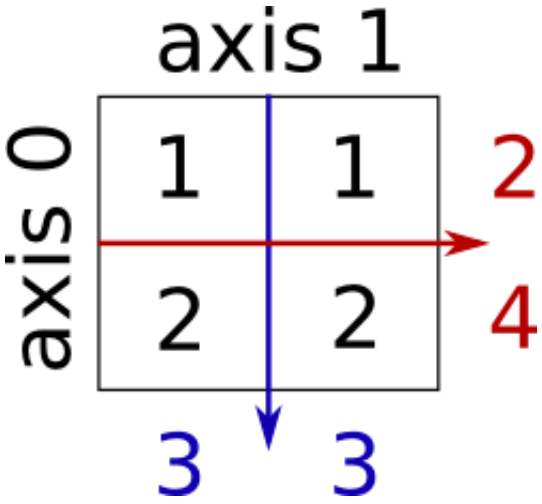
Exercice

Generate arrays `[2**0, 2**1, 2**2, 2**3, 2**4]` and `a_j = 2^(3*j) - j`

3.2.2 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]
```

```
1.14764...
>>> x[0, 1, :].sum()
1.14764...
```

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
```

- 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
```

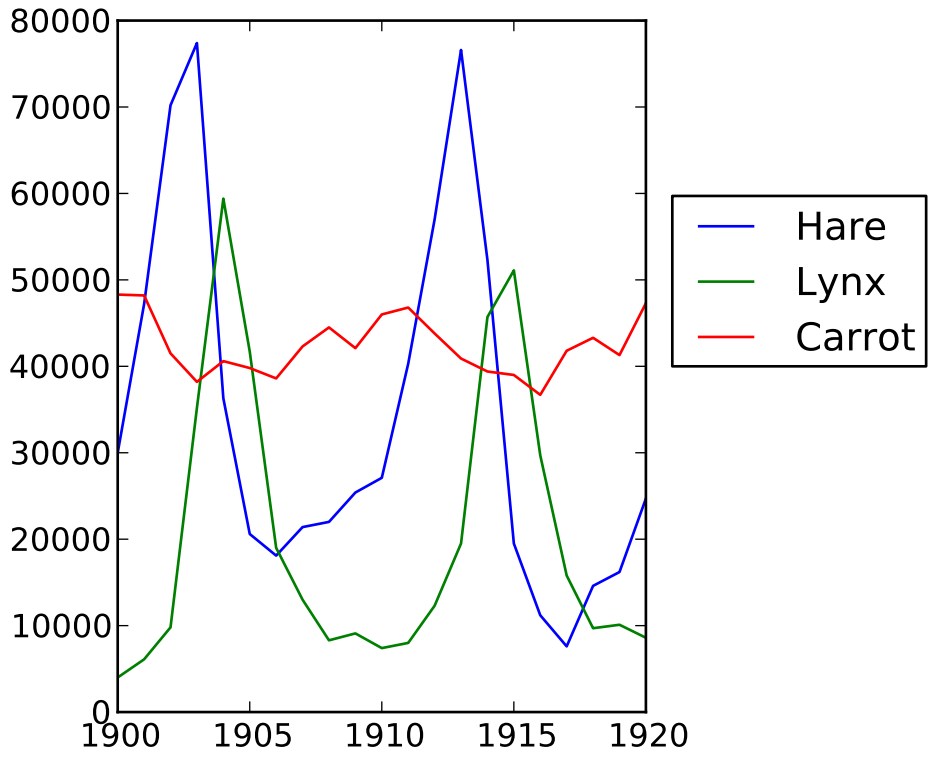
```
>>> a = np.array([1, 2, 3, 2])
>>> b = np.array([2, 2, 3, 2])
>>> c = np.array([6, 4, 4, 5])
>>> ((a <= b) & (b <= c)).all()
True
```

- ... 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

>>> from matplotlib import pyplot as plt
>>> plt.axes([0.2, 0.1, 0.5, 0.8])
<matplotlib.axes.Axes object at ...>
>>> plt.plot(year, hares, year, lynxes, year, carrots)
[<matplotlib.lines.Line2D object at ...>, ...]
>>> plt.legend(('Hare', 'Lynx', 'Carrot'), loc=(1.05, 0.5))
<matplotlib.legend.Legend object at ...>
```



The mean populations over time:

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

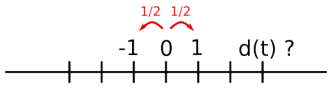
The sample standard deviations:

```
>>> populations.std(axis=0)
array([ 20897.90645809,  16254.59153691,   3322.50622558])
```

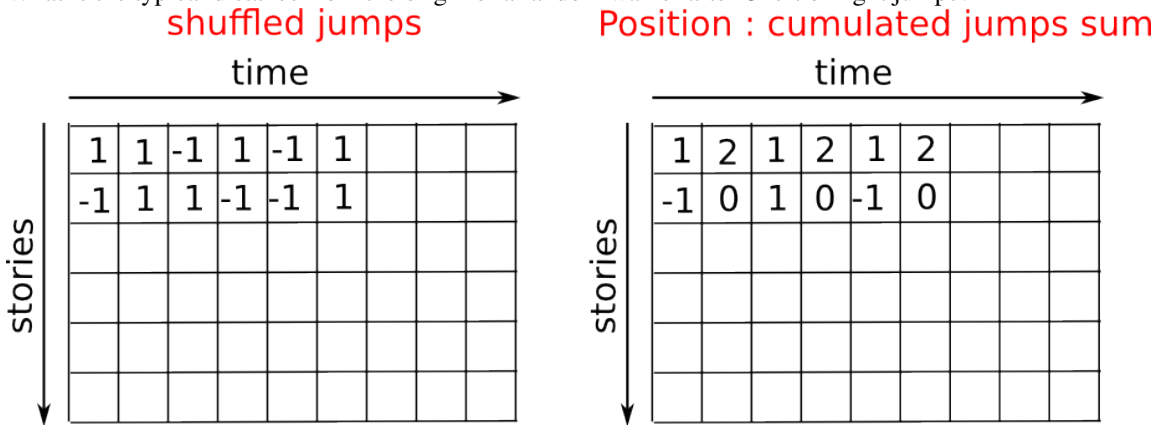
Which species has the highest population each year?

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

Example: diffusion simulation using a random walk algorithm



What is the typical distance from the origin of a random walker after `t` left or right jumps?




```
>>> n_stories = 1000 # number of walkers
>>> t_max = 200      # time during which we follow the walker
```

We randomly choose all the steps 1 or -1 of the walk:

```
>>> t = np.arange(t_max)
>>> steps = 2 * np.random.random_integers(0, 1, (n_stories, t_max)) - 1
>>> np.unique(steps) # Verification: all steps are 1 or -1
array([-1,  1])
```

We build the walks by summing steps along the time:

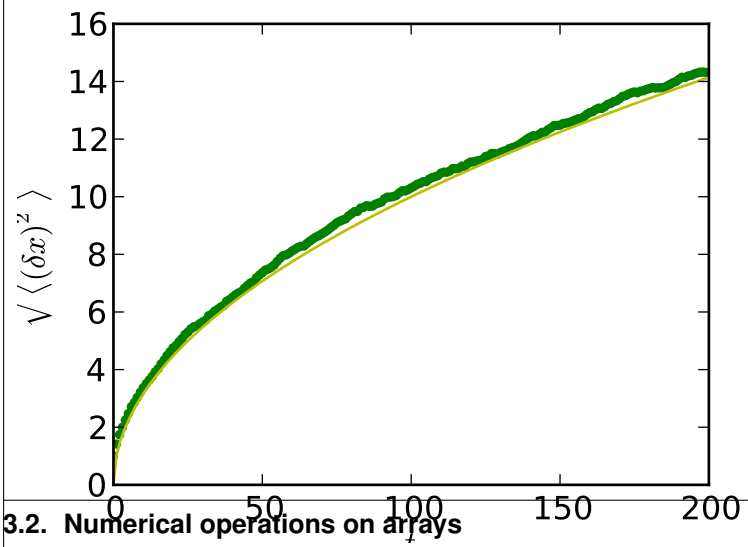
```
>>> positions = np.cumsum(steps, axis=1) # axis = 1: dimension of time
>>> sq_distance = positions**2
```

We get the mean in the axis of the stories:

```
>>> mean_sq_distance = np.mean(sq_distance, axis=0)
```

Plot the results:

```
>>> plt.figure(figsize=(4, 3))
<matplotlib.figure.Figure object at ...>
>>> plt.plot(t, np.sqrt(mean_sq_distance), 'g.', t, np.sqrt(t), 'y-')
[<matplotlib.lines.Line2D object at ...>, <matplotlib.lines.Line2D object at ...>]
>>> plt.xlabel(r"$t$")
<matplotlib.text.Text object at ...>
>>> plt.ylabel(r"$\sqrt{\langle (\delta x)^2 \rangle}$")
<matplotlib.text.Text object at ...>
```



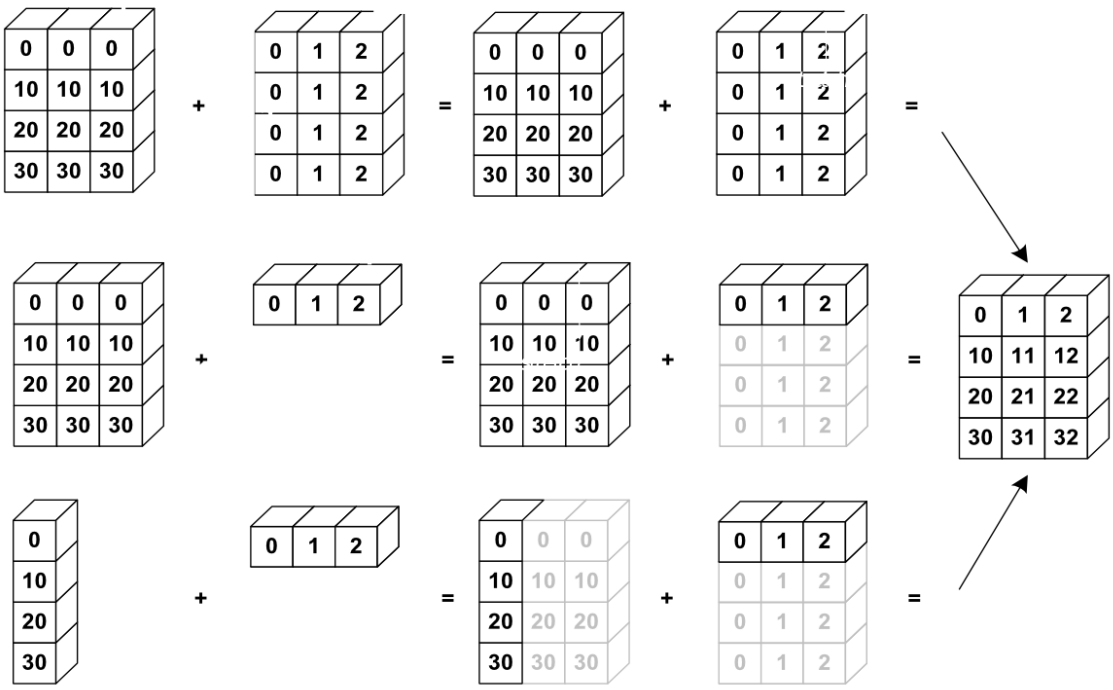
The RMS distance grows as the square root of the time!

3.2.3 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!:

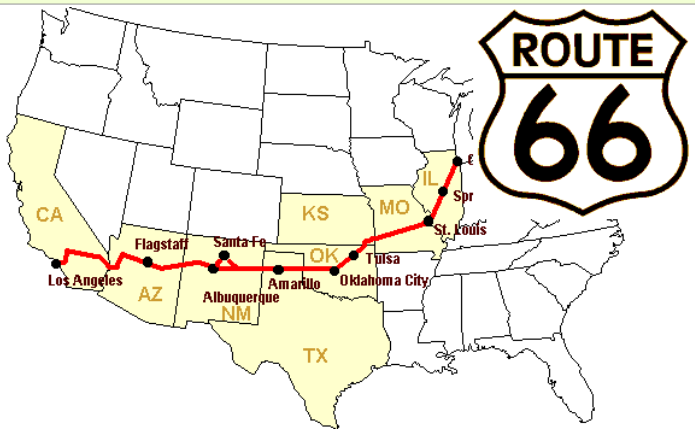
```
>>> a = np.ones((4, 5))
>>> a[0] = 2  # we assign an array of dimension 0 to an array of dimension 1
>>> a
array([[ 2.,  2.,  2.,  2.,  2.],
       [ 1.,  1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.]])
```

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

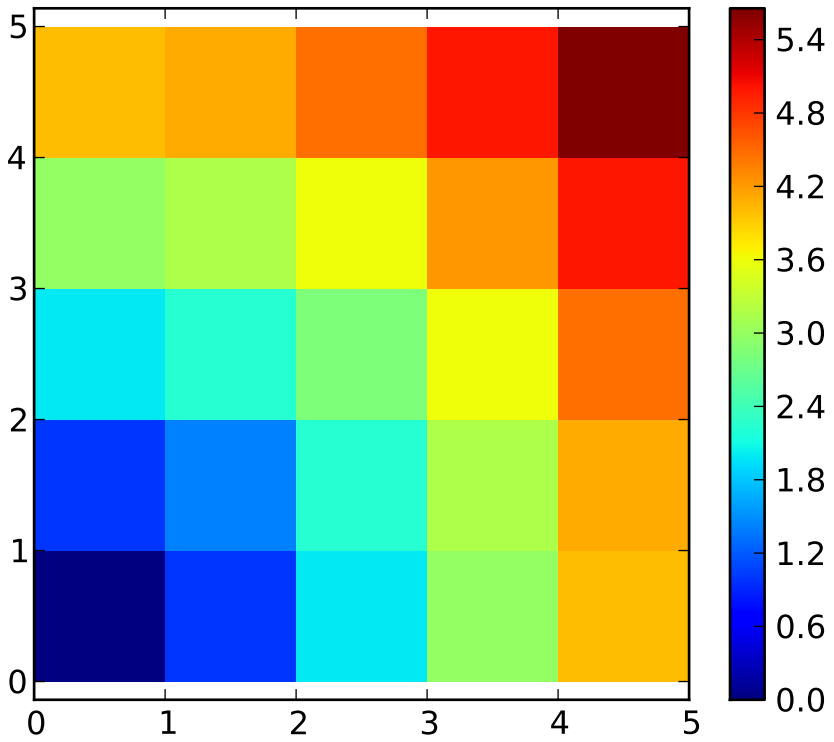
Let's construct an array of distances (in miles) between cities of Route 66: Chicago, Springfield, Saint-Louis, Tulsa, Oklahoma City, Amarillo, Santa Fe, Albuquerque, Flagstaff and Los Angeles.

```
>>> 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]])
```



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 of 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)     # doctest: +ELLIPSIS
   <matplotlib.collections.PolyCollection object at ...>
   >>> plt.colorbar()     # doctest: +ELLIPSIS
   <matplotlib.colorbar.Colorbar instance at ...>
   >>> plt.axis('equal')
   (0.0, 200.0, 0.0, 16.0)
```



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!

3.2.4 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
```

Views and copies

`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: reshape may also return a copy!

```
>>> 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 the section on *the memory layout of an array* (page 76) 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
```

We can use f2py to wrap this fortran code in Python: `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

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

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}
0.0
```

Linear operators on such block vectors have similar block structure:

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

```
>>> 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 4x4 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.

3.2.5 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)
>>> j
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)
```

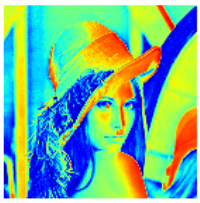
3.2.6 Some exercices

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:

```
>>> from scipy import misc
>>> lena = misc.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 = misc.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, cmap=plt.cm.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`

```
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 we 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: Array 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)
```

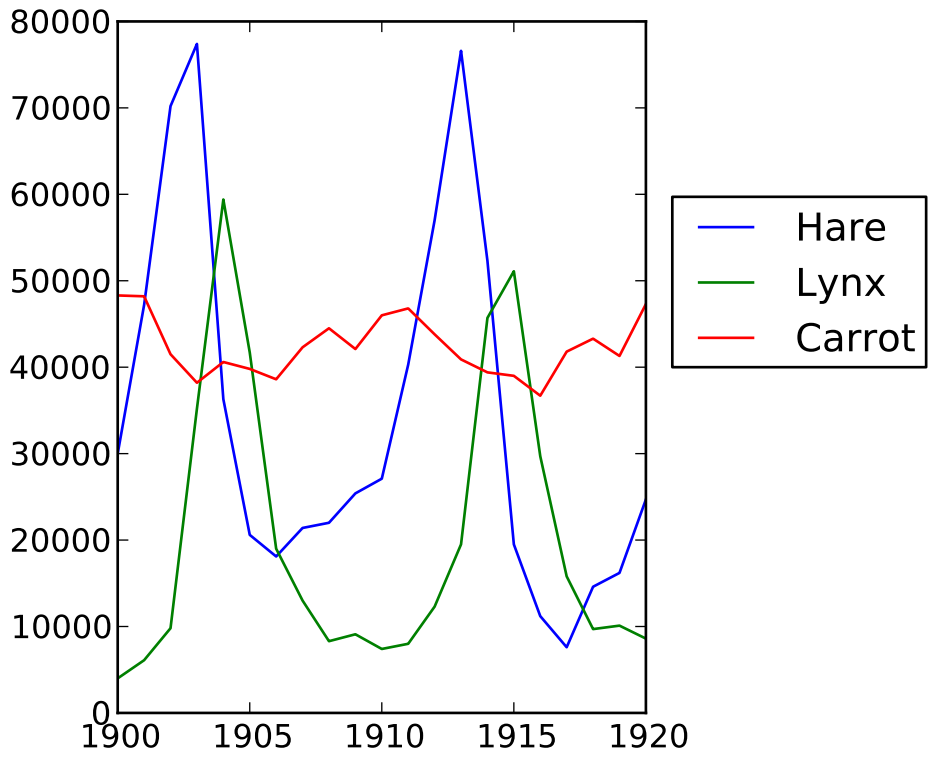
   elementwise with the array `b = np.array([1., 5, 10, 15, 20])`. (Hint: `np.newaxis`).

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: 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])
<matplotlib.axes.Axes object at ...>
>>> plt.plot(year, hares, year, lynxes, year, carrots)
[<matplotlib.lines.Line2D object at ...>, ...]
>>> plt.legend(('Hare', 'Lynx', 'Carrot'), loc=(1.05, 0.5))
<matplotlib.legend.Legend object at ...>
```



Computes and print, 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: Crude integral approximations

Write a function `f(a, b, c)` that returns $a^b - c$. Form a 24x12x6 array containing its values in parameter ranges `[0,1] x [0,1] x [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: $\ln 2 - \frac{1}{2} \approx 0.1931\ldots$ — 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: Mandelbrot set

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

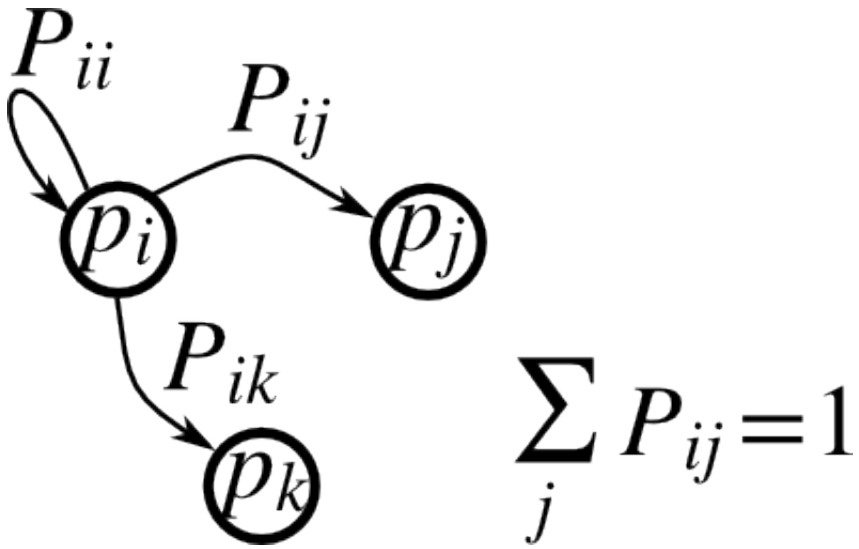
```
N_max = 50
some_threshold = 50

c = x + 1j*y

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

Point (x, y) belongs to the Mandelbrot set if $|c|$ < `some_threshold`.
Do this computation by:

1. Construct a grid of c = x + 1j*y values in range [-2, 1] x [-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])
<matplotlib.image.AxesImage object at ...>
>>> plt.gray()
>>> plt.savefig('mandelbrot.png')
```

Exercise: Markov chain



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

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

Remember to normalize the eigenvector — I didn't...

- Checks if `p_50` and `p_stationary` are equal to tolerance 1e-5

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

3.2.7 Summary

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.

3.3 More elaborate arrays

Section contents

- More data types (page 70)
- Structured data types (page 71)
- Masked arrays (page 72)
- Under the hood: the memory layout of a numpy array (page 76)

3.3.1 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                       # still floating-point
array([ 2.,  1.,  2.])
>>> 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
(4294967295, 4294967295)
>>> np.iinfo(np.uint64).max, 2**64 - 1
(18446744073709551615L, 18446744073709551615L)
```

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)

3.3.2 Structured 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, 0.37), ('BETA', 1, 0.11), ('TAU', 1,   0.13),
...               ('ALFA', 1.5, 0.37), ('ALFA', 3, 0.11), ('TAU', 1.2, 0.13)]
>>> samples
array([('ALFA', 1.0, 0.37), ('BETA', 1.0, 0.11), ('TAU', 1.0, 0.13),
       ('ALFA', 1.5, 0.37), ('ALFA', 3.0, 0.11), ('TAU', 1.2, 0.13)],
      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([ 0.37,  0.11,  0.13,  0.37,  0.11,  0.13])
>>> samples[0]
('ALFA', 1.0, 0.37)

>>> samples[0]['sensor_code'] = 'TAU'
>>> samples[0]
('TAU', 1.0, 0.37)
```

Multiple fields at once:

```
>>> samples[['position', 'value']]
array([(1.0, 0.37), (1.0, 0.11), (1.0, 0.13), (1.5, 0.37), (3.0, 0.11),
       (1.2, 0.13)],
      dtype=[('position', '<f8'), ('value', '<f8')])
```

Fancy indexing works, as usual:

```
>>> samples[samples['sensor_code'] == 'ALFA']
array([('ALFA', 1.5, 0.37), ('ALFA', 3.0, 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.

3.3.3 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 = np.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!

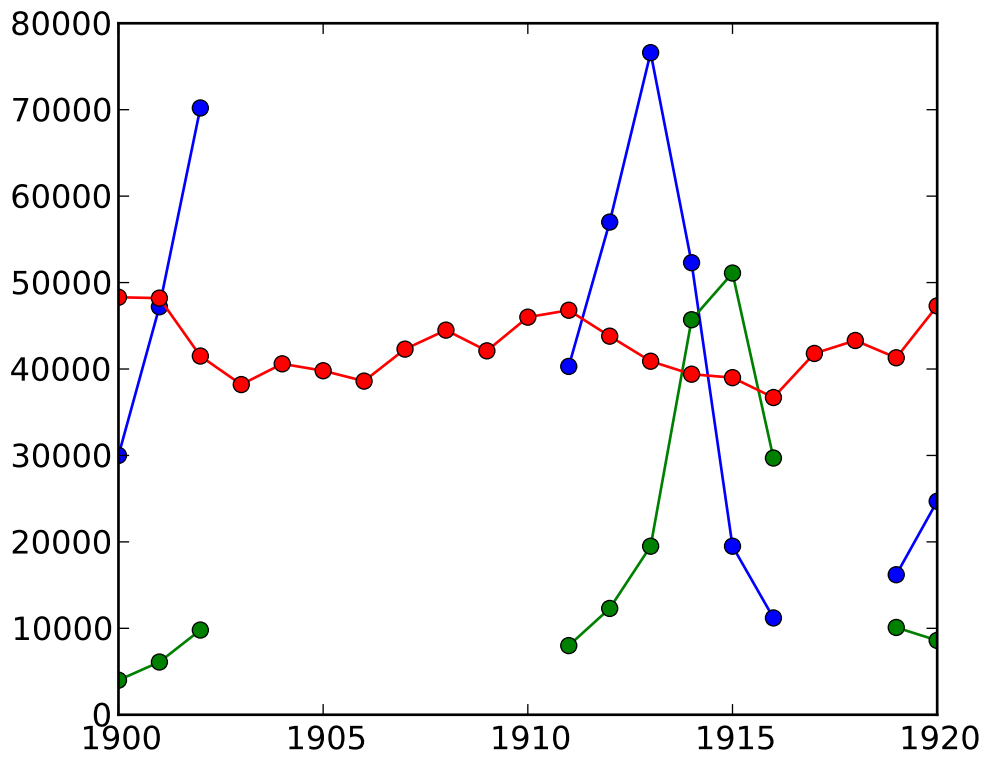
Example: Masked statistics

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)))
>>> # '&' means 'and' and '|' means 'or'
>>> 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-')
[<matplotlib.lines.Line2D object at ...>, ...]
```

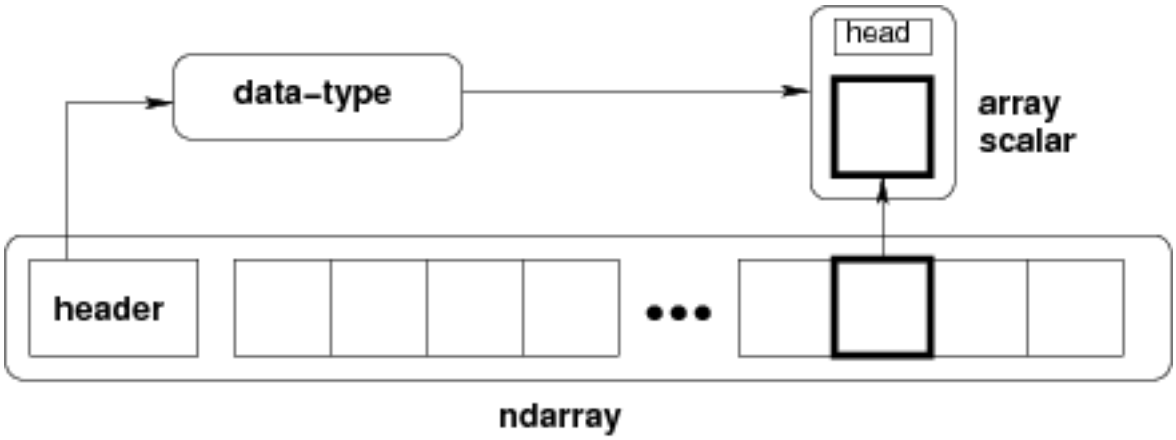


3.3.4 Under the hood: the memory layout of a numpy array

A numpy array is:

block of memory + indexing scheme + data type descriptor

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



Block of memory

```
>>> x = np.array([1, 2, 3, 4], dtype=np.int32)
>>> x.data
<read-write buffer for ..., size 16, offset 0 at ...>
>>> 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[:]
>>> 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 ..., size 4, offset 0 at ...>
>>> 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.

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\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

$$\begin{aligned}\text{shape} &= (d_1, d_2, ..., d_n)\\ \text{strides} &= (s_1, s_2, ..., s_n)\\ s_j^C &= d_{j+1}d_{j+2}...d_n \times \text{itemsize}\\ s_j^F &= d_1 d_2 ... d_{j-1} \times \text{itemsize}\end{aligned}$$

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], dtype=int32)
>>> 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)
```

- 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.

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)

While it is off topic in a chapter on numpy, let's take a moment to recall good coding practice, which really do pay off in the long run:

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.

3.4 Advanced operations

Section contents

- Polynomials (page 79)
- Loading data files (page 81)

3.4.1 Polynomials

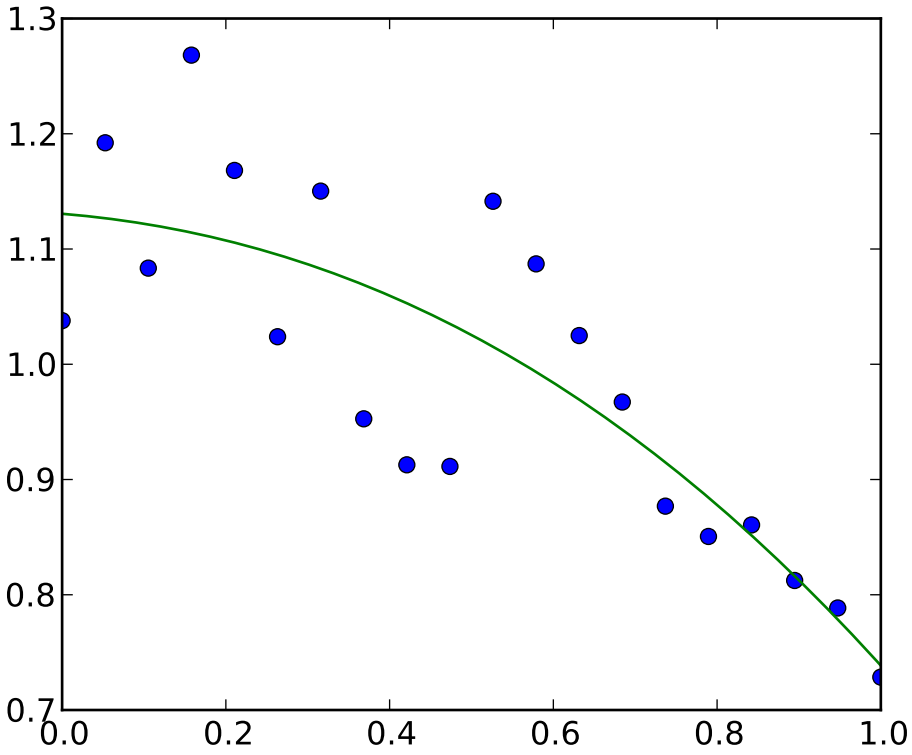
Numpy also contains polynomials in different bases:

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), '-')
[<matplotlib.lines.Line2D object at ...>, <matplotlib.lines.Line2D object at ...>]
```



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

More polynomials (with more bases)

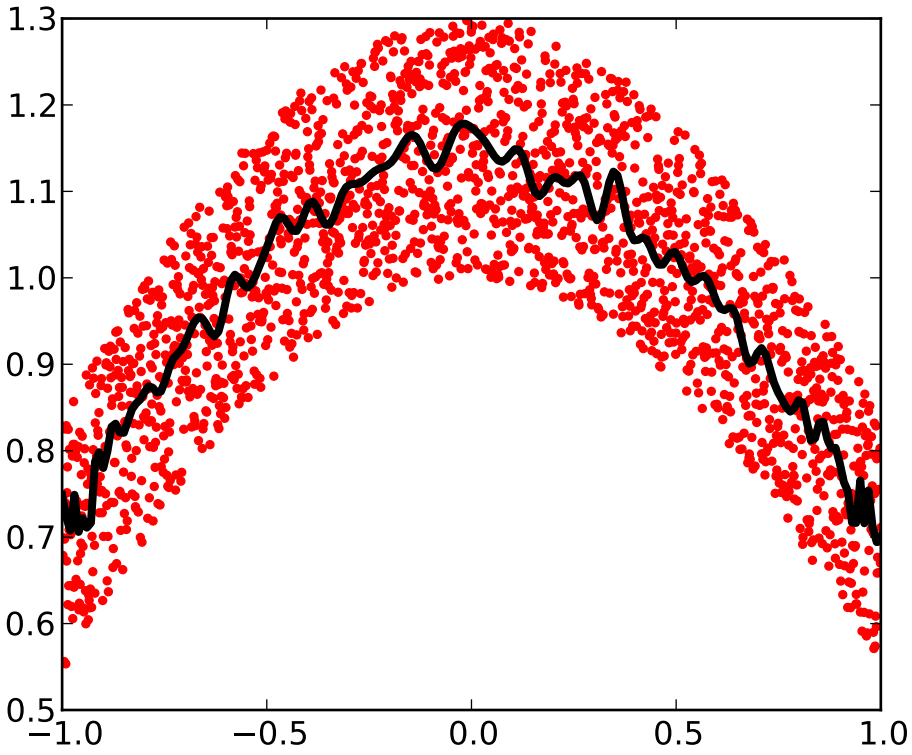
Numpy also has a more sophisticated polynomial interface, which supports e.g. the Chebyshev basis.

$3x^2 + 2x - 1$

```
>>> p = np.polynomial.Polynomial([-1, 2, 3]) # coefs in different order!
>>> p(0)
-1.0
>>> p.roots()
array([-1.        ,  0.33333333])
>>> p.degree()  # In general polynomials do not always expose '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.')
[<matplotlib.lines.Line2D object at ...>]
>>> plt.plot(t, p(t), 'k-', lw=3)
[<matplotlib.lines.Line2D object at ...>]
```



The Chebyshev polynomials have some advantages in interpolation.

3.4.2 Loading data files

Text files

Example: `populations.txt`:

```
1900        30e3    4e3     48300
1901        47.2e3  6.1e3   48200
1902        70.2e3  9.8e3   41500
...
```

```
>>> data = np.loadtxt('data/populations.txt')
>>> data
array([[  1900.,  30000.,   4000.,  48300.],
       [  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 with *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
```

Images

Using Matplotlib:

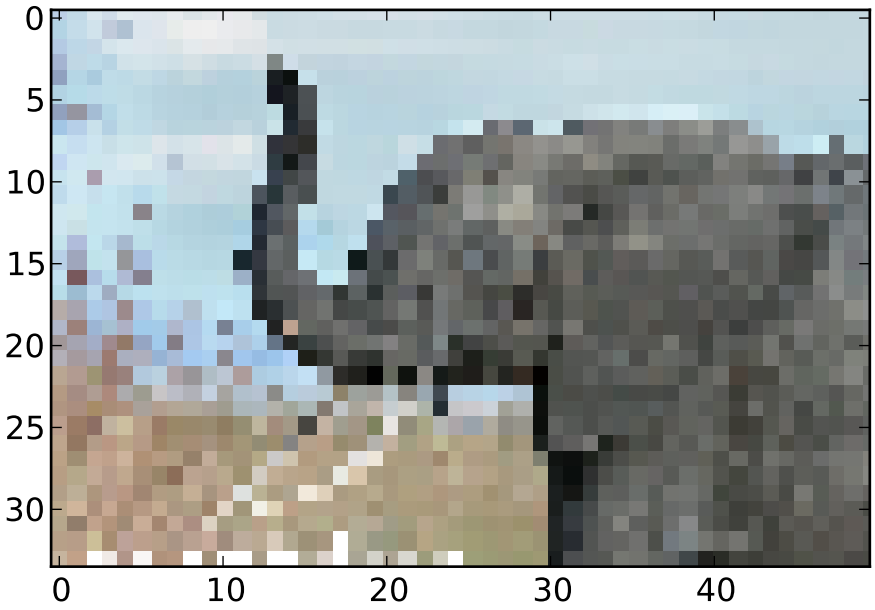
```
>>> img = plt.imread('data/elephant.png')
>>> img.shape, img.dtype
((200, 300, 3), dtype('float32'))
>>> plt.imshow(img)
<matplotlib.image.AxesImage object at ...>
>>> plt.savefig('plot.png')

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

This saved only one channel (of RGB):

```
>>> plt.imshow(plt.imread('red_elephant.png'))
<matplotlib.image.AxesImage object at ...>
```

Other libraries:

```
>>> from scipy.misc import imsave
>>> imsave('tiny_elephant.png', img[::6,::6])
>>> plt.imshow(plt.imread('tiny_elephant.png'), interpolation='nearest')
<matplotlib.image.AxesImage object at ...>
```



Numpy's own format

Numpy has its own binary format, not portable but with efficient I/O:

```
>>> data = np.ones((3, 3))
>>> 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.

Exercise: 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`.

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:

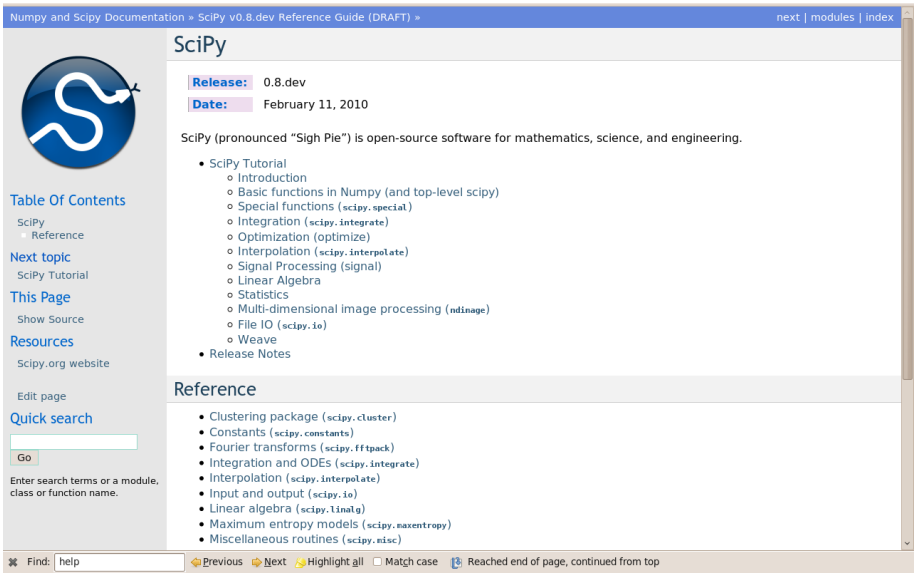
- In Ipython, `help function` opens the docstring of the function. Only type the beginning of the function's name and use tab completion to display the matching functions.

```
In [204]: help np.v
np.vander      np.vdot        np.version     np.void0       np.vstack
np.var         np.vectorize   np.void        np.vsplit

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

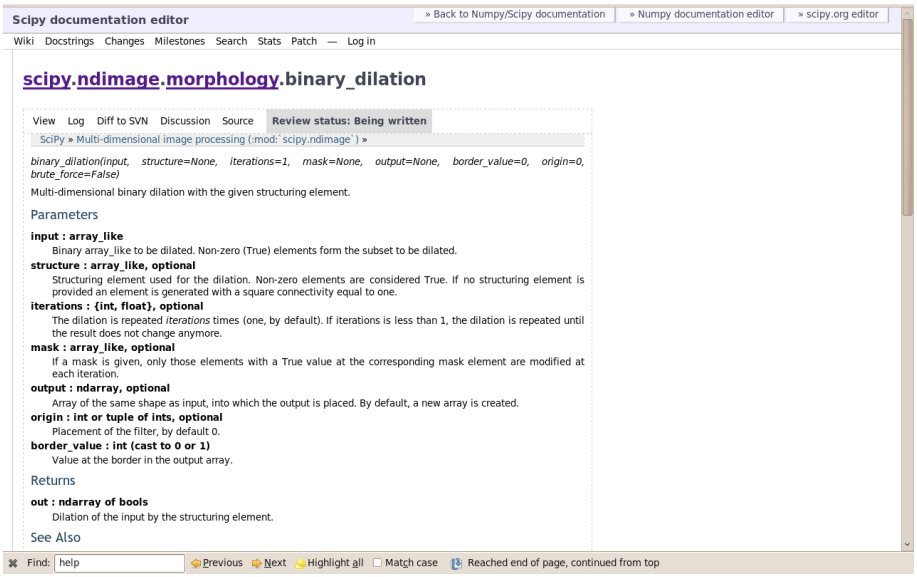
In Ipython it is not possible to open a separated window for help and documentation; however one can always open a second `Ipython` shell just to display help and docstrings...

- 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/).

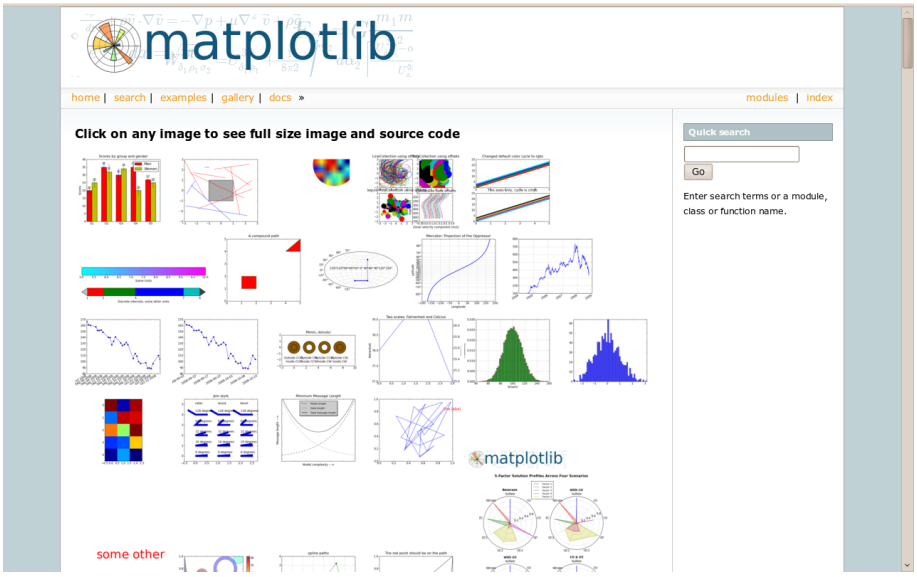
  Tutorials on various topics as well as the complete API with all docstrings are found on this website.



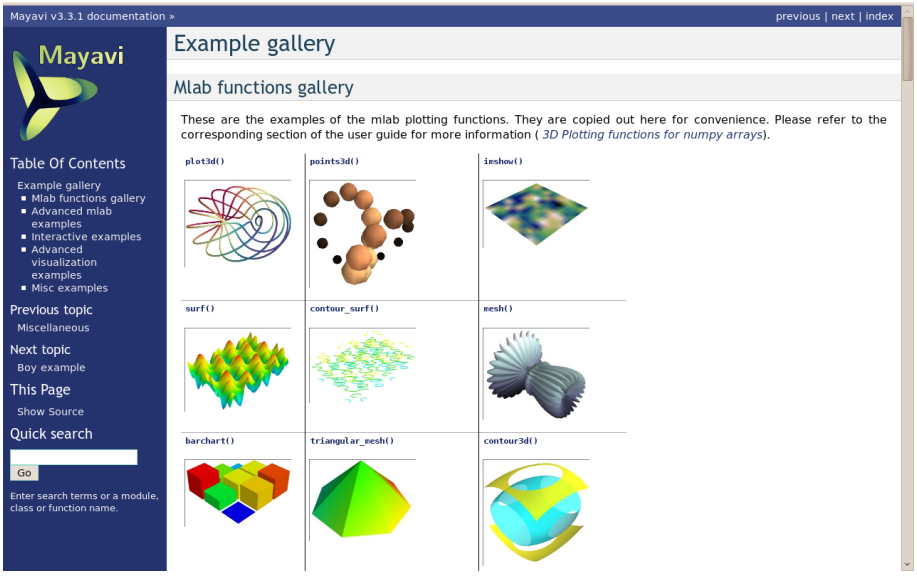
- Numpy's and Scipy's documentation is enriched and updated on a regular basis by users on a wiki http://docs.scipy.org/numpy/. As a result, some docstrings are clearer or more detailed on the wiki, and you may want to read directly the documentation on the wiki instead of the official documentation 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, indexation 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 5

Matplotlib

author Mike Müller

5.1 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.

5.2 IPython and the pylab mode

5.2.1 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` (`--pylab` since IPython version 0.12), it allows interactive `matplotlib` sessions that has Matlab/Mathematica-like functionality.

5.2.2 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.

5.3 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.
```

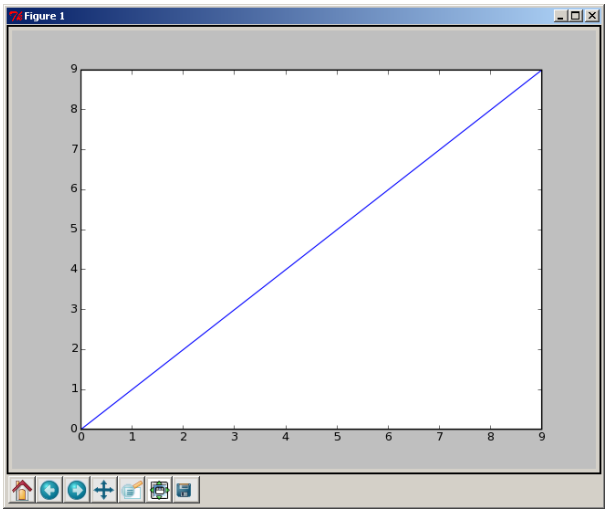
```
help    -> Python's own help system.
object? -> Details about 'object'. ?object also works, ?? prints more.

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()
```

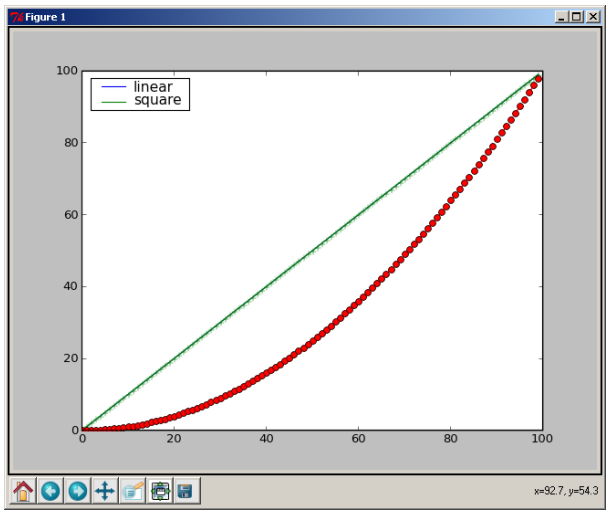
and print it anew providing new line styles (a green dotted line with crosses for the linear and a red dashed line with circles for the square graph):

```
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:



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.

5.4 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 antialised 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

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.

5.5 Text

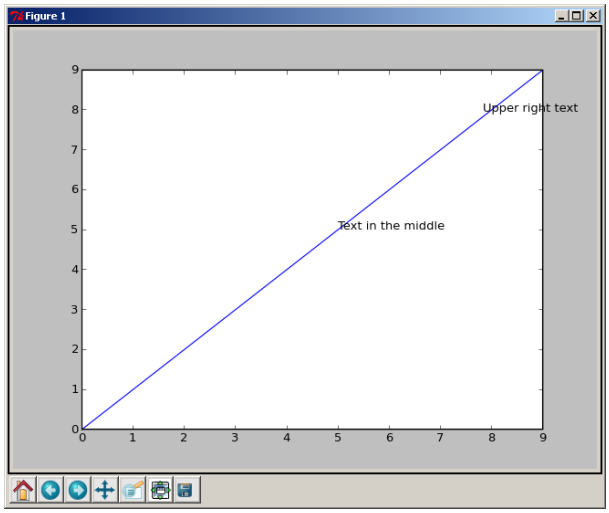
We've already used some commands to add text to our figure: `xlabel` `ylabel`, and `title`.

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 form 0 to 1:

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



`matplotlib` supports TeX mathematical expression. So `r'$\pi$'` will show up as:

π

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'})
```

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

5.6 Ticks

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).

There are several locators for different kind of requirements:

Class	Description
NullLocator	no ticks
IndexLocator	locator for index plots (e.g. where `x = range(len(y))`
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.ticker.Locator`. 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 matplotlib.dates.rrule

Similarly to locators, there are formatters:

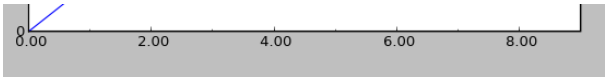
Class	Description
NullFormatter	no labels on the ticks
FixedFormatter	set the strings manually for the labels
FuncFormatter	user defined function sets the labels
FormatStrFormatter	use a sprintf format string
IndexFormatter	cycle through fixed strings by tick position
ScalarFormatter	default formatter 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.ticker.Formatter`. 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:



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.

5.7 Figures, Subplots, and Axes

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.

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

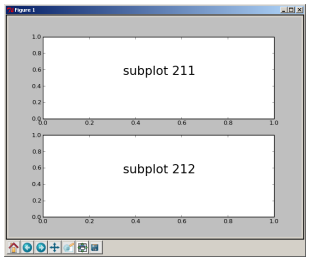
The defaults can be specified in the resource file and will be used most of the time. Only the number of the figure is frequently changed.

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).

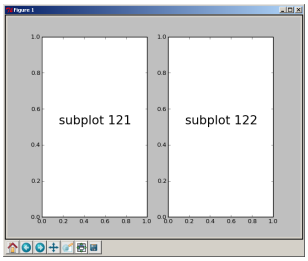
As with other objects, you can set figure properties also `setp` or with the `set_something` methods.

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.

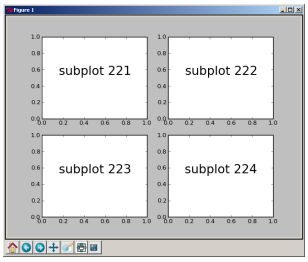
A plot with two rows and one column is created with `subplot(211)` and `subplot(212)`. The result looks like this:



If you want two plots side by side, you create one row and two columns with `subplot(121)` and `subplot(112)`. 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:

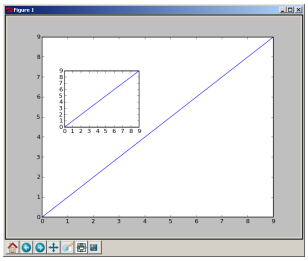


Frequently, you don't want all subplots to have ticks or labels. You can set the `xticklabels` or the `yticklabels` to an empty list (`[]`). Every subplot defines the methods `'is_first_row`, `is_first_col`, `is_last_row`, `is_last_col`. These can help to set ticks and labels only for the outer pots.

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:



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.

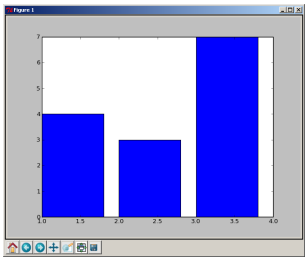
5.8 Other Types of Plots

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.

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:

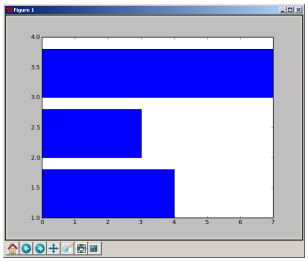


The default column width is 0.8. It can be changed with common methods by setting `width`. As it can be `color` and `bottom`, we can also set an error bar with `yerr` or `xerr`.

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

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

We get:



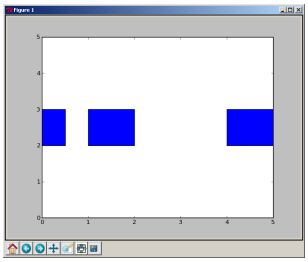
We can also have discontinuous vertical bars with `broken_barh`. We specify start and width of the range in y-direction and all start-width pairs in x-direction:

```
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:



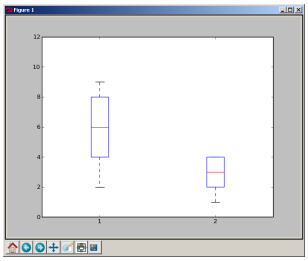
We can draw box and whisker plots:

```
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.

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

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

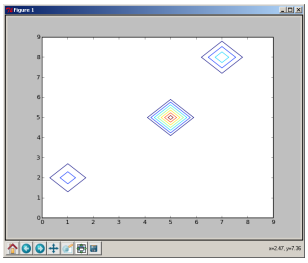
and also a 2D array for z:

```
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.,  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.,  1.,  1.,  4.,  1.,  1.],
       [ 1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.]])
```

Now we can make a simple contour plot:

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

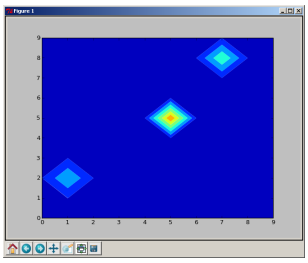
Our plot looks like this:



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

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

Now our plot area is filled:



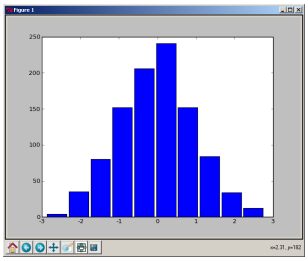
We can make histograms. Let's get some normally distributed random numbers from `numpy`:

```
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:



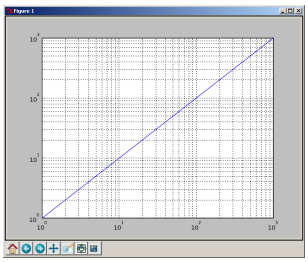
Plots with logarithmic scales are easy:

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

We set the mayor and minor grid:

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

Now we have loglog plot:

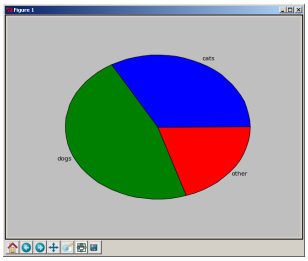


If we want only one axis with a logarithmic scale we can use `semilogx` or `semilogy`.

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:



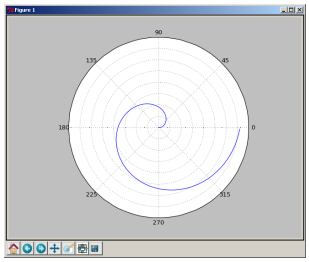
Polar plots are also possible. Let's define our `r` from 0 to 360 and our `theta` from 0 to 360 degrees. We need to convert them to radians:

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

Now plot in polar coordinates:

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

We get a nice spiral:



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)
```

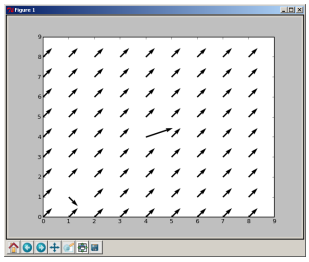
The x and y components of the arrows are specified as 2D arrays:

```
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:



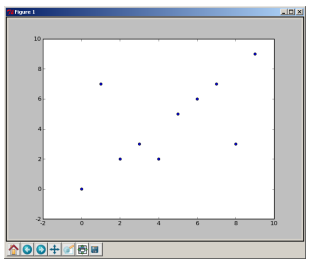
Scatter plots print x vs. y diagrams. We define `x` and `y` and make some point in `y` random:

```
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:

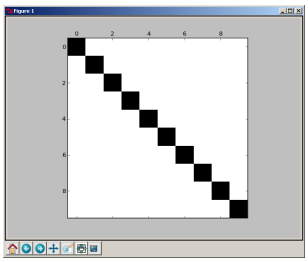


Working with sparse matrices, it is often of interest as how the matrix looks like in terms of sparsity. We take an identity matrix as an example:

```
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]])
```

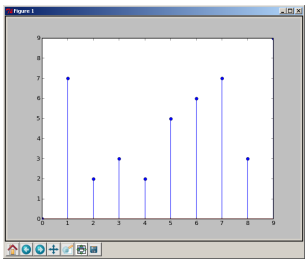
Now we look at it more visually:

```
spy(i)
```



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)
```



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

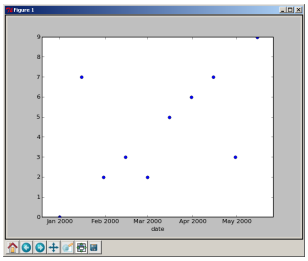
```
import datetime
d1 = datetime.datetime(2000, 1, 1)
delta = datetime.timedelta(15)
dates = [d1 + x * delta for x in range(1
dates
[datetime.datetime(2000, 1, 1, 0, 0),
 datetime.datetime(2000, 1, 16, 0, 0),
 datetime.datetime(2000, 1, 31, 0, 0),
 datetime.datetime(2000, 2, 15, 0, 0),
 datetime.datetime(2000,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



5.9 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.

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.

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.

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

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 cover by the toolbar. If so, please adjust the `figsize` for `pylab` accordingly.

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.

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, if 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.

Chapters contents

- Scipy builds upon Numpy (page 105)
- File input/output: `scipy.io` (page 105)
- Signal processing: `scipy.signal` (page 106)
- Special functions: `scipy.special` (page 107)
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- Interpolation: `scipy.interpolate` (page 115)
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- Summary exercises on scientific computing (page 122)

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

6.1 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 *`.

6.2 File input/output: `scipy.io`

- Loading and saving matlab files:

```
>>> from scipy import io
>>> a = np.ones((3, 3))
>>> io.savemat('file.mat', {'a': a}) # savemat expects a dictionary
>>> data = io.loadmat('file.mat', struct_as_record=True)
>>> data['a']
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
```

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:

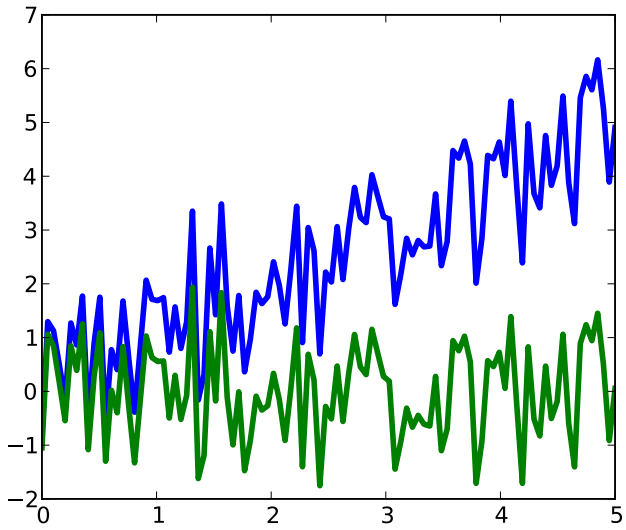
```
np.save/np.load
```

6.3 Signal processing: `scipy.signal`

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

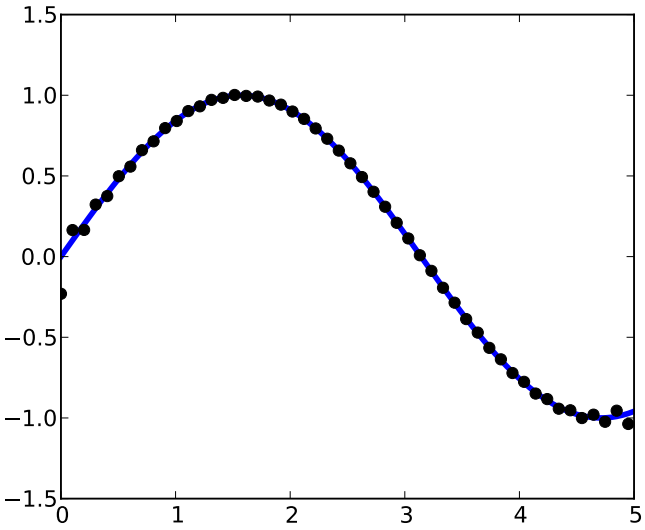
- Detrend: remove linear trend from signal:

```
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)
```



- 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')
```



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.

6.4 Special functions: `scipy.special`

Special functions are transcendal 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`

6.5 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`.

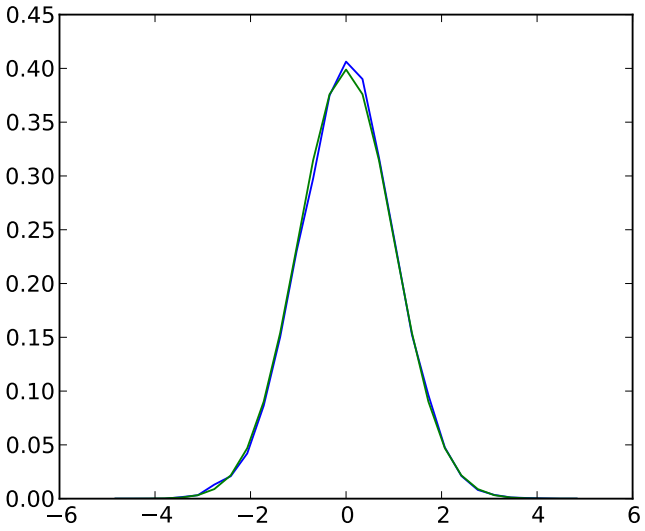
6.5.1 Histogram and probability density function

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)
```



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
-0.045256707490...
>>> std
0.9870331586690...
```

6.5.2 Percentiles

The median is the value with half of the observations below, and half above:

```
>>> np.median(a)
-0.058028034...
```

It is also called the percentile 50, because 50% of the observation are below it:

```
>>> stats.scoreatpercentile(a, 50)
-0.0580280347...
```

Similarly, we can calculate the percentile 90:

```
>>> stats.scoreatpercentile(a, 90)
1.231593551...
```

The percentile is an estimator of the CDF: cumulative distribution function.

6.5.3 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)
(-3.75832707..., 0.00027786...)
```

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.

6.6 Linear algebra operations: `scipy.linalg`

The linalg module provides standard linear algebra operations, relying on an underlying efficient implementation (BLAS).

- 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(9).reshape((3, 3)) + np.diag([1, 0, 1])
>>> uarr, spec, vharr = linalg.svd(arr)
```

The resulting array spectrum is:

```
>>> spec
array([ 14.88982544,   0.45294236,   0.29654967])
```

For the recomposition, an alias for manipulating matrix will first be defined:

```
>>> asmat = np.asmatrix
```

then the steps are:

```
>>> sarr = np.diag(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`.

6.7 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..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)
```

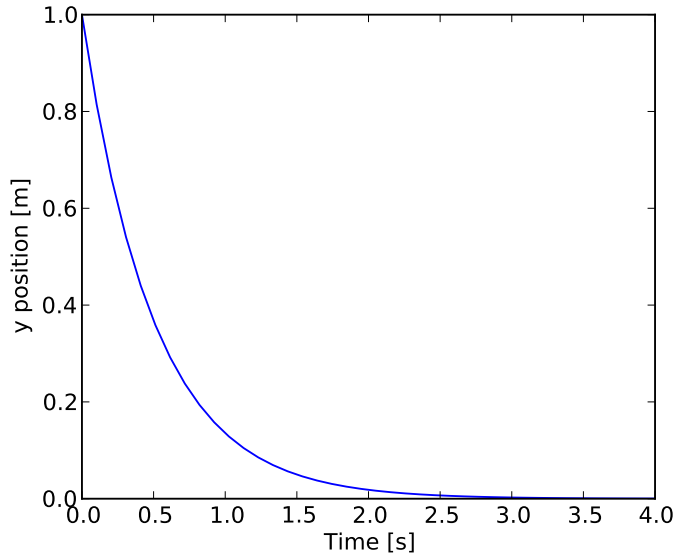
Thus the derivative function has been called more than 40 times:

```
>>> 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:



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 eps wo y' + wo^2 y = 0` with `wo^2 = k/m` being `k` the spring constant, `m` the mass and `eps=c/(2 m wo)` 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
```

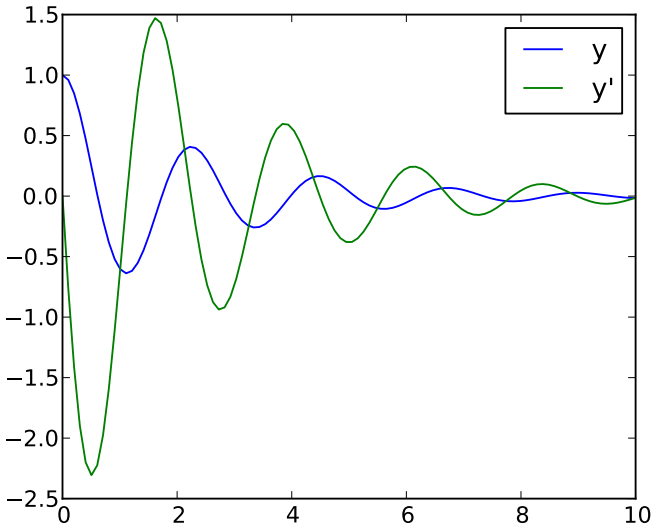
For the `odeint` solver the 2nd order equation needs to be transformed in a system of two first-order equations for the vector `Y=(y, y')`. It will be convenient to define `nu = 2 eps wo = c / m` and `om = wo^2 = k/m`:

```
>>> nu_coef = cviscous/mass
>>> om_coef = kspring/mass
```

Thus the function will calculate the velocity and acceleration by:

```
>>> def calc_deri(yvec, time, nuc, omc):
...     return (yvec[1], -nuc * yvec[1] - omc * yvec[0])
...
>>> time_vec = np.linspace(0, 10, 100)
>>> yarr = odeint(calc_deri, (1, 0), time_vec, args=(nu_coef, om_coef))
```

The final position and velocity are shown on the following Matplotlib figure:



There is no Partial Differential Equations (PDE) solver in scipy. Some PDE packages are written in Python, such as fipy or SfePy.

6.8 Fast Fourier transforms: `scipy.fftpack`

The `fftpack` module allows to compute fast Fourier transforms. As an illustration, an input signal may look like:

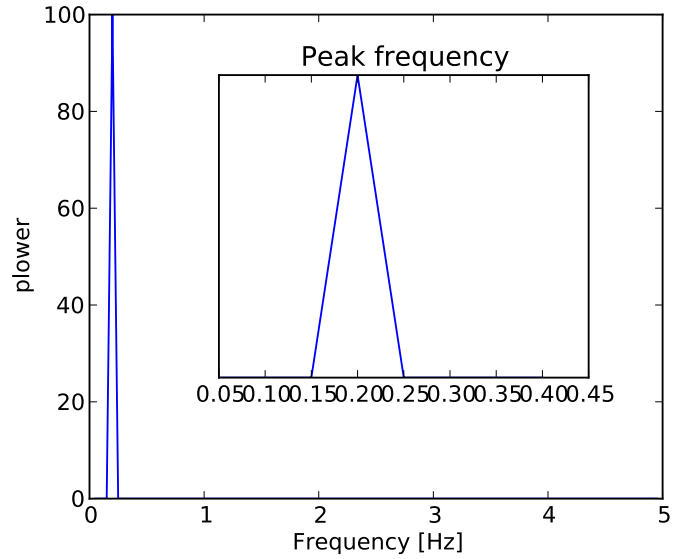
```
>>> time_step = 0.1
>>> period = 5.
>>> time_vec = np.arange(0, 20, time_step)
>>> sig = np.sin(2 * np.pi / period * time_vec) + \
...       np.cos(10 * np.pi * time_vec)
```

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]
```



Thus the signal frequency can be found by:

```
>>> freq = freqs[power.argmax()]
>>> np.allclose(freq, 1./period)
True
```

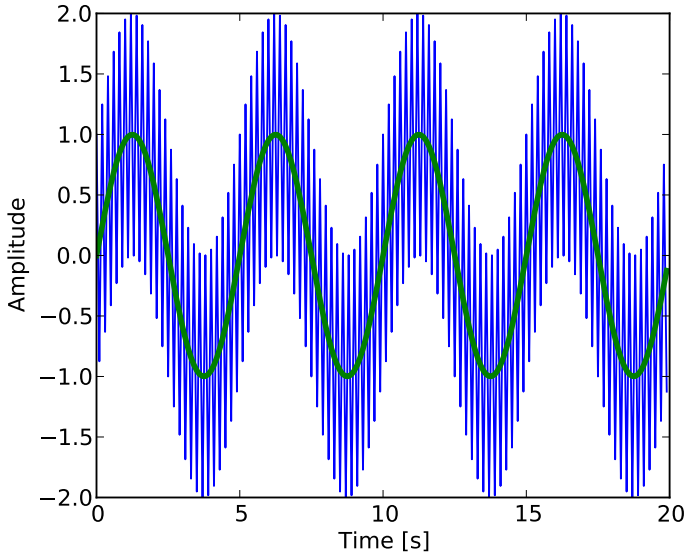
Now only the main signal component will be extracted from the Fourier transform:

```
>>> sig_fft[np.abs(sample_freq) > freq] = 0
```

The resulting signal can be computed by the `ifft` function:

```
>>> main_sig = fftpack.ifft(sig_fft)
```

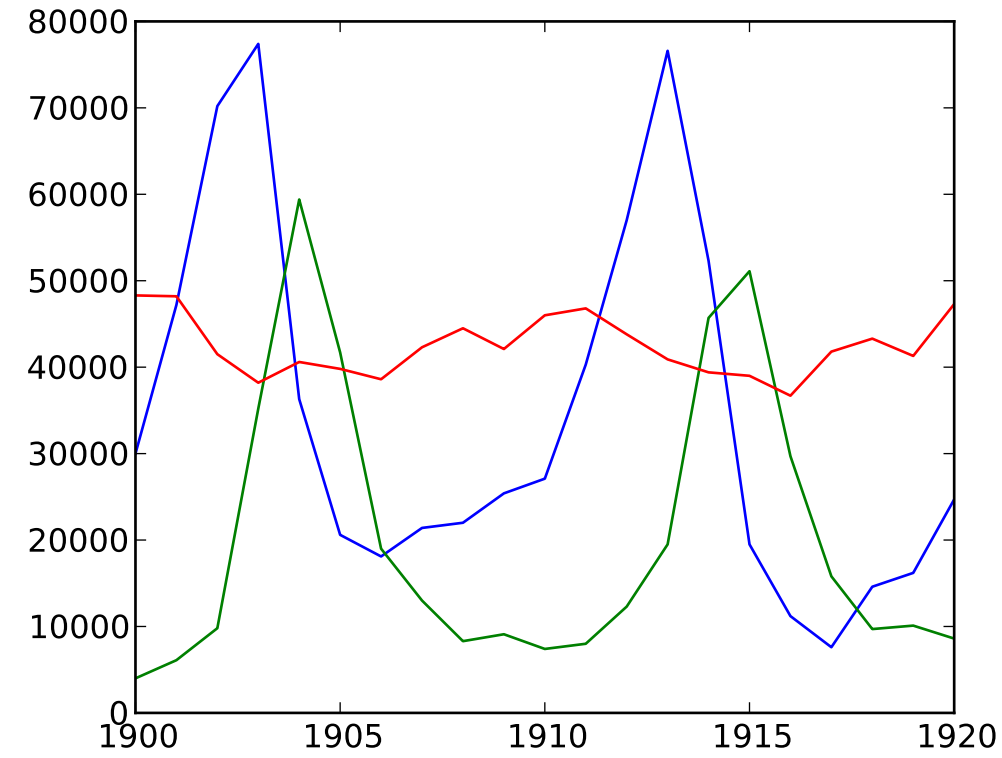
The result is shown on the Matplotlib figure:

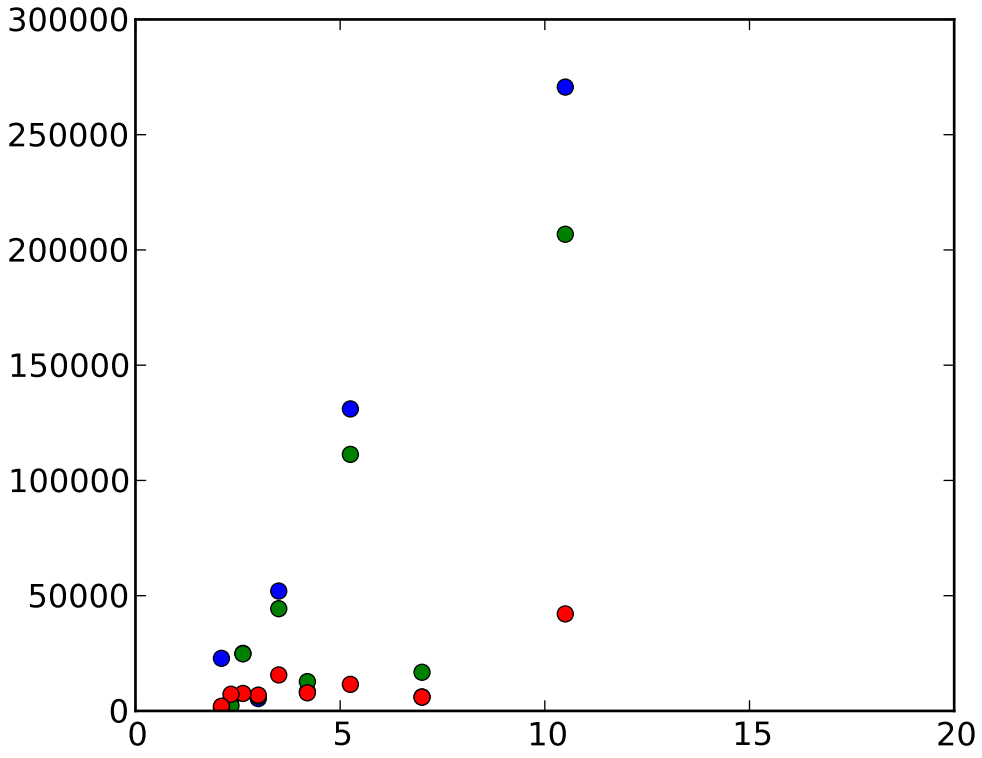


Note: numpy.fft

Numpy also has an implementation of FFT. However, in general the scipy one should be prefered, as it uses more efficient underlying implementations.

Worked example: Crude periodicity finding



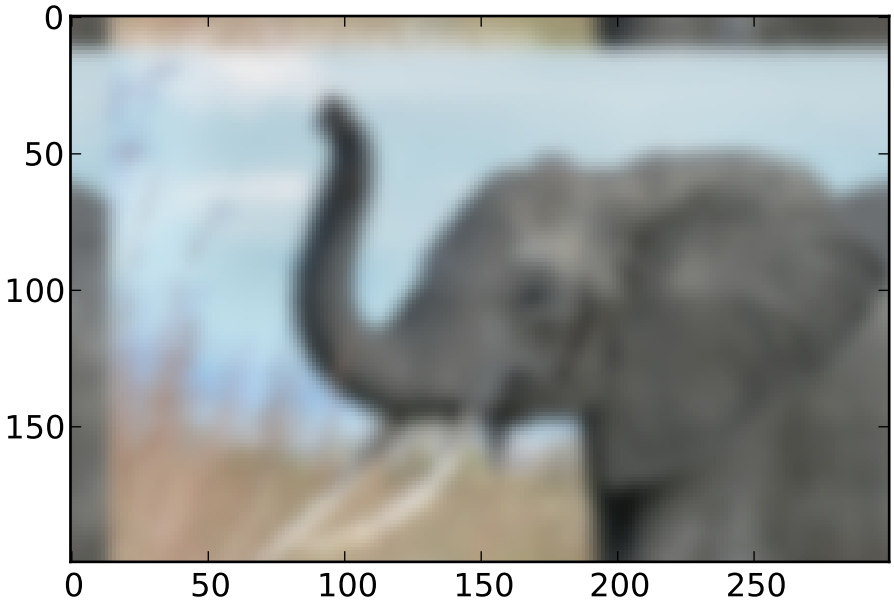


Worked example: Gaussian image blur

Convolution:

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

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



6.9 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)
```

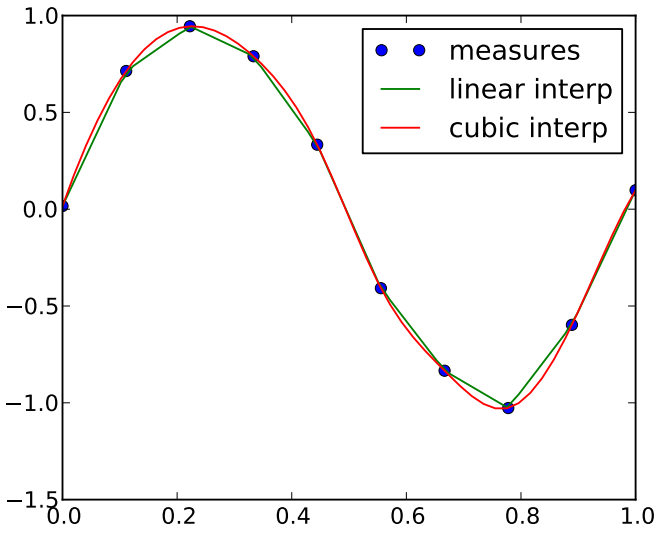
Then the `linear_interp` instance needs to be evaluated on time of interest:

```
>>> 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:



`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 122) for a more advance spline interpolation example.

6.10 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.

```
>>> from scipy import optimize
```

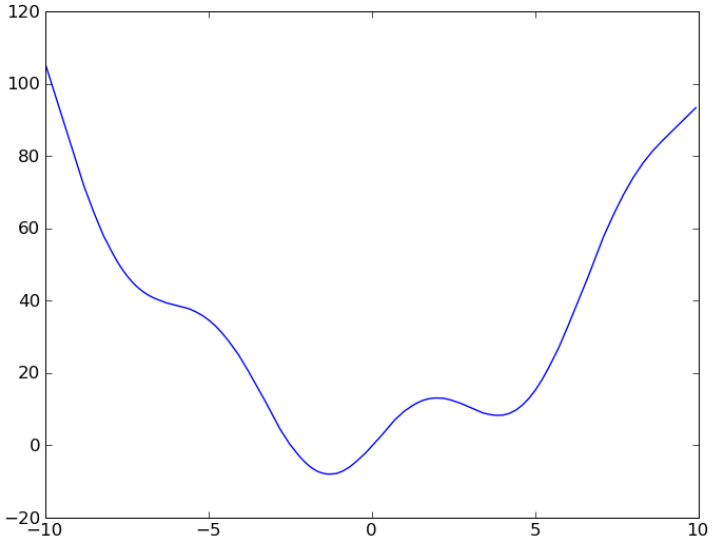
Example: Minimizing a scalar function using different algorithms

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.

6.10.1 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.

6.10.2 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)
3.8374671...
```

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 126) for a more advanced example.

6.11 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.

6.11.1 Geometrical transformations on images

Changing orientation, resolution, ..

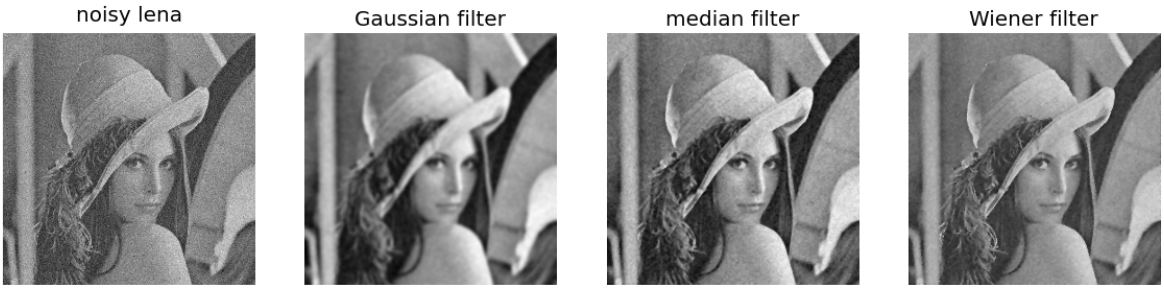
```
>>> from scipy import misc
>>> lena = misc.lena()
>>> shifted_lena = ndimage.shift(lena, (50, 50))
>>> shifted_lena2 = ndimage.shift(lena, (50, 50), mode='nearest')
>>> rotated_lena = ndimage.rotate(lena, 30)
>>> cropped_lena = lena[50:-50, 50:-50]
>>> zoomed_lena = ndimage.zoom(lena, 2)
>>> zoomed_lena.shape
(1024, 1024)
```

```
In [35]: subplot(151)
Out[35]: <matplotlib.axes.AxesSubplot object at 0x925f46c>

In [36]: pl.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.
```

6.11.2 Image filtering

```
>>> from scipy import misc
>>> lena = misc.lena()
>>> import numpy as np
>>> noisy_lena = np.copy(lena).astype(np.float)
```

```
>>> 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)
>>> from scipy import signal
>>> wiener_lena = signal.wiener(blurred_lena, (5,5))
```



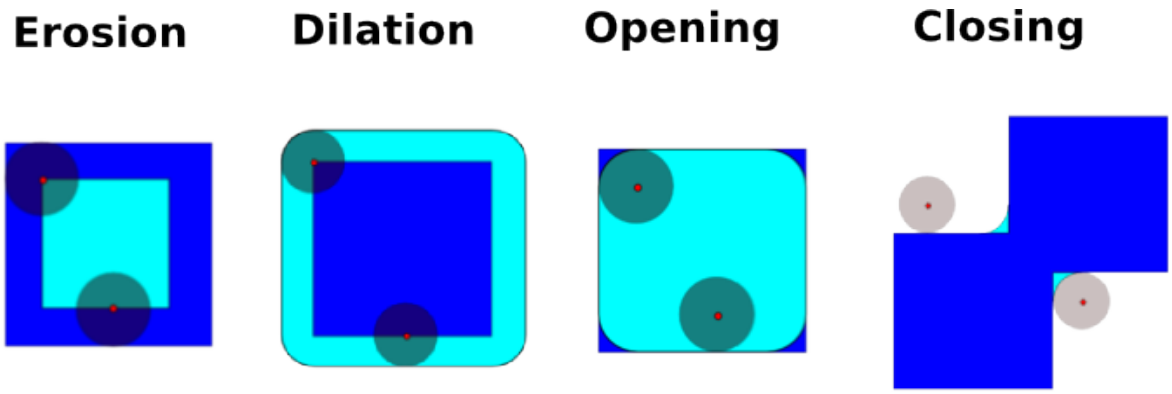
And many other filters in `scipy.ndimage.filters` and `scipy.signal` can be applied to images

Exercise

Compare histograms for the different filtered images.

6.11.3 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.



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.,  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]])
```

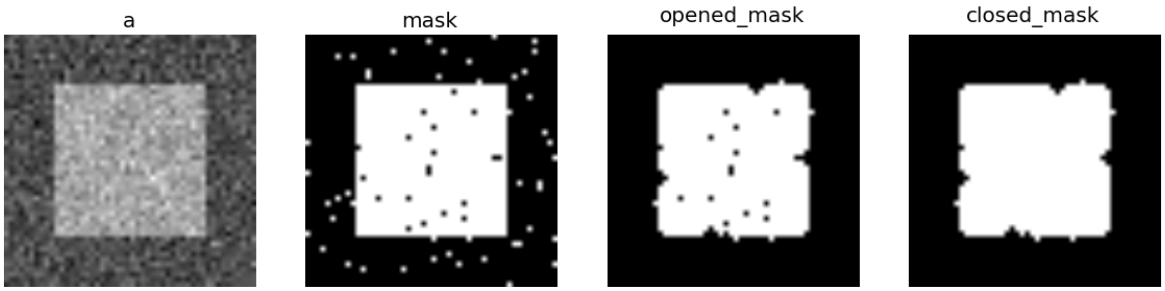
- **Closing:** `ndimage.binary_closing`

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]])
```

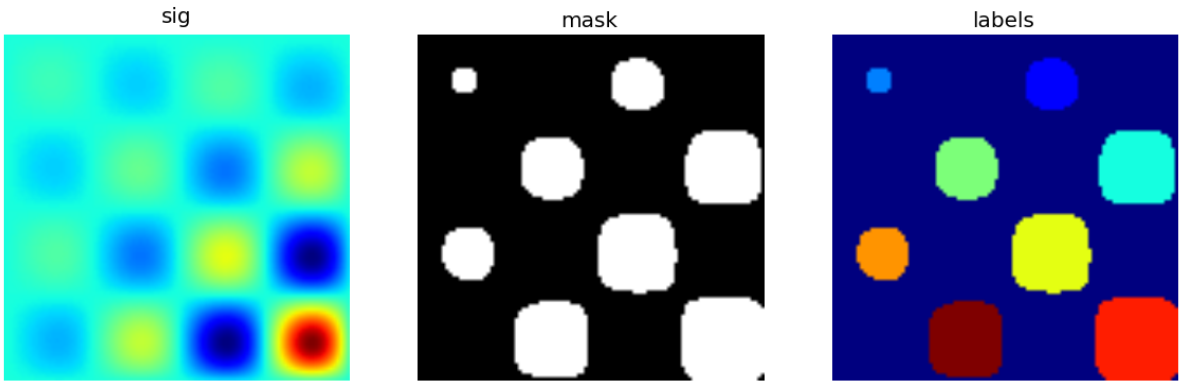
6.11.4 Measurements on images

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.**2)**2
>>> 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
array([ 190.,   45.,  424.,  278.,  459.,  190.,  549.,  424.])
>>> maxima = ndimage.maximum(sig, labels, xrange(1, labels.max()+1))
>>> maxima
array([  1.80238238,   1.13527605,   5.51954079,   2.49611818,
         6.71673619,   1.80238238,  16.76547217,   5.51954079])
>>> ndimage.find_objects(labels==4)
[(slice(30L, 48L, None), slice(30L, 48L, None))]
>>> sl = ndimage.find_objects(labels==4)
>>> import pylab as pl
>>> pl.imshow(sig[sl[0]])
<matplotlib.image.AxesImage object at ...>
```



See the summary exercise on *Image processing application: counting bubbles and unmolten grains* (page 130) for a more advanced example.

6.12 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.

6.12.1 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 `examples/max-speeds.npy`, thus they will be loaded by using numpy:

```
>>> import numpy as np
>>> max_speeds = np.load('intro/summary-exercises/examples/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
32.97989825...
```

The results are now gathered on a Matplotlib figure:

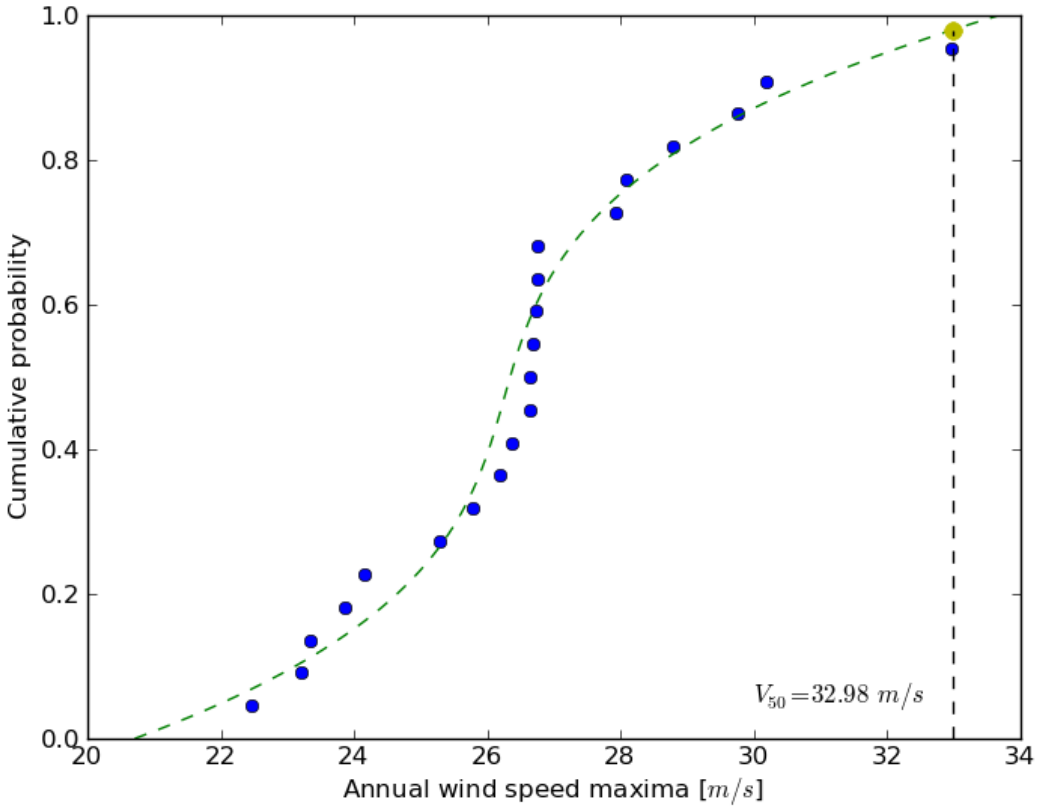


Figure 6.1: Solution: *Python source file*

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 `examples/sprog-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.
- 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.

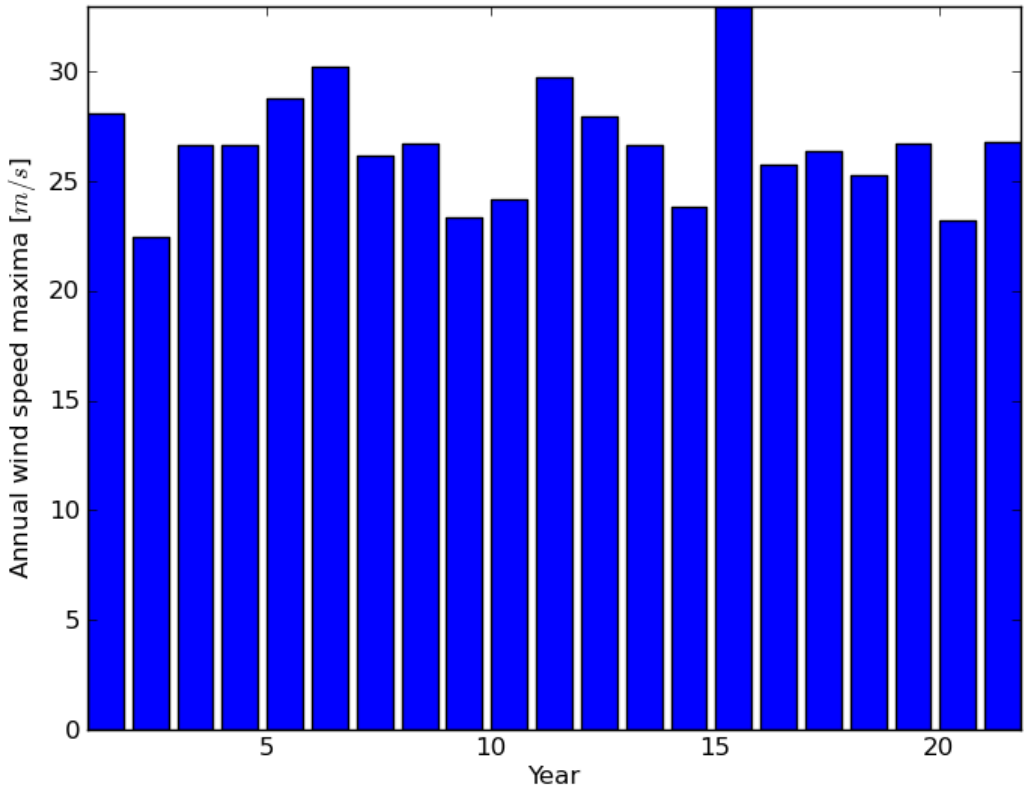


Figure 6.2: Solution: *Python source file*

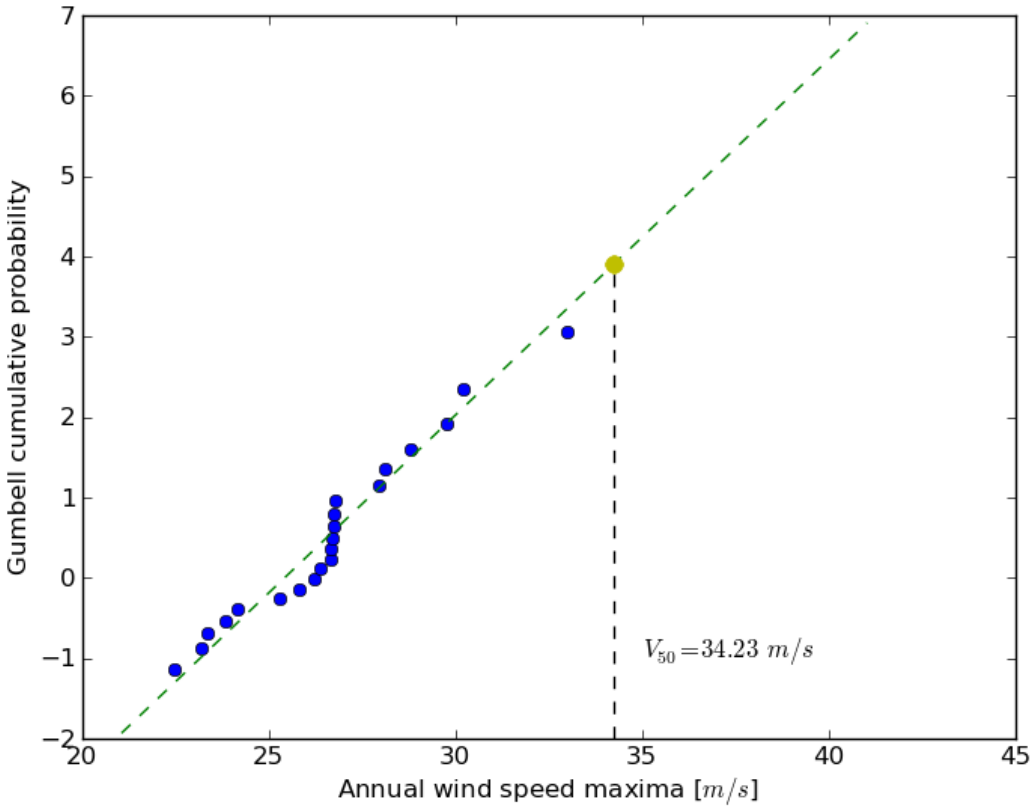


Figure 6.3: Solution: *Python source file*

- The last step will be to find 34.23 m/s for the maximum wind speed occurring every 50 years.

6.12.2 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 127).

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 [1] for more details).

In this tutorial, the goal is to analyze the waveform recorded by the lidar system [2]. 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

[1] Mallet, C. and Bretar, F. Full-Waveform Topographic Lidar: State-of-the-Art. *ISPRS Journal of Photogrammetry and Remote Sensing* 64(1), pp.1-16, January 2009 http://dx.doi.org/10.1016/j.isprsjprs.2008.09.007

[2] 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.

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.

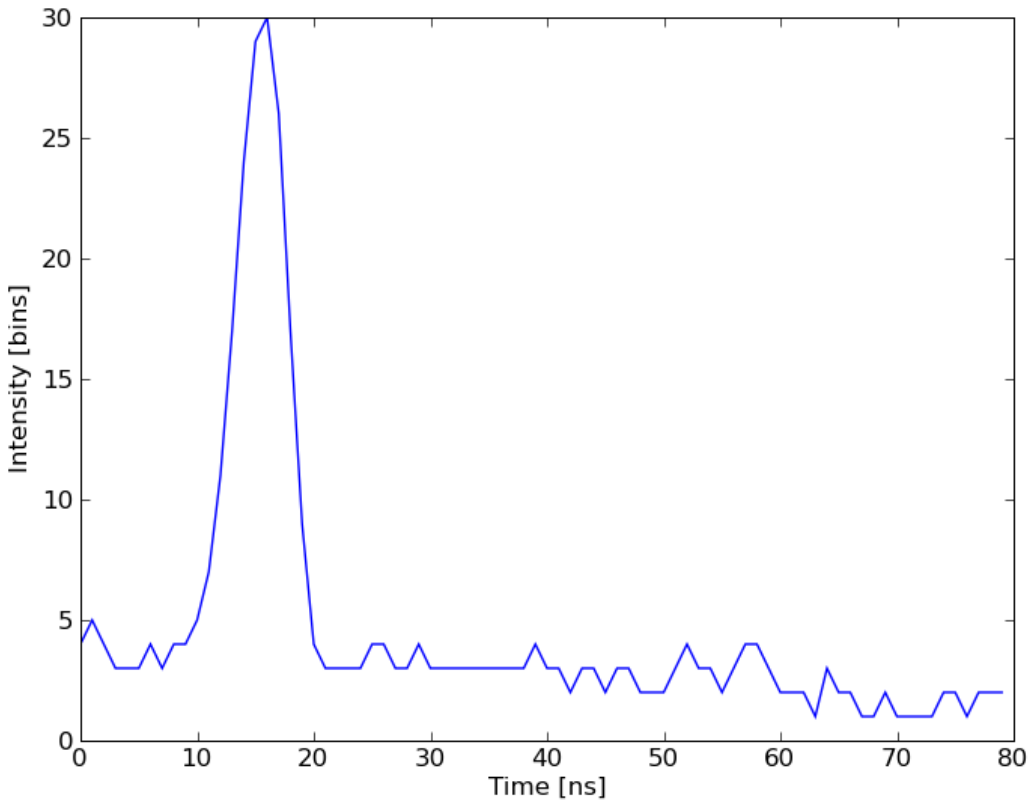
Loading and visualization

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()
```



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]
```

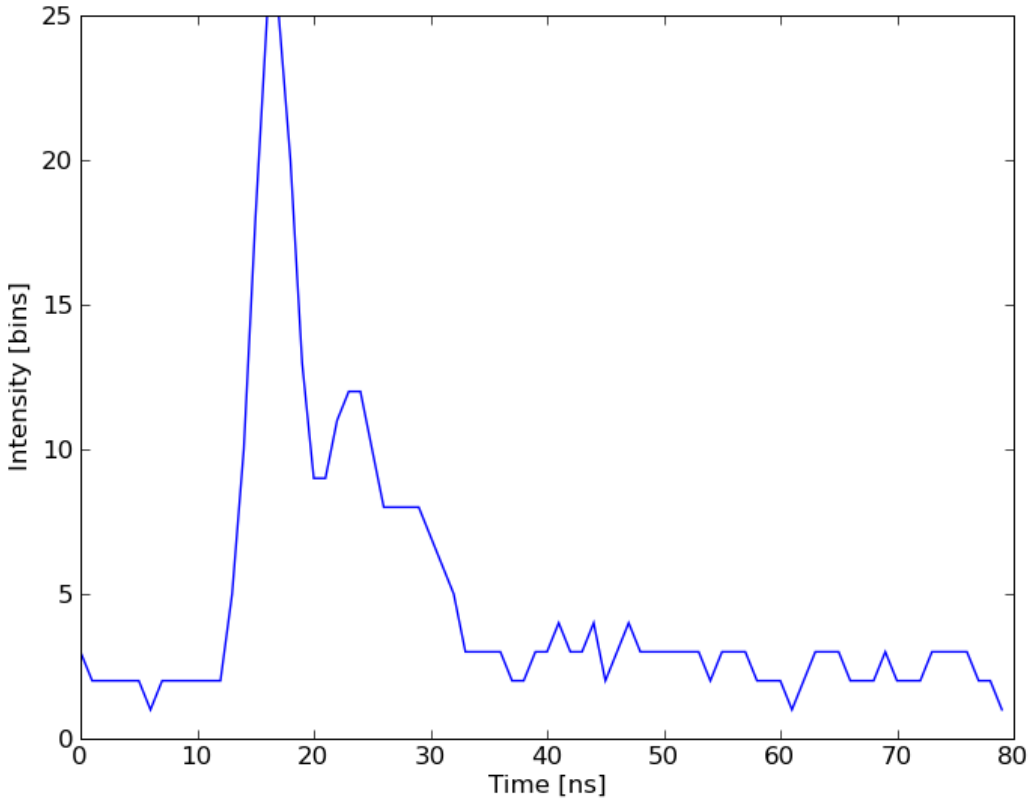
And visualize the solution:

```
>>> 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.



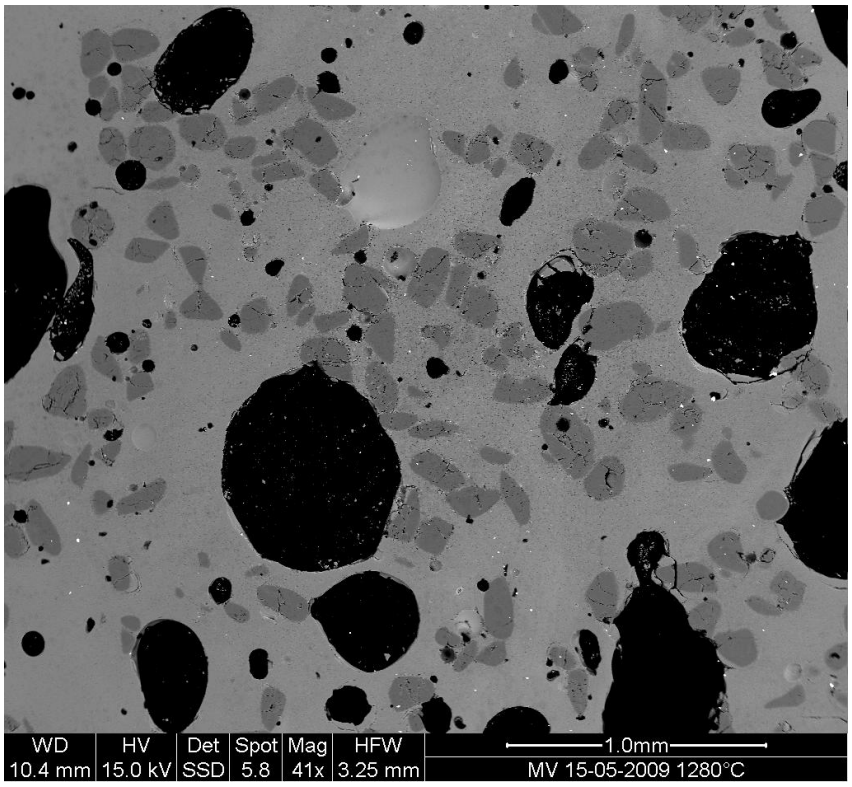
- In some cases, writing an explicit function to compute the Jacobian is faster than letting `leastsq` estimate it numerically. Create a function to compute the Jacobian of the residuals and use it as an input for `leastsq`.
- When we want to detect very small peaks in the signal, or when the initial 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.

6.12.3 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.

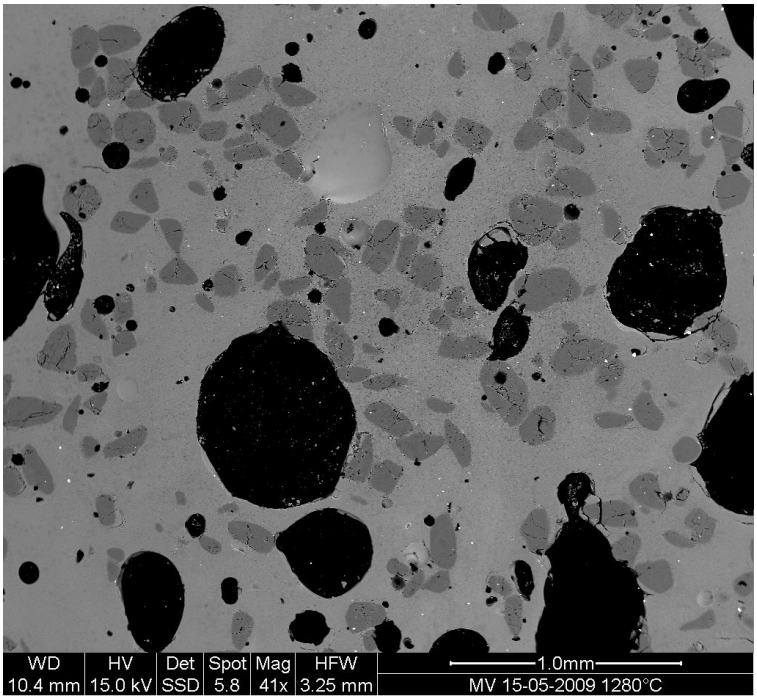
7. Attribute labels to all bubbles and sand grains, and remove from the sand mask grains that are smaller than 10 pixels. To do so, use `ndimage.sum` or `np.bincount` to compute the grain sizes.

8. Compute the mean size of bubbles.

Proposed solution

```
>>> import numpy as np
>>> import pylab as pl
>>> from scipy import ndimage
```

6.12.4 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).

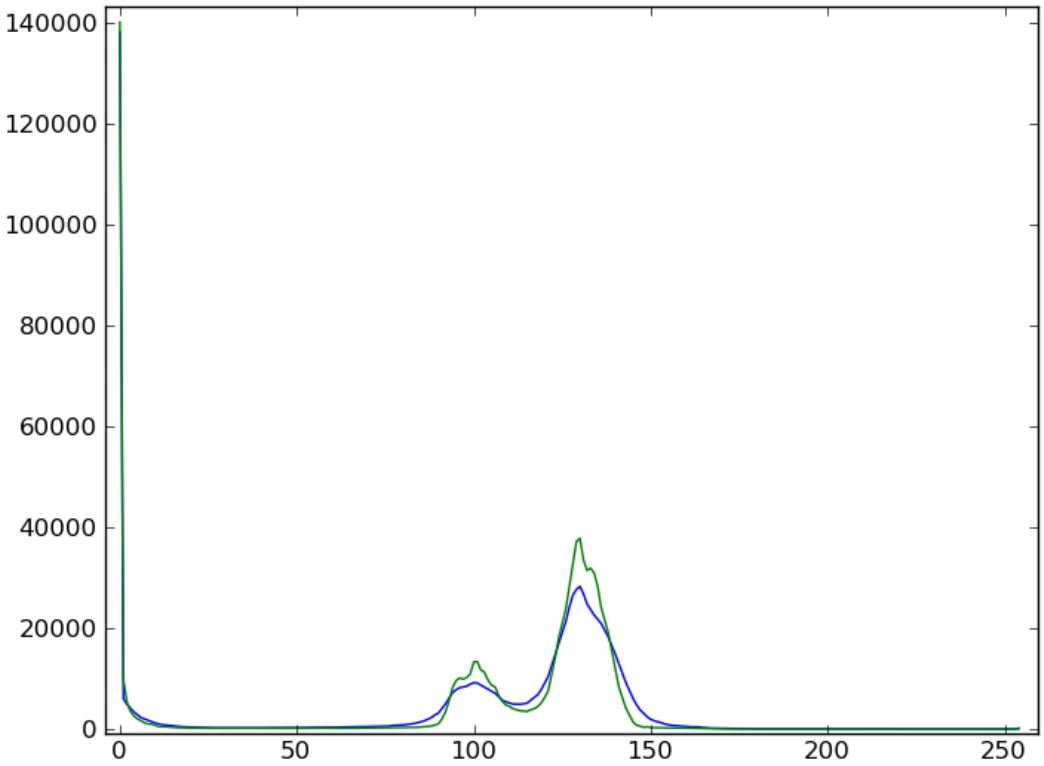
```
>>> dat = pl.imread('data/MV_HFV_012.jpg')
```

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))
```

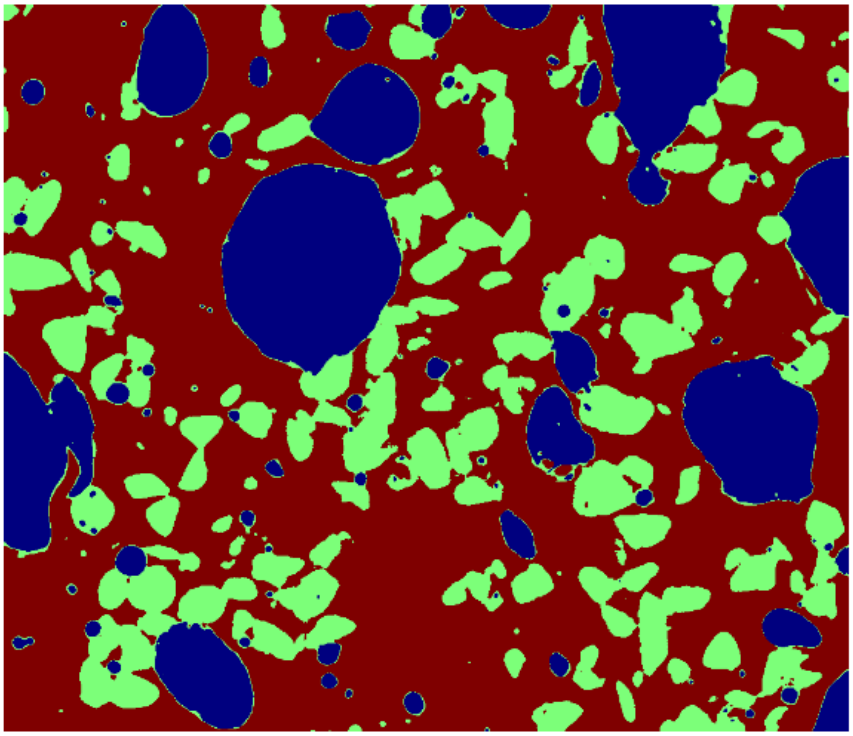


4. Using the histogram of the filtered image, determine thresholds that allow to define masks for sand pixels, glass pixels and bubble pixels. Other option (homework): write a function that determines automatically the thresholds from the minima of the histogram.

```
>>> 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)
```

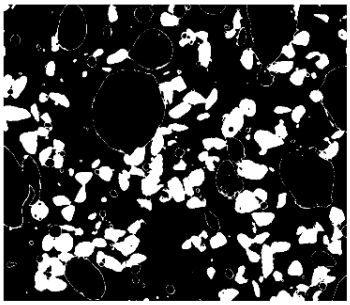


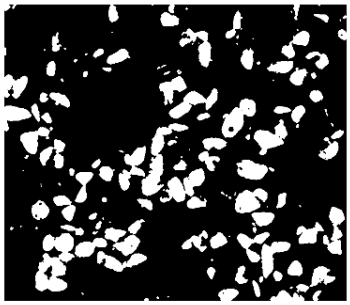
6. Use mathematical morphology to clean the different phases.

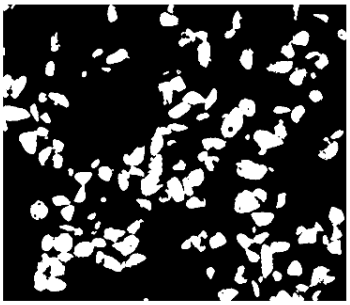
```
>>> sand_op = ndimage.binary_opening(sand, iterations=2)
```

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)
>>> mean_bubble_size, median_bubble_size
```

```
    (1699.875, 65.0)
```

Part II

Advanced topics

CHAPTER 7

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.

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7.1 Iterators, generator expressions and generators

7.1.1 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 it's `__iter__` method doesn't create a separate object: only a single thread of sequential access is allowed.

7.1.2 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.

7.1.3 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 of 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, is 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.

7.1.4 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 %i--' % i
...         try:
...             ans = yield i
...         except GeneratorExit:
...             print '--closing--'
...             raise
...         except Exception as e:
...             print '--yield raised %r--' % e
...         else:
...             print '--yield returned %s--' % 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.

7.1.5 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**, 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.

7.2 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 is 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 sound like more typing, and it is, and also the name of the decorated function dubbling 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 its 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 `@` is 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.

7.2.1 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 if 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.

7.2.2 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 argument-less 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.

7.2.3 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.

7.2.4 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 a 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).

7.2.5 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()                       # doctest: +SKIP
    ... 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                         # doctest: +SKIP
    ... 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
```

7.2.6 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:

```
def 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
```

7.2.7 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.

7.2.8 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

7.3 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 :( )

7.3.1 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']
```

7.3.2 Using generators to define context managers

When discussing generators (page 138), 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 139), 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!

CHAPTER 8

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 153)
  - It's... (page 153)
  - Block of memory (page 154)
  - Data types (page 154)
  - Indexing scheme: strides (page 159)
  - Findings in dissection (page 165)
- Universal functions (page 165)
  - What they are? (page 165)
  - Exercise: building an ufunc from scratch (page 166)
  - Solution: building an ufunc from scratch (page 169)
  - Generalized ufuncs (page 172)
- Interoperability features (page 174)
  - Sharing multidimensional, typed data (page 174)
  - The old buffer protocol (page 174)
  - The old buffer protocol (page 174)
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- Summary (page 177)
- Contributing to Numpy/Scipy (page 177)
  - Why (page 177)
  - Reporting bugs (page 177)
  - Contributing to documentation (page 178)
  - Contributing features (page 179)
  - How to help, in general (page 180)

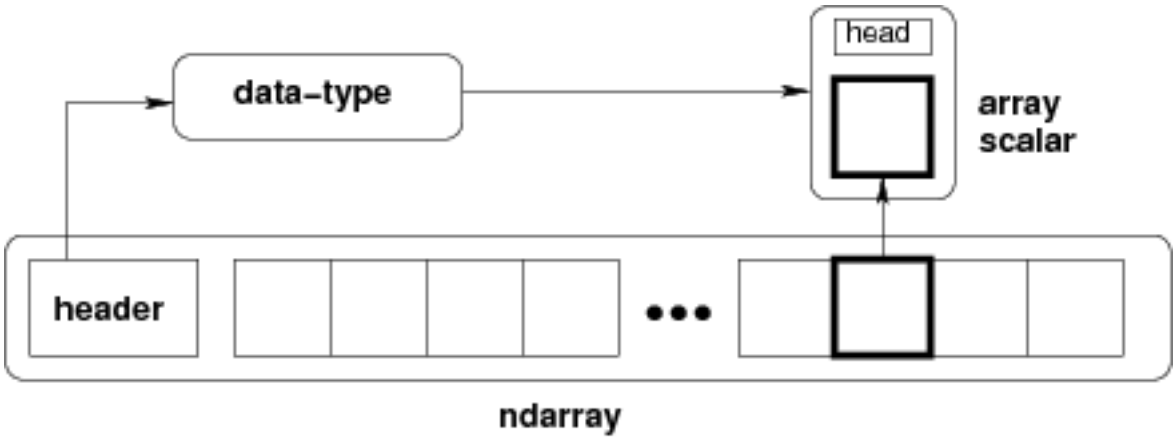
8.1 Life of ndarray

8.1.1 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;
```

8.1.2 Block of memory

```
>>> x = np.array([1, 2, 3, 4], dtype=np.int32)
>>> x.data
<read-write buffer for ..., size 16, offset 0 at ...>
>>> 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]
64803824
```

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 ..., size 4, offset 0 at ...>
>>> 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.

8.1.3 Data types

The descriptor

`dtype` describes a single item in the array:

type	**scalar type** of the data, one of: int8, int16, float64, *et al.* (fixed size) str, unicode, void (flexible size)
itemsize	**size** of the data block
byteorder	**byte order**: big-endian > / little-endian < / not applicable |
fields	sub-dtypes, if it's a **structured data type**
shape	shape of the array, if it's a **sub-array**

```
>>> np.dtype(int).type
<type 'numpy.int64'>
>>> np.dtype(int).itemsize
8
>>> 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 ...>
>>> 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

Exercice

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('data/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']], 17
>>> 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([257, 258, 259, 260], dtype=int32)
```

- 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?

1. 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

2. Create a new view:

```
>>> y = x.view("<i4")
>>> y
array([67305985], dtype=int32)
>>> 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], dtype=int32)
>>> 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)
```

8.1.4 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

$$\begin{aligned}\text{shape} &= (d_1, d_2, ..., d_n)\\ \text{strides} &= (s_1, s_2, ..., s_n)\\ s_j^C &= d_{j+1}d_{j+2}...d_n \times \text{itemsize}\\ s_j^F &= d_1 d_2 ... d_{j-1} \times \text{itemsize}\end{aligned}$$

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], dtype=int32)
```

```
>>> 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], dtype=int32)
```

Slice first, to adjust the data pointer:

```
>>> as_strided(x[0, 1:], shape=(2, ), strides=((3+1)*x.itemsize, ))
array([2, 6], dtype=int32)

>>> as_strided(x[1:, 0], shape=(2, ), strides=((3+1)*x.itemsize, ))
array([4, 8], dtype=int32)
```

Note:

```
>>> y = np.diag(x, k=1)
>>> y
array([2, 6], dtype=int32)
```

However,

```
>>> y.flags.owndata
True
```

It makes a copy?!

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()
```

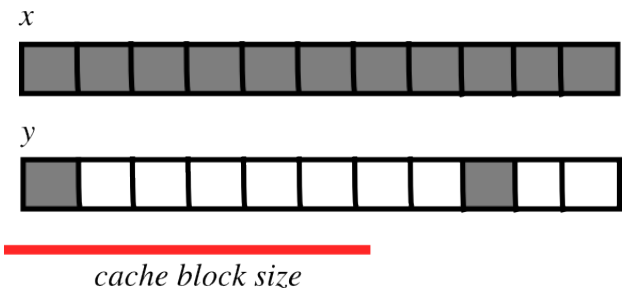
CPU cache effects

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?



- 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

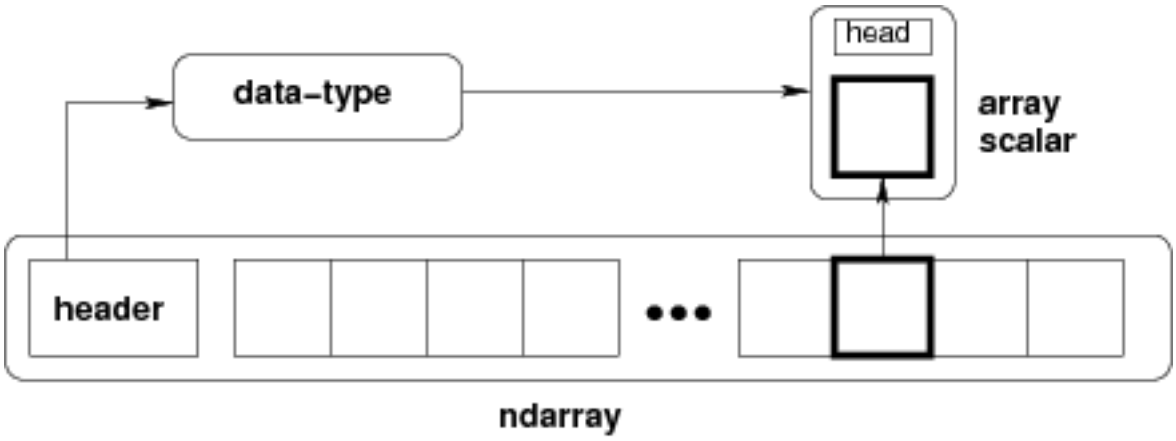
```
>>> a -= b.copy()
```

```
>>> 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 re-appears on the RHS

8.1.5 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

8.2 Universal functions

8.2.1 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];
        }
    }
```

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_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(npy_cdouble *input, npy_cdouble* output)
PyUfunc_DD_D	elementwise_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

8.2.2 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.real**2 + z.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 nout,
        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* o
# ===============  =======================================================
#
# 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_LONGDOUBLE, 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_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* 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_LONGDOUBLE, NPY_CFLOAT, NPY_CDOUBLE, NPY_CLONGDOUBLE, NPY_DATETIME,
NPY_TIMEDELTA, NPY_OBJECT, NPY_STRING, NPY_UNICODE, NPY_VOID
```

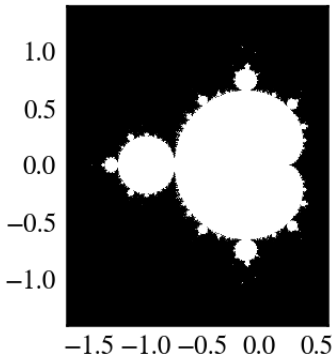
8.2.3 Solution: building an ufunc from scratch

```
# 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(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_func,
    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
    )
```

8.2.4 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) -> (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];
    }
}
```

8.3 Interoperability features

8.3.1 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**)

8.3.2 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
>>> data = np.zeros((200, 200, 4), dtype=np.int8)
>>> data[:, :] = [255, 0, 0, 255] # Red
>>> # In PIL, RGBA images consist of 32-bit integers whose bytes are [RR,GG,BB,AA]
>>> data = data.view(np.int32).squeeze()
>>> img = Image.frombuffer("RGBA", (200, 200), data)
>>> img.save('test.png')
```

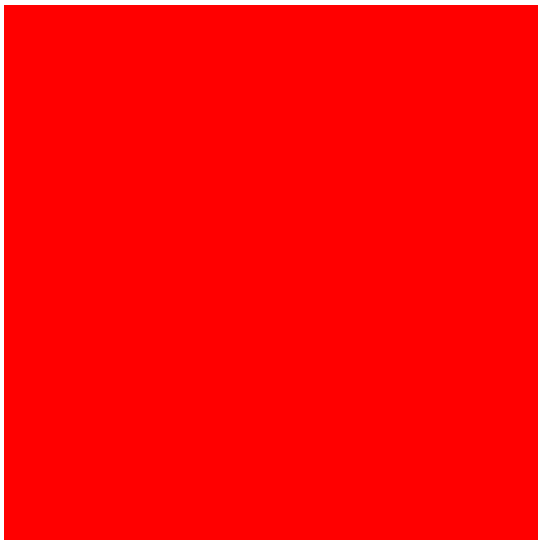
Q:

Check what happens if `data` is now modified, and `img` saved again.

8.3.3 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')
```



8.3.4 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',                 # same, in another form
 'strides': None,                  # strides; or None if in C-order
 'shape': (2, 2),
 'version': 3,
}
```

```
>>> import Image
>>> img = Image.open('data/test.png')
>>> img.__array_interface__
{'data': ...,
 '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.

8.4 Siblings: `chararray`, `maskedarray`, `matrix`

```
>>> 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

---

- 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!

```
>>> 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])
```

- 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]])
```

8.5 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

8.6 Contributing to Numpy/Scipy

Get this tutorial: http://www.euroscipy.org/talk/882

8.6.1 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?"

8.6.2 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.

```
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([ 6, 11,  4, 10,  2,  8,  1,  7,  9,  3,  0,  5])
    >>> np.random.permutation(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 np.__version__
2...
```

Check that the following is what you expect

```
>>> print np.__file__
/...
```

In case you have old/broken Numpy installations lying around.

If unsure, try to remove existing Numpy installations, and reinstall...

8.6.3 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

8.6.4 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
```

8.6.5 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

      http://scipy.org/Developer_Zone/UG_Toc
- Ask on communication channels:
  - `numpy-discussion` list
  - `scipy-dev` list

CHAPTER 9

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 181)
  - Coding best practices to avoid getting in trouble (page 181)
  - pyflakes: fast static analysis (page 182)
    - Running pyflakes on the current edited file (page 182)
    - A type-as-go spell-checker like integration (page 183)
- Debugging workflow (page 183)
- Using the Python debugger (page 184)
  - Invoking the debugger (page 184)
    - Postmortem (page 184)
    - Step-by-step execution (page 186)
    - Other ways of starting a debugger (page 187)
  - Debugger commands and interaction (page 188)
- Debugging segmentation faults using gdb (page 188)

9.1 Avoiding bugs

9.1.1 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)

9.1.2 pyflakes: fast static analysis

They 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

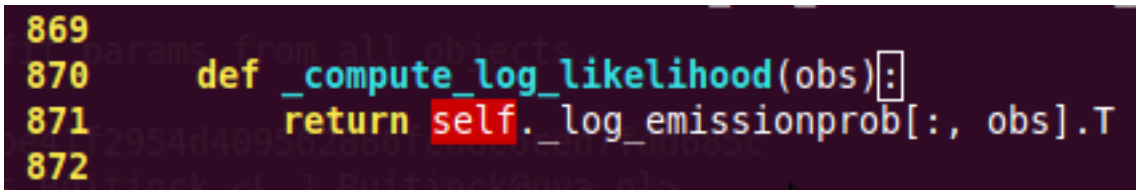
- **In vim** In your `vimrc` (binds F5 to `pyflakes`):

```
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



- **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)
```

9.2 Debugging workflow

I 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.

9.3 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.

9.3.1 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_erro
      3 def index_error():
      4     lst = list('foobar')
----> 5     print lst[len(lst)]
      6
      7 if __name__ == '__main__':

IndexError: list index out of range

In [2]: %debug
> /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/index_error.py(5)index_erro
      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>
File "index_error.py", line 8, 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_er
-> 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_f
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(4)
      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_f
```

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

```
ipdb> c
> /home/varoquau/dev/scipy-lecture-notes/advanced/debugging_optimizing/wiener_filtering.py(34
     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(35
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(36
     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(37
     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 than 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.

9.3.2 Debugger commands and interaction

`l(list)`	Lists the code at the current position
`u(p)`	Walk up the call stack
`d(own)`	Walk down the call stack
`n(ext)`	Execute the next line (does not go down in new functions)
`s(tep)`	Execute the next statement (goes down in new functions)
`bt`	Print the call stack
`a`	Print the local variables
`!command`	Exectute 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 then your local variable when typing code in the debugger**.

9.4 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 `gbdinit`. 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(dit->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
    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
    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`

CHAPTER 10

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 191)
- Profiling Python code (page 192)
  - Timeit (page 192)
  - Profiler (page 192)
  - Line-profiler (page 193)
- Making code go faster (page 194)
  - Algorithmic optimization (page 194)
    - Example of the SVD (page 194)
- Writing faster numerical code (page 195)

10.1 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 bottleneck, 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.

10.2 Profiling Python code

No optimization without measuring!

- **Measure:** profiling, timing
- You'll have surprises: the fastest code is not always what you think

10.2.1 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

---

10.2.2 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' objects
     1    0.017    0.017    0.021    0.021 function_base.py:645(asarray_chkfinite)
    54    0.011    0.000    0.011    0.000 {numpy.core._dotblas.dot}
     2    0.005    0.002    0.005    0.002 {method 'any' of 'numpy.ndarray' objects}
     6    0.001    0.000    0.001    0.000 ica.py:195(gprime)
     6    0.001    0.000    0.001    0.000 ica.py:192(g)
    14    0.001    0.000    0.001    0.000 {numpy.linalg.lapack_lite.dsyevd}
    19    0.001    0.000    0.001    0.000 twodim_base.py:204(diag)
     1    0.001    0.001    0.008    0.008 ica.py:69(_ica_par)
     1    0.001    0.001   14.551   14.551 {execfile}
   107    0.000    0.000    0.001    0.000 defmatrix.py:239(__array_finalize__)
     7    0.000    0.000    0.004    0.001 ica.py:58(_sym_decorrelation)
     7    0.000    0.000    0.002    0.000 linalg.py:841(eigh)
   172    0.000    0.000    0.000    0.000 {isinstance}
     1    0.000    0.000   14.551   14.551 demo.py:1(<module>)
    29    0.000    0.000    0.000    0.000 numeric.py:180(asarray)
    35    0.000    0.000    0.000    0.000 defmatrix.py:193(__new__)
    35    0.000    0.000    0.001    0.000 defmatrix.py:43(asmatrix)
    21    0.000    0.000    0.001    0.000 defmatrix.py:287(__mul__)
    41    0.000    0.000    0.000    0.000 {numpy.core.multiarray.zeros}
    28    0.000    0.000    0.000    0.000 {method 'transpose' of 'numpy.ndarray' objects}
     1    0.000    0.000    0.008    0.008 ica.py:97(fastica)
     ...
```

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.

10.2.3 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 `-` 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.

10.3 Making code go faster

Once we have identified the bottlenecks, we need to make the corresponding code go faster.

10.3.1 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 then 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.

10.4 Writing faster numerical code

A complete discussion on advanced use of numpy is found in chapter *Advanced Numpy* (page 152), 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 162) 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 163)):

```
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:

```
In [5]: a = np.random.rand(20, 2**18)

In [6]: b = np.random.rand(20, 2**18)

In [7]: %timeit np.dot(b, a.T)
1 loops, best of 3: 194 ms per loop

In [8]: c = np.ascontiguousarray(a.T)
```

```
In [9]: %timeit np.dot(b, c)
10 loops, best of 3: 84.2 ms per loop
```

Note that copying the data to work around this effect may not be worth it:

```
In [10]: %timeit c = np.ascontiguousarray(a.T)
10 loops, best of 3: 106 ms per loop
```

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.

CHAPTER 11

Sparse Matrices in SciPy

author Robert Cimrman

11.1 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 (*)

11.1.1 Why Sparse Matrices?

- the memory, that grows like `n**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)
[<matplotlib.lines.Line2D object at ...>]
>>> plt.xlabel('size n')
<matplotlib.text.Text object at ...>
>>> plt.ylabel('memory [MB]')
<matplotlib.text.Text object at ...>
```

11.1.2 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

11.1.3 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`
- ...

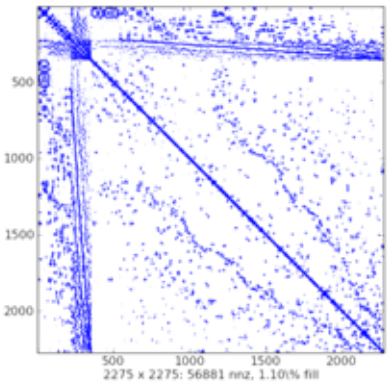
11.1.4 Prerequisites

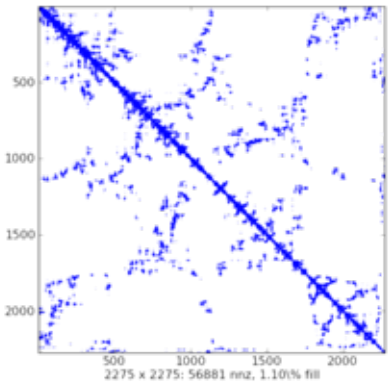
recent versions of

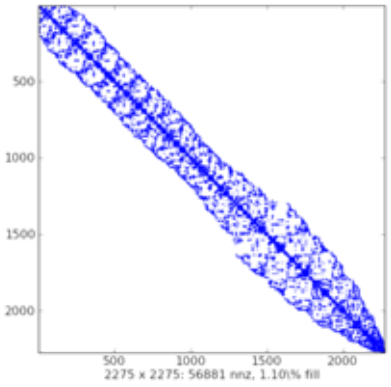
- `numpy`
- `scipy`
- `matplotlib` (optional)
- `ipython` (the enhancements come handy)

11.1.5 Sparsity Structure Visualization

- `spy()` from `matplotlib`
- example plots:







11.2 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 sparsetools 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

11.2.1 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

11.2.2 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 (sparsetools)
- **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 = sparse.dia_matrix((data, offsets), shape=(4, 4))
>>> mtx
<4x4 sparse matrix of type '<type 'numpy.int64'>'
        with 9 stored elements (3 diagonals) in DIAgonal format>
>>> mtx.todense()
matrix([[1, 0, 3, 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 = sparse.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], dtype=int32)
>>> 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 = sparse.lil_matrix((4, 5))
```

- prepare random data:

```
>>> from numpy.random import rand
>>> data = np.round(rand(2, 3))
>>> data
array([[ 1.,  1.,  1.],
       [ 1.,  0.,  1.]])
```

- assign the data using fancy indexing:

```
>>> mtx[:2, [1, 2, 3]] = data
>>> mtx
<4x5 sparse matrix of type '<type 'numpy.float64'>'
        with 5 stored elements in LInked List format>
>>> print mtx
  (0, 1)  1.0
  (0, 2)  1.0
  (0, 3)  1.0
  (1, 1)  1.0
  (1, 3)  1.0
>>> mtx.todense()
matrix([[ 0.,  1.,  1.,  1.,  0.],
        [ 0.,  1.,  0.,  1.,  0.],
        [ 0.,  0.,  0.,  0.,  0.],
        [ 0.,  0.,  0.,  0.,  0.]])
>>> mtx.toarray()
array([[ 0.,  1.,  1.,  1.,  0.],
       [ 0.,  1.,  0.,  1.,  0.],
       [ 0.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.]])
```

- more slicing and indexing:

```
>>> mtx = sparse.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.int64'>'
  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 = sparse.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 20 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.]])
```

- 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):
 ...
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 (sparsetools)
- **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 = sparse.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 = sparse.coo_matrix((data, (row, col)), shape=(4, 4))
>>> mtx
<4x4 sparse matrix of type '<type 'numpy.int64'>'
        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 = sparse.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):
...
TypeError: 'coo_matrix' object ...
```

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 (sparsetools)
- **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)

Examples

- create empty CSR matrix:

```
>>> mtx = sparse.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 = sparse.csr_matrix((data, (row, col)), shape=(3, 3))
>>> mtx
<3x3 sparse matrix of type '<type 'numpy.int64'>'
        with 6 stored elements in Compressed Sparse Row format>
>>> mtx.todense()
matrix([[1, 0, 2],
        [0, 0, 3],
        [4, 5, 6]])
```

```
>>> mtx.data
array([1, 2, 3, 4, 5, 6])
>>> mtx.indices
array([0, 2, 2, 0, 1, 2], dtype=int32)
>>> mtx.indptr
array([0, 2, 3, 6], dtype=int32)
```

- 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 = sparse.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 (sparsetools)
- **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 CSC matrix:

```
>>> mtx = sparse.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 = sparse.csc_matrix((data, (row, col)), shape=(3, 3))
>>> mtx
<3x3 sparse matrix of type '<type 'numpy.int64'>'
        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], dtype=int32)
>>> mtx.indptr
array([0, 2, 3, 6], dtype=int32)
```

- 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 = sparse.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 (sparsetools)
- **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 = sparse.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 = sparse.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 = sparse.bsr_matrix((data, (row, col)), shape=(3, 3))
>>> mtx
<3x3 sparse matrix of type '<type 'numpy.int64'>'
        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]]])
>>> mtx.indices
array([0, 2, 2, 0, 1, 2], dtype=int32)
>>> mtx.indptr
array([0, 2, 3, 6], dtype=int32)
```

- 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 = sparse.bsr_matrix((data, indices, indptr), shape=(6, 6))
>>> mtx.todense()
matrix([[1, 1, 0, 0, 2, 2],
        [1, 1, 0, 0, 2, 2],
        [0, 0, 0, 0, 3, 3],
        [0, 0, 0, 0, 3, 3],
        [4, 4, 5, 5, 6, 6],
        [4, 4, 5, 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]]])
```

11.2.3 Summary

Table 11.1: 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

11.3 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']
```

11.3.1 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:

```
>>> from scipy.sparse.linalg import dsolve
>>> help(dsolve)
```

- both superlu and umfpack can be used (if the latter is installed) as follows:
  - prepare a linear system:

```
>>> import numpy as np
>>> from scipy import sparse
>>> mtx = sparse.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 = dsolve.spsolve(mtx1, rhs, use_umfpack=False)
>>> print x
[ 106.   -21.     5.5   -1.5    1. ]
>>> print "Error: ", mtx1 * x - rhs
Error:  [ 0.  0.  0.  0.  0.]
```

- solve as double precision real:

```
>>> mtx2 = mtx.astype(np.float64)
>>> x = dsolve.spsolve(mtx2, rhs, use_umfpack=True)
>>> print x
[ 106.   -21.     5.5   -1.5    1. ]
>>> print "Error: ", mtx2 * x - rhs
Error:  [ 0.  0.  0.  0.  0.]
```

- solve as single precision complex:

```
>>> mtx1 = mtx.astype(np.complex64)
>>> x = dsolve.spsolve(mtx1, rhs, use_umfpack=False)
>>> print x
[ 106.0+0.j  -21.0+0.j    5.5+0.j   -1.5+0.j    1.0+0.j]
>>> print "Error: ", mtx1 * x - rhs
Error:  [ 0.+0.j  0.+0.j  0.+0.j  0.+0.j  0.+0.j]
```

- solve as double precision complex:

```
>>> mtx2 = mtx.astype(np.complex128)
>>> x = dsolve.spsolve(mtx2, rhs, use_umfpack=True)
>>> print x
[ 106.0+0.j  -21.0+0.j    5.5+0.j   -1.5+0.j    1.0+0.j]
>>> print "Error: ", mtx2 * x - rhs
Error:  [ 0.+0.j  0.+0.j  0.+0.j  0.+0.j  0.+0.j]
```

```
"""
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 'rezidual:', np.linalg.norm(mtx * x - rhs)
```

- `examples/direct_solve.py`

11.3.2 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()`

11.3.3 Eigenvalue Problem Solvers

The `eigen` module

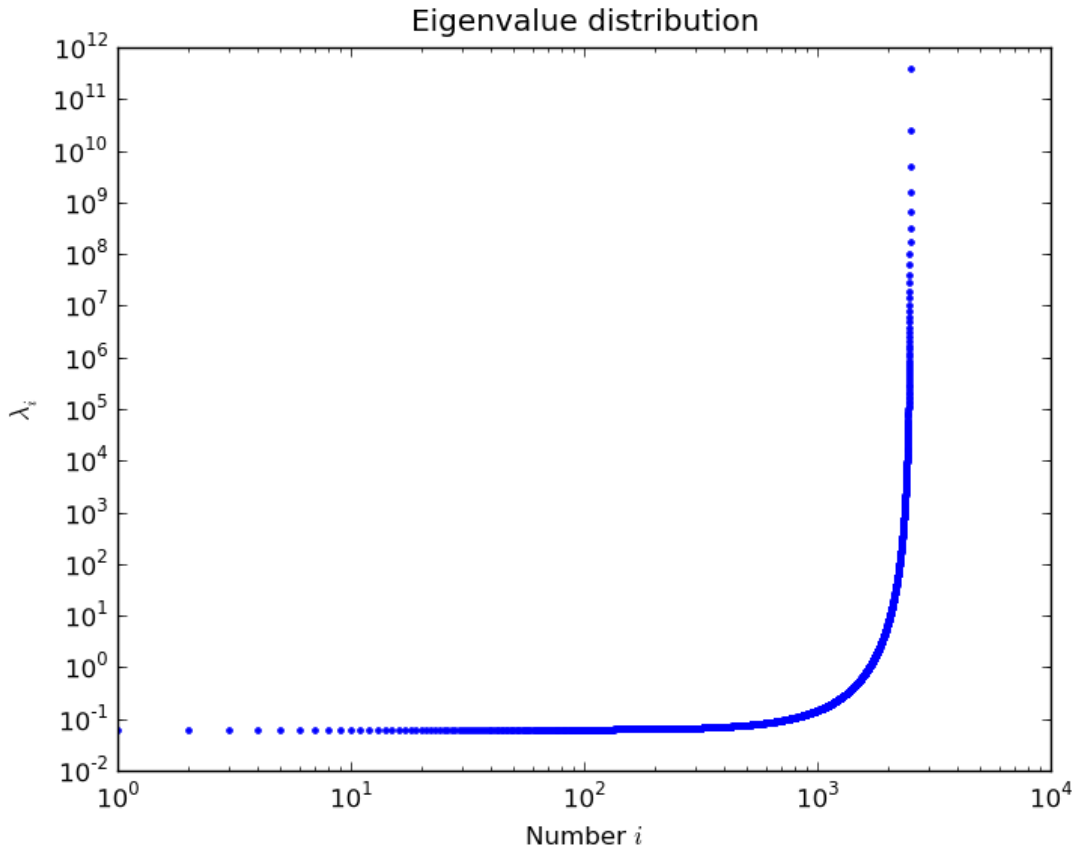
- `arpack` * a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems
- `lobpcg` (Locally Optimal Block Preconditioned Conjugate Gradient Method) * works very well in combination with PyAMG * example by Nathan Bell:

```
    """
    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
```



11.4 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

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- Displaying images (page 219)
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  - Statistical information (page 221)
  - Geometrical transformations (page 222)
- Image filtering (page 222)
  - Blurring/smoothing (page 222)
  - Sharpening (page 223)
  - Denoising (page 223)
  - Mathematical morphology (page 224)
- Feature extraction (page 227)
  - Edge detection (page 227)
  - Segmentation (page 228)
- Measuring objects properties (page 230)

12.1 Opening and writing to image files

Writing an array to a file:

```
from scipy import misc
l = misc.lena()
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

```
>>> for i in range(10):
...     im = np.random.random_integers(0, 255, 10000).reshape((100, 100))
...     misc.imsave('random_%02d.png' % i, im)
>>> from glob import glob
>>> filelist = glob('random*.png')
>>> filelist.sort()
```

12.2 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:

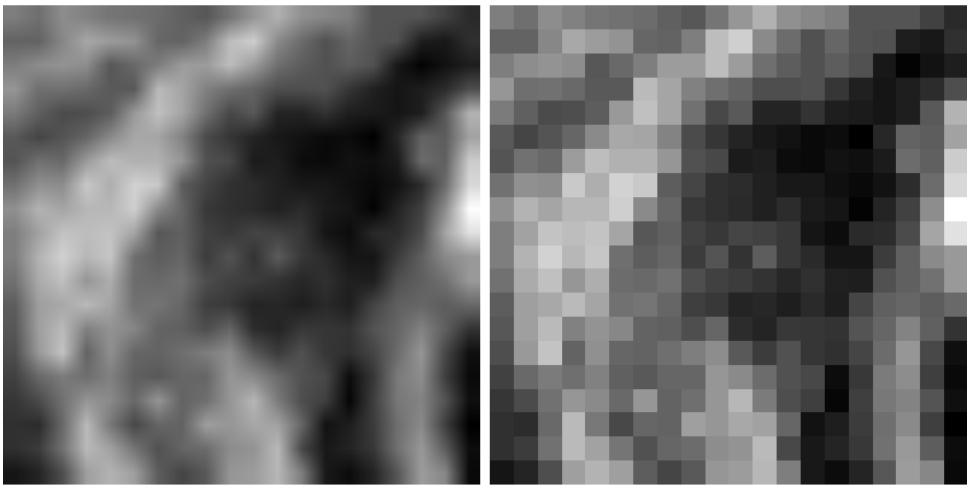
```
>>> plt.imshow(l, cmap=plt.cm.gray, vmin=30, vmax=200)
<matplotlib.image.AxesImage object at 0x33ef750>
>>> # Remove axes and ticks
>>> plt.axis('off')
(-0.5, 511.5, 511.5, -0.5)
```

Draw contour lines:

```
>>> plt.contour(l, [60, 211])
<matplotlib.contour.ContourSet instance at 0x33f8c20>
```

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')
```



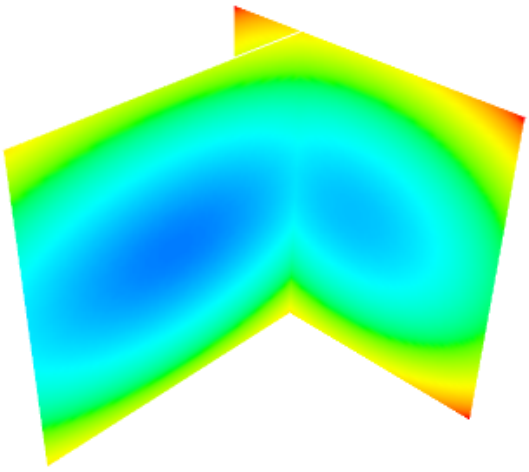
Other packages sometimes use graphical toolkits for visualization (GTK, Qt):

```
>>> 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 254) and *Volumetric data* (page 257).

- Image plane widgets
- Isosurfaces
- ...



12.3 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
```

12.3.1 Statistical information

```
>>> lena = scipy.lena()
>>> lena.mean()
124.04678344726562
>>> lena.max(), lena.min()
(245, 25)
```

`np.histogram`

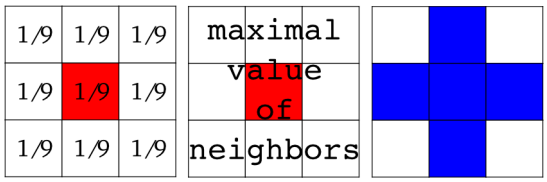
12.3.2 Geometrical transformations

```
>>> 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)
```

12.4 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*.



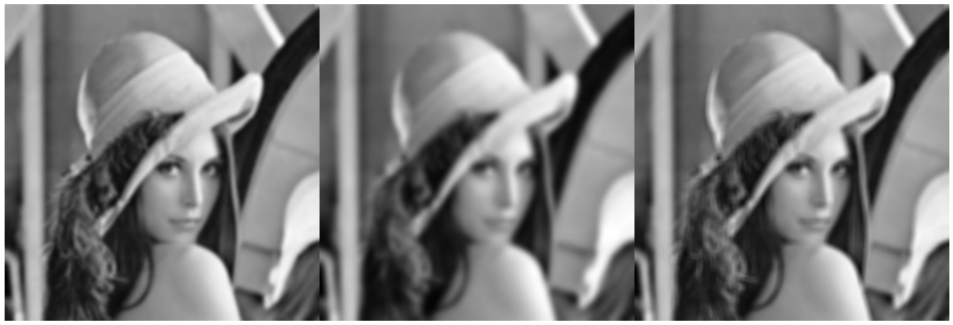
12.4.1 Blurring/smoothing

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)
```



12.4.2 Sharpening

Sharpen a blurred image:

```
>>> lena = scipy.lena()
>>> blurred_l = ndimage.gaussian_filter(lena, 3)
```

increase the weight of edges by adding an approximation of the Laplacian:

```
>>> filter_blurred_l = ndimage.gaussian_filter(blurred_l, 1)
>>> alpha = 30
>>> sharpened = blurred_l + alpha * (blurred_l - filter_blurred_l)
```



12.4.3 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:

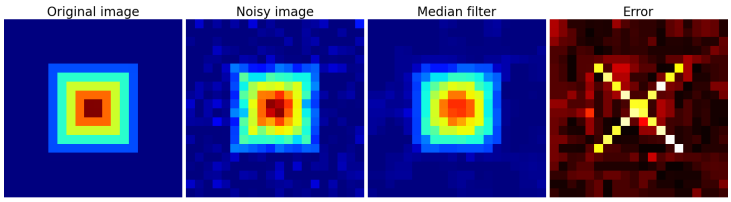
```
>>> med_denoised = ndimage.median_filter(noisy, 3)
```

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)
```

Other rank filter: `ndimage.maximum_filter`, `ndimage.percentile_filter`

Other local non-linear filters: Wiener (`scipy.signal.wiener`), etc.

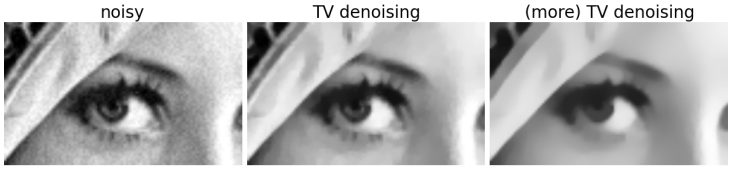


Non-local filters

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.



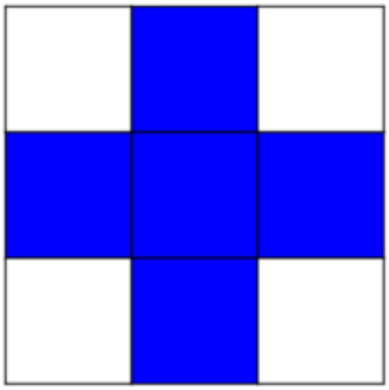
12.4.4 Mathematical morphology

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.

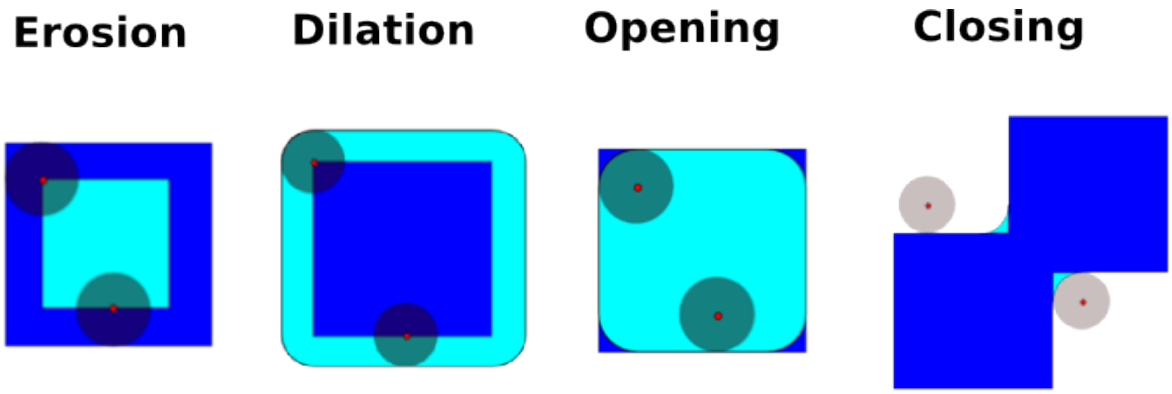
Structuring element:

```
>>> 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, 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]])
```



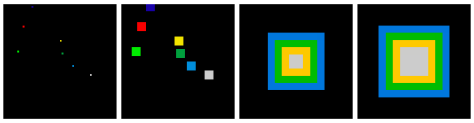
Dilation: maximum filter:

```
>>> 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.]])
>>> ndimage.binary_dilation(a).astype(a.dtype)
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.]])
```

Also works for grey-valued images:

```
>>> np.random.seed(2)
>>> x, y = (63*np.random.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)))
```



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.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)
```

Closing: dilation + erosion

Many other mathematical morphology operations: hit and miss transform, tophat, etc.

12.5 Feature extraction

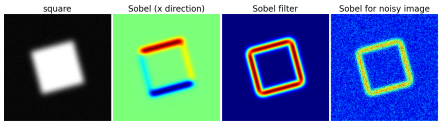
12.5.1 Edge detection

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:

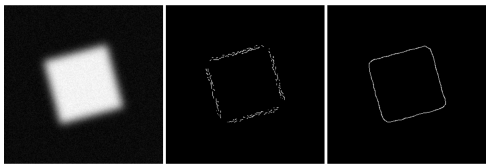
```
>>> sx = ndimage.sobel(im, axis=0, mode='constant')
>>> sy = ndimage.sobel(im, axis=1, mode='constant')
>>> sob = np.hypot(sx, sy)
```



Canny filter

The Canny filter is available in the `scikits.image` (doc), 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
```

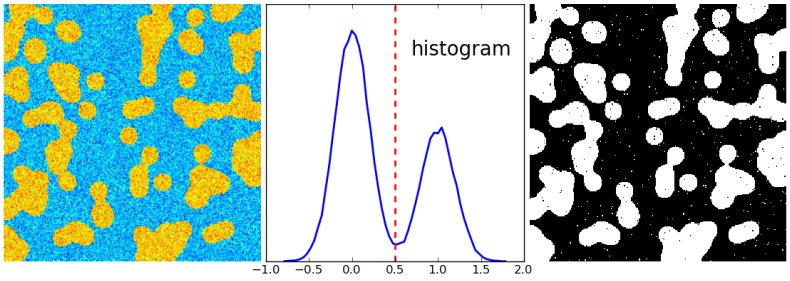


Several parameters need to be adjusted... risk of overfitting

12.5.2 Segmentation

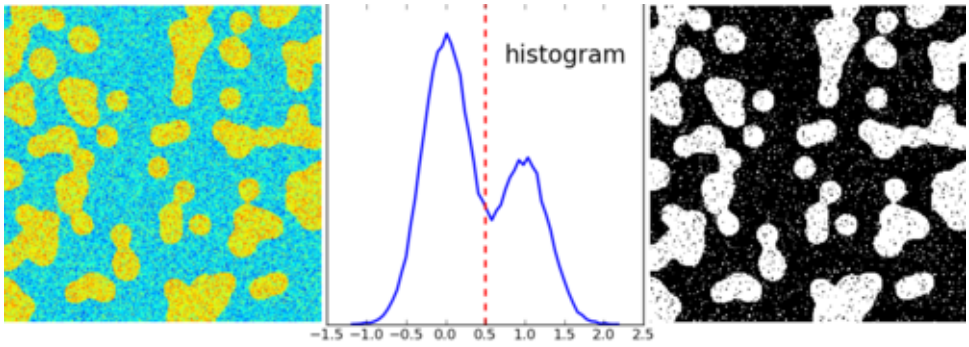
- **Histogram-based** segmentation (no spatial information)

```
>>> 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=l/(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
```



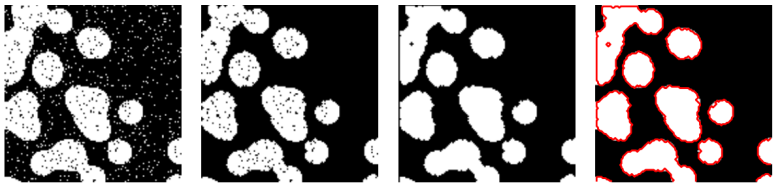
Automatic thresholding: use Gaussian mixture model:

```
>>> 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)
```



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()
0.0042572021484375
```

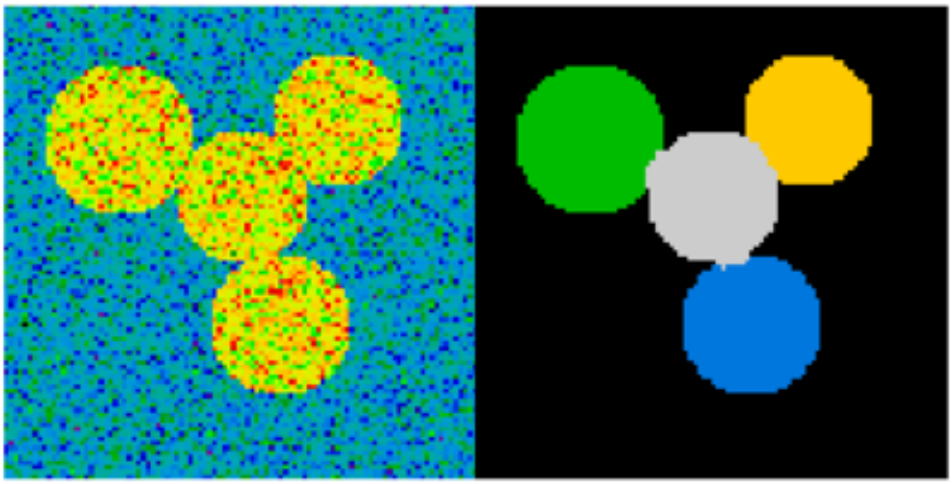
Exercise

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
```



12.6 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=l/(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>
```

Compute size, mean_value, etc. of each region:

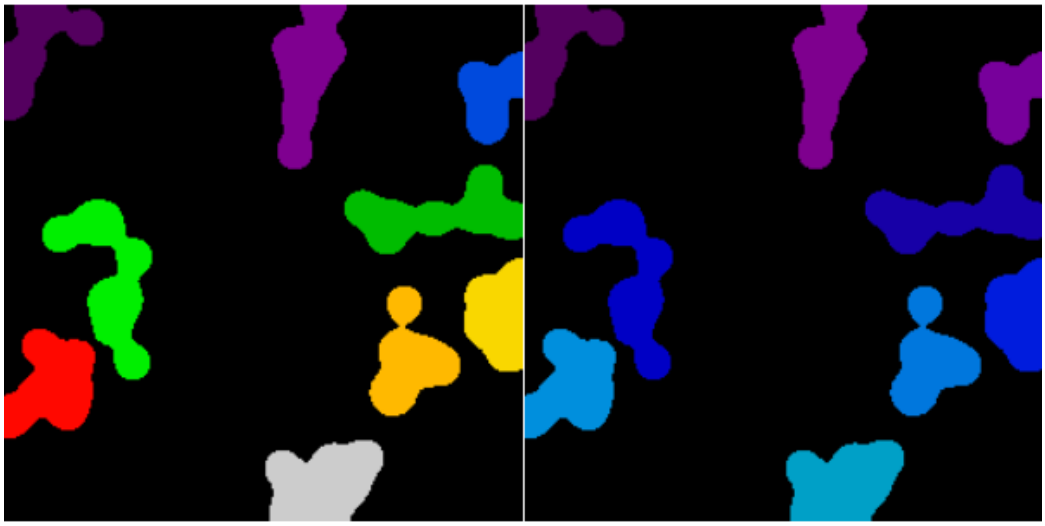
```
>>> sizes = ndimage.sum(mask, label_im, range(nb_labels + 1))
>>> mean_vals = ndimage.sum(im, label_im, range(1, nb_labels + 1))
```

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)
```

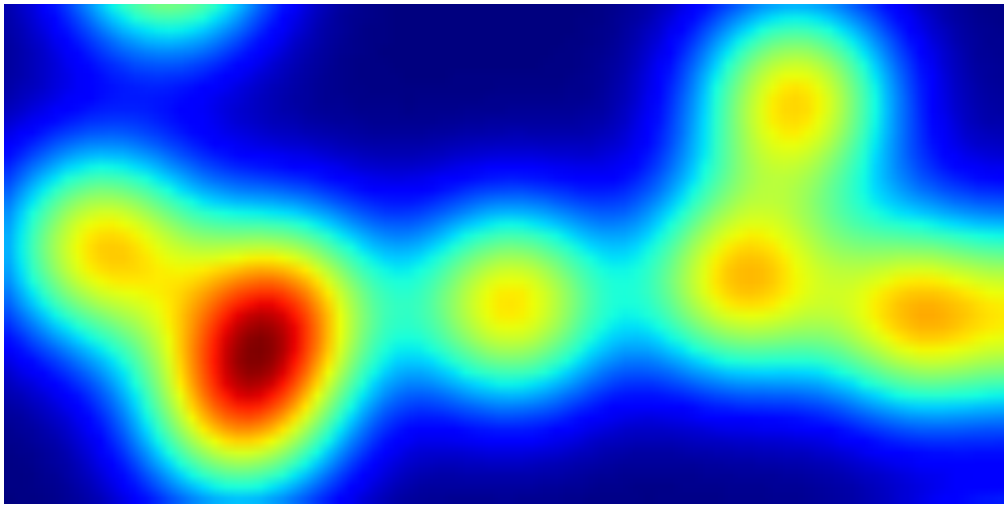
Now reassign labels with `np.searchsorted`:

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



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)
```



Other spatial measures: `ndimage.center_of_mass`, `ndimage.maximum_position`, etc.

Can be used outside the limited scope of segmentation applications.

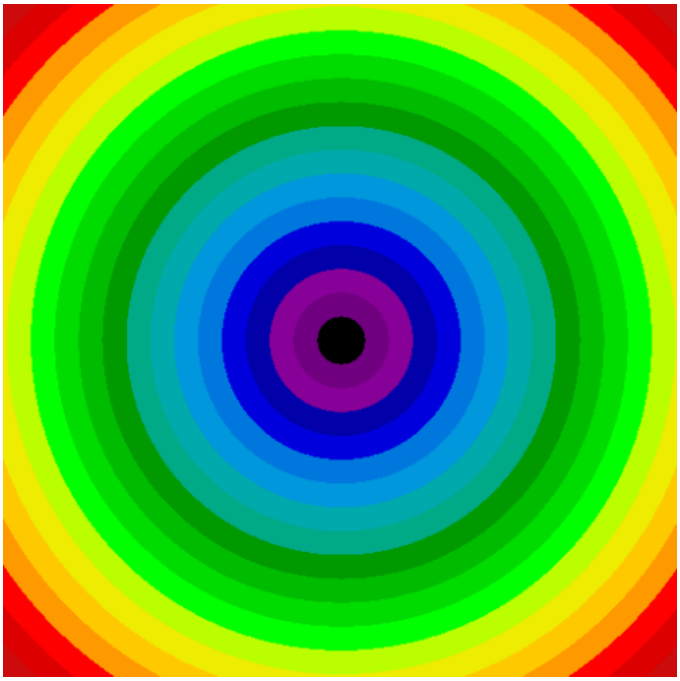
Example: block mean:

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

When regions are regular blocks, it is more efficient to use stride tricks (*Example: fake dimensions with strides* (page 161)).

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))
```

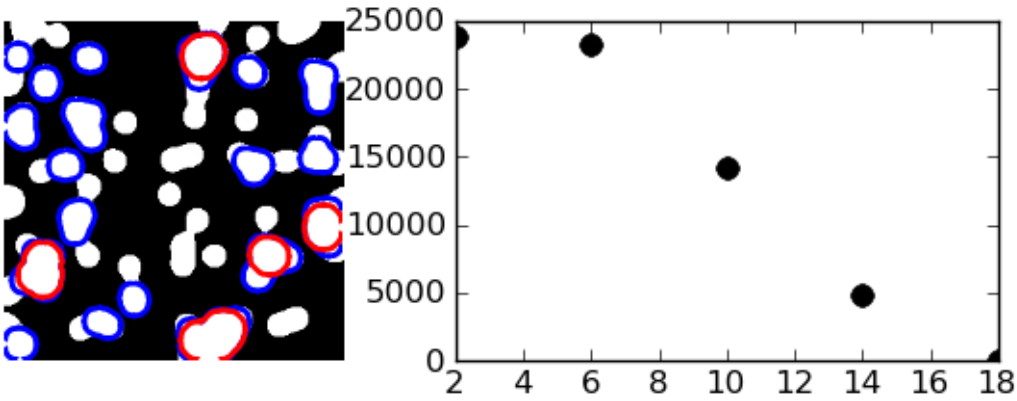


- **Other measures**

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=l/(4.*n))
>>>
>>> mask = im > im.mean()
>>>
>>> granulo = granulometry(mask, sizes=np.arange(2, 19, 4))
```


25000
20000
15000
10000
5000
0
2
4
6
8
10
12
14
16
18

CHAPTER 13

Traits

author Didrik Pinte

The Traits project allows you to simply add validation, initialization, delegation, notification and a graphical user interface to Python object attributes. In this tutorial we will explore the Traits toolset and learn how to dramatically reduce the amount of boilerplate code you write, do rapid GUI application development, and understand the ideas which underly other parts of the Enthought Tool Suite.

Traits and the Enthought Tool Suite are open source projects licensed under a BSD-style license.

Intended Audience

Intermediate to advanced Python programmers

Requirements

- Python 2.6 or 2.7 (www.python.org)
- Either wxPython (http://www.wxpython.org/) or PyQt (http://www.riverbankcomputing.co.uk/software/pyqt/intro)
- Numpy and Scipy (http://www.scipy.org)
- Enthought Tool Suite 3.x or higher (http://code.enthought.com/projects)
- All required software can be obtained by installing the EPD Free (http://www.enthought.com/products/epd.php)

Tutorial content

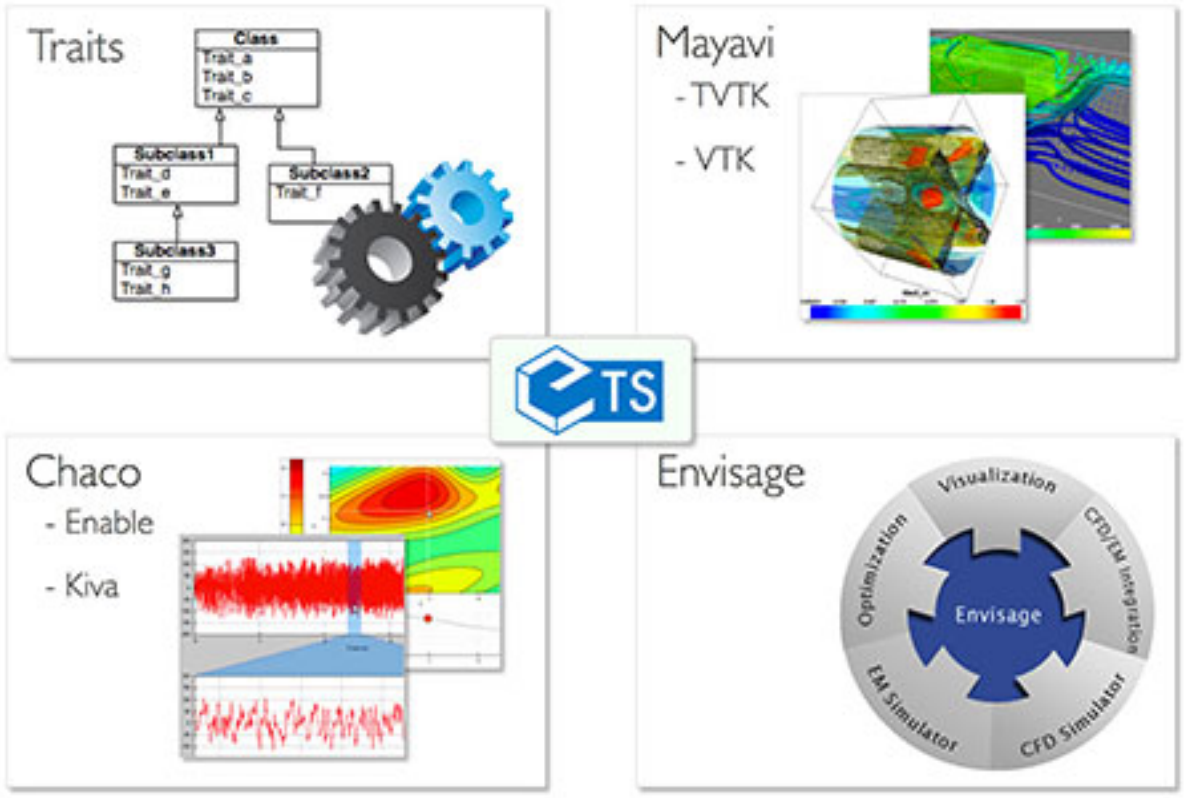
- Introduction (page 236)
- Example (page 236)
- What are Traits (page 237)
  - Initialisation (page 238)
  - Validation (page 238)
  - Documentation (page 239)
  - Visualisation (page 240)
  - Deferral (page 241)
  - Notification (page 246)
  - Some more advanced traits (page 249)
- References (page 252)

13.1 Introduction

The Enthought Tool Suite enable the construction of sophisticated application frameworks for data analysis, 2D plotting and 3D visualization. These powerful, reusable components are released under liberal BSD-style licenses.

The main packages are:

- Traits - component based approach to build our applications.
- Kiva - 2D primitives supporting path based rendering, affine transforms, alpha blending and more.
- Enable - object based 2D drawing canvas.
- Chaco - plotting toolkit for building complex interactive 2D plots.
- Mayavi - 3D visualization of scientific data based on VTK.
- Envisage - application plugin framework for building scriptable and extensible applications



In this tutorial, we will focus on Traits.

13.2 Example

Throughout this tutorial, we will use an example based on a water resource management simple case. We will try to model a dam and reservoir system. The reservoir and the dams do have a set of parameters :

- Name
- Minimal and maximal capacity of the reservoir [hm3]
- Height and length of the dam [m]
- Catchment area [km2]
- Hydraulic head [m]

- Power of the turbines [MW]
- Minimal and maximal release [m3/s]
- Efficiency of the turbines

The reservoir has a known behaviour. One part is related to the energy production based on the water released. A simple formula for approximating electric power production at a hydroelectric plant is $P = \rho hrgk$, where:

- P is Power in watts,
- ρ is the density of water (~1000 kg/m3),
- h is height in meters,
- r is flow rate in cubic meters per second,
- g is acceleration due to gravity of 9.8 m/s2,
- k is a coefficient of efficiency ranging from 0 to 1.

Annual electric energy production depends on the available water supply. In some installations the water flow rate can vary by a factor of 10:1 over the course of a year.

The second part of the behaviour is the state of the storage that depends on controlled and uncontrolled parameters :

$$storage_{t+1} = storage_t + inflows - release - spillage - irrigation$$

Warning: The data used in this tutorial are not real and might even not have sense in the reality.

13.3 What are Traits

A trait is a type definition that can be used for normal Python object attributes, giving the attributes some additional characteristics:

- **Standardization:**
  - Initialization
  - Validation
  - Deferral
- Notification
- Visualization
- Documentation

A class can freely mix trait-based attributes with normal Python attributes, or can opt to allow the use of only a fixed or open set of trait attributes within the class. Trait attributes defined by a class are automatically inherited by any subclass derived from the class.

The common way of creating a traits class is by extending from the **HasTraits** base class and defining class traits :

```
from traits.api import HasTraits, Str, Float

class Reservoir(HasTraits):

    name = Str
    max_storage = Float
```

Warning: For Traits 3.x users
If using Traits 3.x, you need to adapt the namespace of the traits packages:
- traits.api should be enthought.traits.api
- traitsui.api should be enthought.traits.ui.api

Using a traits class like that is as simple as any other Python class. Note that the trait value are passed using keyword arguments:

```
reservoir = Reservoir(name='Lac de Vouglans', max_storage=605)
```

13.3.1 Initialisation

All the traits do have a default value that initialise the variables. For example, the basic python types do have the following trait equivalents:

Trait	Python Type	Built-in Default Value
Bool	Boolean	False
Complex	Complex number	0+0j
Float	Floating point number	0.0
Int	Plain integer	0
Long	Long integer	0L
Str	String	''
Unicode	Unicode	u''

A number of other predefined trait type do exist : Array, Enum, Range, Event, Dict, List, Color, Set, Expression, Code, Callable, Type, Tuple, etc.

Custom default values can be defined in the code:

```
from traits.api import HasTraits, Str, Float

class Reservoir(HasTraits):

    name = Str
    max_storage = Float(100)

reservoir = Reservoir(name='Lac de Vouglans')
```

Note: Complex initialisation

When a complex initialisation is required for a trait, a _XXX_default magic method can be implemented. It will be lazily called when trying to access the XXX trait. For example:

```
def _name_default(self):
    """ Complex initialisation of the reservoir name. """

    return 'Undefined'
```

13.3.2 Validation

Every trait does validation when the user tries to set its content:

```
reservoir = Reservoir(name='Lac de Vouglans', max_storage=605)

reservoir.max_storage = '230'
---------------------------------------------------------------------------
TraitError                                 Traceback (most recent call last)
/Users/dpinte/projects/scipy-lecture-notes/advanced/traits/<ipython-input-7-979bdff9974a> in <modu
```

```
----> 1 reservoir.max_storage = '230'

/Users/dpinte/projects/ets/traits/traits/trait_handlers.pyc in error(self, object, name, value)
    166         """
    167         raise TraitError( object, name, self.full_info( object, name, value ),
--> 168                           value )
    169
    170     def arg_error ( self, method, arg_num, object, name, value ):

TraitError: The 'max_storage' trait of a Reservoir instance must be a float, but a value of '23'
```

13.3.3 Documentation

By essence, all the traits do provide documentation about the model itself. The declarative approach to the creation of classes makes it self-descriptive:

```
from traits.api import HasTraits, Str, Float

class Reservoir(HasTraits):

    name = Str
    max_storage = Float(100)
```

The **desc** metadata of the traits can be used to provide a more descriptive information about the trait :

```
from traits.api import HasTraits, Str, Float

class Reservoir(HasTraits):

    name = Str
    max_storage = Float(100, desc='Maximal storage [hm3]')
```

Let's now define the complete reservoir class:

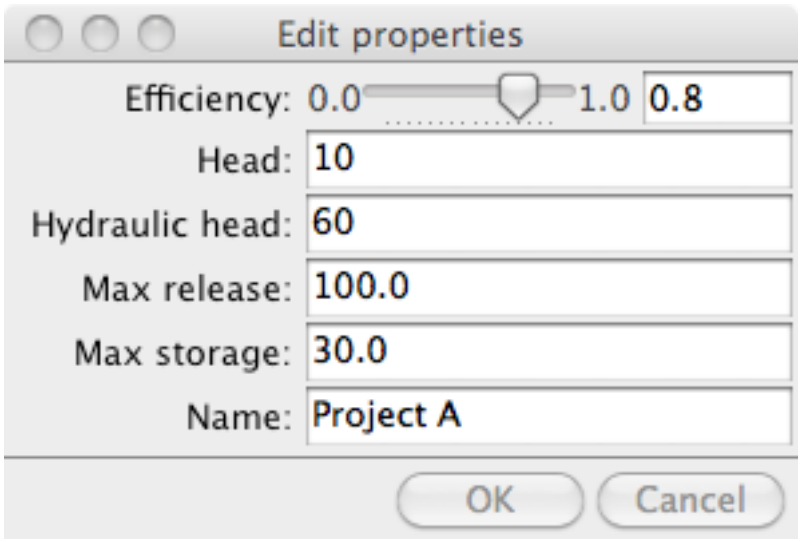
```
from traits.api import HasTraits, Str, Float, Range

class Reservoir(HasTraits):
    name = Str
    max_storage = Float(1e6, desc='Maximal storage [hm3]')
    max_release = Float(10, desc='Maximal release [m3/s]')
    head = Float(10, desc='Hydraulic head [m]')
    efficiency = Range(0, 1.)

    def energy_production(self, release):
        ''' Returns the energy production [Wh] for the given release [m3/s]
        '''
        power = 1000 * 9.81 * self.head * release * self.efficiency
        return power * 3600


if __name__ == '__main__':
    reservoir = Reservoir(
                        name = 'Project A',
                        max_storage = 30,
                        max_release = 100.0,
                        head = 60,
                        efficiency = 0.8
                    )

    release = 80
    print 'Releasing {} m3/s produces {} kWh'.format(
```

```
                        release, reservoir.energy_production(release)
                    )
```

13.3.4 Visualisation

The Traits library is also aware of user interfaces and can pop up a default view for the Reservoir class:

```
reservoir1 = Reservoir()
reservoir1.edit_traits()
```

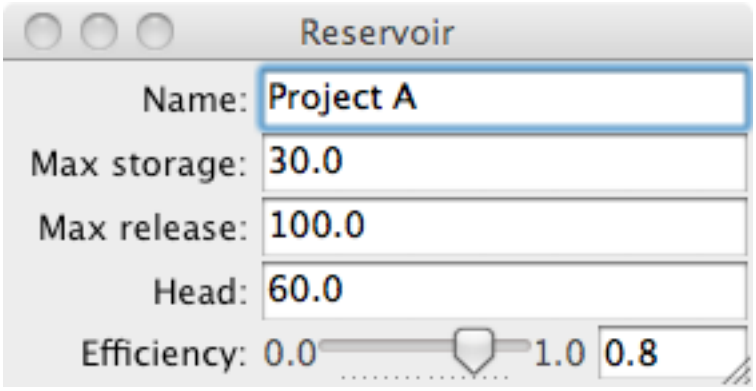


TraitsUI simplifies the way user interfaces are created. Every trait on a HasTraits class has a default editor that will manage the way the trait is rendered to the screen (e.g. the Range trait is displayed as a slider, etc.).

In the very same vein as the Traits declarative way of creating classes, TraitsUI provides a declarative interface to build user interfaces code:

```
from traits.api import HasTraits, Str, Float, Range
from traitsui.api import View

class Reservoir(HasTraits):
    name = Str
    max_storage = Float(1e6, desc='Maximal storage [hm3]')
    max_release = Float(10, desc='Maximal release [m3/s]')
    head = Float(10, desc='Hydraulic head [m]')
    efficiency = Range(0, 1.)

    traits_view = View(
        'name', 'max_storage', 'max_release', 'head', 'efficiency',
        title = 'Reservoir',
        resizable = True,
    )

    def energy_production(self, release):
        ''' Returns the energy production [Wh] for the given release [m3/s]
        '''
        power = 1000 * 9.81 * self.head * release * self.efficiency
        return power * 3600


if __name__ == '__main__':
    reservoir = Reservoir(
                        name = 'Project A',
                        max_storage = 30,
```

```
                        max_release = 100.0,
                        head = 60,
                        efficiency = 0.8
                    )

    reservoir.configure_traits()
```



13.3.5 Deferral

Being able to defer the definition of a trait and its value to another object is a powerful feature of Traits.

```
from traits.api import HasTraits, Instance, DelegatesTo, Float, Range

from reservoir import Reservoir

class ReservoirState(HasTraits):
    """Keeps track of the reservoir state given the initial storage.
    """
    reservoir = Instance(Reservoir, ())
    min_storage = Float
    max_storage = DelegatesTo('reservoir')
    min_release = Float
    max_release = DelegatesTo('reservoir')

    # state attributes
    storage = Range(low='min_storage', high='max_storage')

    # control attributes
    inflows =  Float(desc='Inflows [hm3]')
    release = Range(low='min_release', high='max_release')
    spillage = Float(desc='Spillage [hm3]')

    def print_state(self):
        print 'Storage\tRelease\tInflows\tSpillage'
        str_format = '\t'.join(['{:7.2f}'for i in range(4)])
        print str_format.format(self.storage, self.release, self.inflows,
                self.spillage)
        print '-' * 79


if __name__ == '__main__':
    projectA = Reservoir(
            name = 'Project A',
            max_storage = 30,
            max_release = 100.0,
            hydraulic_head = 60,
            efficiency = 0.8
        )
```

```
    state = ReservoirState(reservoir=projectA, storage=10)
    state.release = 90
    state.inflows = 0
    state.print_state()

    print 'How do we update the current storage ?'
```

A special trait allows to manage events and trigger function calls using the magic **_xxxx_fired** method:

```
from traits.api import HasTraits, Instance, DelegatesTo, Float, Range, Event

from reservoir import Reservoir

class ReservoirState(HasTraits):
    """Keeps track of the reservoir state given the initial storage.

    For the simplicity of the example, the release is considered in
    hm3/timestep and not in m3/s.
    """
    reservoir = Instance(Reservoir, ())
    min_storage = Float
    max_storage = DelegatesTo('reservoir')
    min_release = Float
    max_release = DelegatesTo('reservoir')

    # state attributes
    storage = Range(low='min_storage', high='max_storage')

    # control attributes
    inflows =  Float(desc='Inflows [hm3]')
    release = Range(low='min_release', high='max_release')
    spillage = Float(desc='Spillage [hm3]')

    update_storage = Event(desc='Updates the storage to the next time step')

    def _update_storage_fired(self):
        # update storage state
        new_storage = self.storage - self.release  + self.inflows
        self.storage = min(new_storage, self.max_storage)
        overflow = new_storage - self.max_storage
        self.spillage = max(overflow, 0)

    def print_state(self):
        print 'Storage\tRelease\tInflows\tSpillage'
        str_format = '\t'.join(['{:7.2f}'for i in range(4)])
        print str_format.format(self.storage, self.release, self.inflows,
                self.spillage)
        print '-' * 79


if __name__ == '__main__':
    projectA = Reservoir(
        name = 'Project A',
        max_storage = 30,
        max_release = 5.0,
        hydraulic_head = 60,
        efficiency = 0.8
    )

    state = ReservoirState(reservoir=projectA, storage=15)
    state.release = 5
    state.inflows = 0
```

```
    # release the maximum amount of water during 3 time steps
    state.update_storage = True
    state.print_state()
    state.update_storage = True
    state.print_state()
    state.update_storage = True
    state.print_state()
```

Dependency between objects can be made automatic using the trait **Property**. The **depends_on** attribute expresses the dependency between the property and other traits. When the other traits gets changed, the property is invalidated. Again, Traits uses magic method names for the property :

- _get_XXX for the getter of the XXX Property trait
- _set_XXX for the setter of the XXX Property trait

```
from traits.api import HasTraits, Instance, DelegatesTo, Float, Range
from traits.api import Property

from reservoir import Reservoir

class ReservoirState(HasTraits):
    """Keeps track of the reservoir state given the initial storage.

    For the simplicity of the example, the release is considered in
    hm3/timestep and not in m3/s.
    """
    reservoir = Instance(Reservoir, ())
    max_storage = DelegatesTo('reservoir')
    min_release = Float
    max_release = DelegatesTo('reservoir')

    # state attributes
    storage = Property(depends_on='inflows, release')

    # control attributes
    inflows =  Float(desc='Inflows [hm3]')
    release = Range(low='min_release', high='max_release')
    spillage = Property(
            desc='Spillage [hm3]', depends_on=['storage', 'inflows', 'release']
        )

    ### Private traits. ########################################################
    _storage = Float

    ### Traits property implementation. ########################################
    def _get_storage(self):
        new_storage = self._storage - self.release + self.inflows
        return min(new_storage, self.max_storage)

    def _set_storage(self, storage_value):
        self._storage = storage_value

    def _get_spillage(self):
        new_storage = self._storage - self.release  + self.inflows
        overflow = new_storage - self.max_storage
        return max(overflow, 0)

    def print_state(self):
        print 'Storage\tRelease\tInflows\tSpillage'
        str_format = '\t'.join(['{:7.2f}'for i in range(4)])
        print str_format.format(self.storage, self.release, self.inflows,
                self.spillage)
        print '-' * 79
```

```
if __name__ == '__main__':
    projectA = Reservoir(
                    name = 'Project A',
                    max_storage = 30,
                    max_release = 5,
                    hydraulic_head = 60,
                    efficiency = 0.8
                )

    state = ReservoirState(reservoir=projectA, storage=25)
    state.release = 4
    state.inflows = 0

    state.print_state()
```

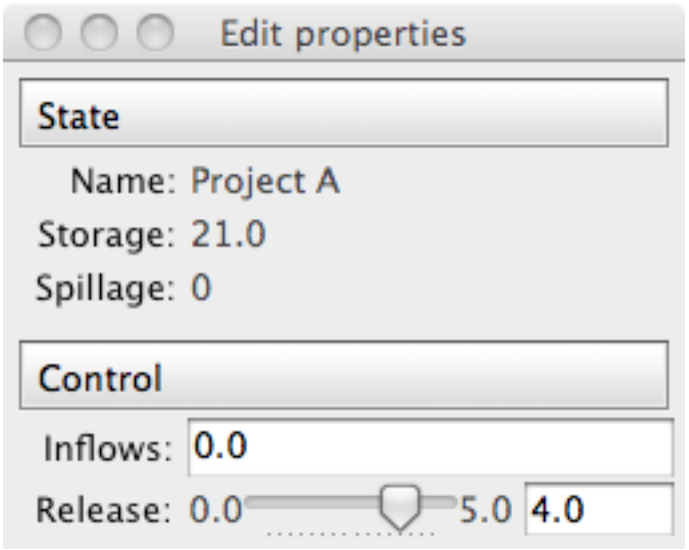
Note: Caching property

Heavy computation or long running computation might be a problem when accessing a property where the inputs have not changed. The @cached_property decorator can be used to cache the value and only recompute them once invalidated.

Let's extend the TraitsUI introduction with the ReservoirState example:

```
from traits.api import HasTraits, Instance, DelegatesTo, Float, Range, Property
from traitsui.api import View, Item, Group, VGroup

from reservoir import Reservoir

class ReservoirState(HasTraits):
    """Keeps track of the reservoir state given the initial storage.

    For the simplicity of the example, the release is considered in
    hm3/timestep and not in m3/s.
    """
    reservoir = Instance(Reservoir, ())
    name = DelegatesTo('reservoir')
    max_storage = DelegatesTo('reservoir')
    max_release = DelegatesTo('reservoir')
    min_release = Float

    # state attributes
    storage = Property(depends_on='inflows, release')

    # control attributes
    inflows =  Float(desc='Inflows [hm3]')
    release = Range(low='min_release', high='max_release')
    spillage = Property(
            desc='Spillage [hm3]', depends_on=['storage', 'inflows', 'release']
        )

    ### Traits view ###########################################################
    traits_view = View(
        Group(
            VGroup(Item('name'), Item('storage'), Item('spillage'),
                label = 'State', style = 'readonly'
            ),
            VGroup(Item('inflows'), Item('release'), label='Control'),
        )
    )

    ### Private traits. #######################################################
```

```
    _storage = Float

    ### Traits property implementation. ####################################
    def _get_storage(self):
        new_storage = self._storage - self.release + self.inflows
        return min(new_storage, self.max_storage)

    def _set_storage(self, storage_value):
        self._storage = storage_value

    def _get_spillage(self):
        new_storage = self._storage - self.release  + self.inflows
        overflow = new_storage - self.max_storage
        return max(overflow, 0)

    def print_state(self):
        print 'Storage\tRelease\tInflows\tSpillage'
        str_format = '\t'.join(['{:7.2f}'for i in range(4)])
        print str_format.format(self.storage, self.release, self.inflows,
                self.spillage)
        print '-' * 79

if __name__ == '__main__':
    projectA = Reservoir(
        name = 'Project A',
        max_storage = 30,
        max_release = 5,
        hydraulic_head = 60,
        efficiency = 0.8
    )

    state = ReservoirState(reservoir=projectA, storage=25)
    state.release = 4
    state.inflows = 0

    state.print_state()
    state.configure_traits()
```



Some use cases need the delegation mechanism to be broken by the user when setting the value of the trait. The **PrototypeFrom** trait implements this behaviour.

```
from traits.api import HasTraits, Str, Float, Range, PrototypedFrom, Instance

class Turbine(HasTraits):
```

```
    turbine_type = Str
    power = Float(1.0, desc='Maximal power delivered by the turbine [Mw]')


class Reservoir(HasTraits):
    name = Str
    max_storage = Float(1e6, desc='Maximal storage [hm3]')
    max_release = Float(10, desc='Maximal release [m3/s]')
    head = Float(10, desc='Hydraulic head [m]')
    efficiency = Range(0, 1.)

    turbine = Instance(Turbine)
    installed_capacity = PrototypedFrom('turbine', 'power')


if __name__ == '__main__':
    turbine = Turbine(turbine_type='type1', power=5.0)

    reservoir = Reservoir(
            name = 'Project A',
            max_storage = 30,
            max_release = 100.0,
            head = 60,
            efficiency = 0.8,
            turbine = turbine,
        )

    print 'installed capacity is initialised with turbine.power'
    print reservoir.installed_capacity

    print '-' * 15
    print 'updating the turbine power updates the installed capacity'
    turbine.power = 10
    print reservoir.installed_capacity

    print '-' * 15
    print 'setting the installed capacity breaks the link between turbine.power'
    print 'and the installed_capacity trait'

    reservoir.installed_capacity = 8
    print turbine.power, reservoir.installed_capacity
```

13.3.6 Notification

Traits implements a Listener pattern. For each trait a list of static and dynamic listeners can be fed with callbacks. When the trait does change, all the listeners are called.

Static listeners are defined using the _XXX_changed magic methods:

```
from traits.api import HasTraits, Instance, DelegatesTo, Float, Range

from reservoir import Reservoir

class ReservoirState(HasTraits):
    """Keeps track of the reservoir state given the initial storage.
    """
    reservoir = Instance(Reservoir, ())
    min_storage = Float
    max_storage = DelegatesTo('reservoir')
    min_release = Float
    max_release = DelegatesTo('reservoir')
```

```
    # state attributes
    storage = Range(low='min_storage', high='max_storage')

    # control attributes
    inflows =  Float(desc='Inflows [hm3]')
    release = Range(low='min_release', high='max_release')
    spillage = Float(desc='Spillage [hm3]')

    def print_state(self):
        print 'Storage\tRelease\tInflows\tSpillage'
        str_format = '\t'.join(['{:7.2f}'for i in range(4)])
        print str_format.format(self.storage, self.release, self.inflows,
                self.spillage)
        print '-' * 79

    ### Traits listeners ####################################################
    def _release_changed(self, new):
        """When the release is higher than zero, warn all the inhabitants of
        the valley.
        """

        if new > 0:
            print 'Warning, we are releasing {} hm3 of water'.format(new)


if __name__ == '__main__':
    projectA = Reservoir(
            name = 'Project A',
            max_storage = 30,
            max_release = 100.0,
            hydraulic_head = 60,
            efficiency = 0.8
        )

    state = ReservoirState(reservoir=projectA, storage=10)
    state.release = 90
    state.inflows = 0
    state.print_state()
```

The static trait notification signatures can be:

- **def _release_changed(self):** pass
- **def _release_changed(self, new):** pass
- **def _release_changed(self, old, new):** pass
- **def _release_changed(self, name, old, new** pass

Note: Listening to all the changes

To listen to all the changes on a HasTraits class, the magic **_any_trait_changed** method can be implemented.

In many situations, you do not know in advance what type of listeners need to be activated. Traits offers the ability to register listeners on the fly with the dynamic listeners

```
from reservoir import Reservoir
from reservoir_state_property import ReservoirState

def wake_up_watchman_if_spillage(new_value):
    if new_value > 0:
        print 'Wake up watchman! Spilling {} hm3'.format(new_value)

if __name__ == '__main__':
```

```
    projectA = Reservoir(
                        name = 'Project A',
                        max_storage = 30,
                        max_release = 100.0,
                        hydraulic_head = 60,
                        efficiency = 0.8
                    )

    state = ReservoirState(reservoir=projectA, storage=10)

    #register the dynamic listener
    state.on_trait_change(wake_up_watchman_if_spillage, name='spillage')

    state.release = 90
    state.inflows = 0
    state.print_state()

    print 'Forcing spillage'
    state.inflows = 100
    state.release = 0

    print 'Why do we have two executions of the callback ?'
```

The dynamic trait notification signatures are not the same as the static ones :

- **def wake_up_watchman():** pass
- **def wake_up_watchman(new):** pass
- **def wake_up_watchman(name, new):** pass
- **def wake_up_watchman(object, name, new):** pass
- **def wake_up_watchman(object, name, old, new):** pass

Removing a dynamic listener can be done by:

- calling the remove_trait_listener method on the trait with the listener method as argument,
- calling the on_trait_change method with listener method and the keyword remove=True,
- deleting the instance that holds the listener.

Listeners can also be added to classes using the **on_trait_change** decorator:

```
from traits.api import HasTraits, Instance, DelegatesTo, Float, Range
from traits.api import Property, on_trait_change

from reservoir import Reservoir

class ReservoirState(HasTraits):
    """Keeps track of the reservoir state given the initial storage.

    For the simplicity of the example, the release is considered in
    hm3/timestep and not in m3/s.
    """
    reservoir = Instance(Reservoir, ())
    max_storage = DelegatesTo('reservoir')
    min_release = Float
    max_release = DelegatesTo('reservoir')

    # state attributes
    storage = Property(depends_on='inflows, release')

    # control attributes
    inflows =  Float(desc='Inflows [hm3]')
    release = Range(low='min_release', high='max_release')
```

```
    spillage = Property(
            desc='Spillage [hm3]', depends_on=['storage', 'inflows', 'release']
        )


    ### Private traits. ###################################################
    _storage = Float

    ### Traits property implementation. ###################################
    def _get_storage(self):
        new_storage = self._storage - self.release + self.inflows
        return min(new_storage, self.max_storage)

    def _set_storage(self, storage_value):
        self._storage = storage_value

    def _get_spillage(self):
        new_storage = self._storage - self.release  + self.inflows
        overflow = new_storage - self.max_storage
        return max(overflow, 0)

    @on_trait_change('storage')
    def print_state(self):
        print 'Storage\tRelease\tInflows\tSpillage'
        str_format = '\t'.join(['{:7.2f}'for i in range(4)])
        print str_format.format(self.storage, self.release, self.inflows,
                self.spillage)
        print '-' * 79

if __name__ == '__main__':
    projectA = Reservoir(
                        name = 'Project A',
                        max_storage = 30,
                        max_release = 5,
                        hydraulic_head = 60,
                        efficiency = 0.8
                    )

    state = ReservoirState(reservoir=projectA, storage=25)
    state.release = 4
    state.inflows = 0
```

The patterns supported by the on_trait_change method and decorator are powerful. The reader should look at the docstring of HasTraits.on_trait_change for the details.

13.3.7 Some more advanced traits

The following example demonstrate the usage of the Enum and List traits :

```
from traits.api import HasTraits, Str, Float, Range, Enum, List
from traitsui.api import View, Item

class IrrigationArea(HasTraits):
    name = Str
    surface = Float(desc='Surface [ha]')
    crop = Enum('Alfalfa', 'Wheat', 'Cotton')


class Reservoir(HasTraits):
    name = Str
    max_storage = Float(1e6, desc='Maximal storage [hm3]')
    max_release = Float(10, desc='Maximal release [m3/s]')
```

```
    head = Float(10, desc='Hydraulic head [m]')
    efficiency = Range(0, 1.)
    irrigated_areas = List(IrrigationArea)

    def energy_production(self, release):
        ''' Returns the energy production [Wh] for the given release [m3/s]
        '''
        power = 1000 * 9.81 * self.head * release * self.efficiency
        return power * 3600

    traits_view = View(
        Item('name'),
        Item('max_storage'),
        Item('max_release'),
        Item('head'),
        Item('efficiency'),
        Item('irrigated_areas'),
        resizable = True
    )

if __name__ == '__main__':
    upper_block = IrrigationArea(name='Section C', surface=2000, crop='Wheat')

    reservoir = Reservoir(
                    name='Project A',
                    max_storage=30,
                    max_release=100.0,
                    head=60,
                    efficiency=0.8,
                    irrigated_areas=[upper_block]
                )

    release = 80
    print 'Releasing {} m3/s produces {} kWh'.format(
        release, reservoir.energy_production(release)
    )
```

Trait listeners can be used to listen to changes in the content of the list to e.g. keep track of the total crop surface on linked to a given reservoir.

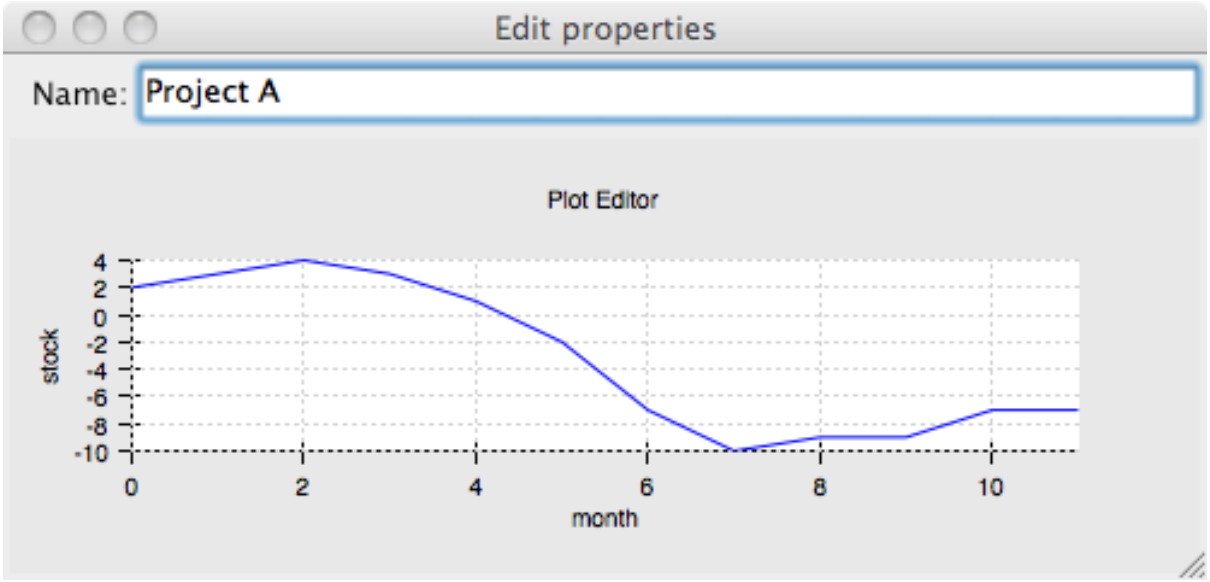
```
from traits.api import HasTraits, Str, Float, Range, Enum, List, Property
from traitsui.api import View, Item

class IrrigationArea(HasTraits):
    name = Str
    surface = Float(desc='Surface [ha]')
    crop = Enum('Alfalfa', 'Wheat', 'Cotton')


class Reservoir(HasTraits):
    name = Str
    max_storage = Float(1e6, desc='Maximal storage [hm3]')
    max_release = Float(10, desc='Maximal release [m3/s]')
    head = Float(10, desc='Hydraulic head [m]')
    efficiency = Range(0, 1.)

    irrigated_areas = List(IrrigationArea)


    total_crop_surface = Property(depends_on='irrigated_areas.surface')

    def _get_total_crop_surface(self):
        return sum([iarea.surface for iarea in self.irrigated_areas])
```

```
    def energy_production(self, release):
        ''' Returns the energy production [Wh] for the given release [m3/s]
        '''
        power = 1000 * 9.81 * self.head * release * self.efficiency
        return power * 3600

    traits_view = View(
        Item('name'),
        Item('max_storage'),
        Item('max_release'),
        Item('head'),
        Item('efficiency'),
        Item('irrigated_areas'),
        Item('total_crop_surface'),
        resizable = True
    )

if __name__ == '__main__':
    upper_block = IrrigationArea(name='Section C', surface=2000, crop='Wheat')

    reservoir = Reservoir(
                        name='Project A',
                        max_storage=30,
                        max_release=100.0,
                        head=60,
                        efficiency=0.8,
                        irrigated_areas=[upper_block],
                    )

    release = 80
    print 'Releasing {} m3/s produces {} kWh'.format(
        release, reservoir.energy_production(release)
    )
```

The next example shows how the Array trait can be used to feed a specialised TraitsUI Item, the ChacoPlotItem:

```
import numpy as np

from traits.api import HasTraits, Array, Instance, Float, Property
from traits.api import DelegatesTo
from traitsui.api import View, Item, Group
from chaco.chaco_plot_editor import ChacoPlotItem

from reservoir import Reservoir


class ReservoirEvolution(HasTraits):
    reservoir = Instance(Reservoir)

    name = DelegatesTo('reservoir')

    inflows = Array(dtype=np.float64, shape=(None))
    releass = Array(dtype=np.float64, shape=(None))

    initial_stock = Float
    stock = Property(depends_on='inflows, releases, initial_stock')

    month = Property(depends_on='stock')

    ### Traits view ###########################################################
    traits_view = View(
        Item('name'),
        Group(
```

```
            ChacoPlotItem('month', 'stock', show_label=False),
        ),
        width = 500,
        resizable = True
    )

    ### Traits properties ##################################################
    def _get_stock(self):
        """
        fixme: should handle cases where we go over the max storage
        """
        return  self.initial_stock + (self.inflows - self.releases).cumsum()

    def _get_month(self):
        return np.arange(self.stock.size)

if __name__ == '__main__':
    reservoir = Reservoir(
                            name = 'Project A',
                            max_storage = 30,
                            max_release = 100.0,
                            head = 60,
                            efficiency = 0.8
                        )

    initial_stock = 10.
    inflows_ts = np.array([6., 6, 4, 4, 1, 2, 0, 0, 3, 1, 5, 3])
    releases_ts = np.array([4., 5, 3, 5, 3, 5, 5, 3, 2, 1, 3, 3])

    view = ReservoirEvolution(
                                reservoir = reservoir,
                                inflows = inflows_ts,
                                releases = releases_ts
                            )
    view.configure_traits()
```



13.4 References

- ETS repositories: http://github.com/enthought

- Traits manual: http://github.enthought.com/traits/traits_user_manual/index.html
- Traits UI manual: http://github.enthought.com/traitsui/traitsui_user_manual/index.html
- Mailing list : enthought-dev@enthought.com

3D plotting with Mayavi

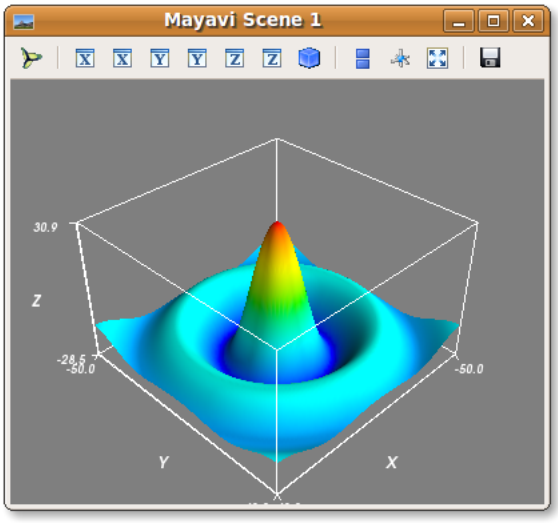
author Gaël Varoquaux

14.1 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()
```

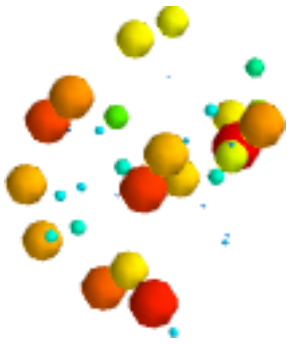
np.mgrid[-10:10:100j, -10:10:100j] creates an x,y grid, going from -10 to 10, with 100 steps in each directions.



14.2 3D plotting functions

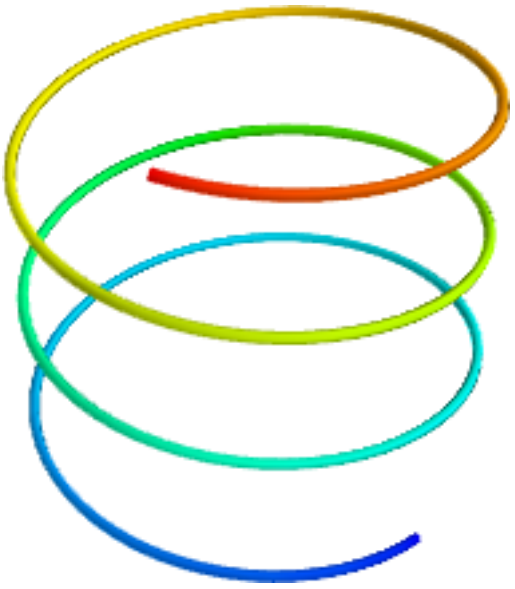
14.2.1 Points

```
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>
```



14.2.2 Lines

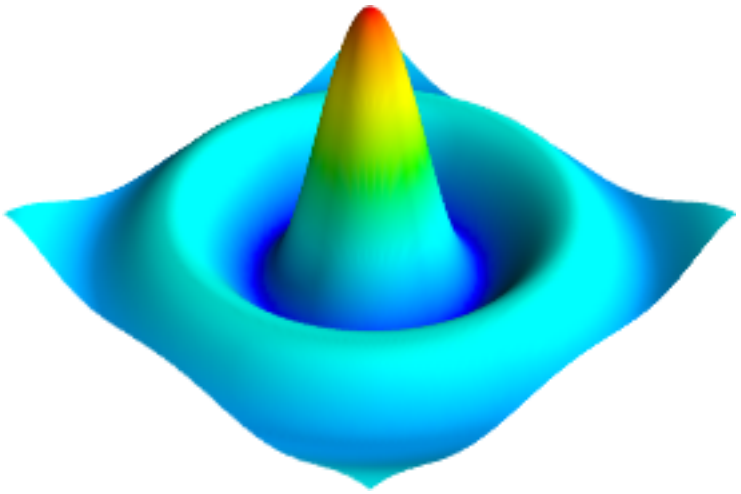
```
In [5]: mlab.clf()

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>
```



14.2.3 Elevation surface

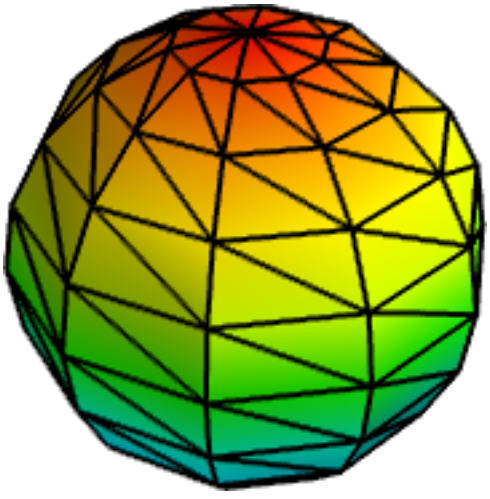
```
In [8]: mlab.clf()
```

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

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

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

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



14.2.4 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>
```



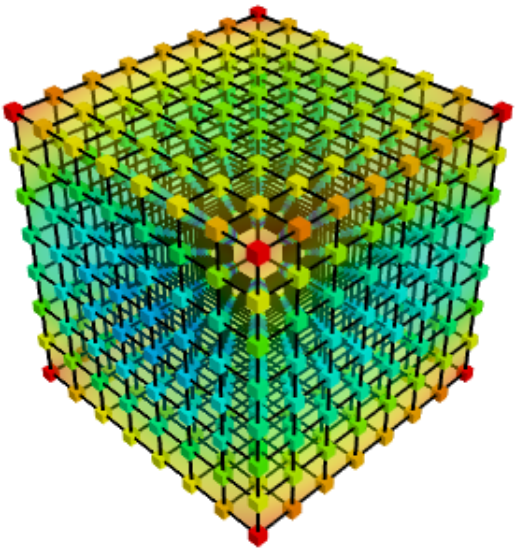
Note: A surface is defined by points **connected** to form triangles or polygones. In *mlab.func* and *mlab.mesh*, the connectivity is implicity given by the layout of the arrays. See also *mlab.triangular_mesh*.

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

14.2.5 Volumetric data

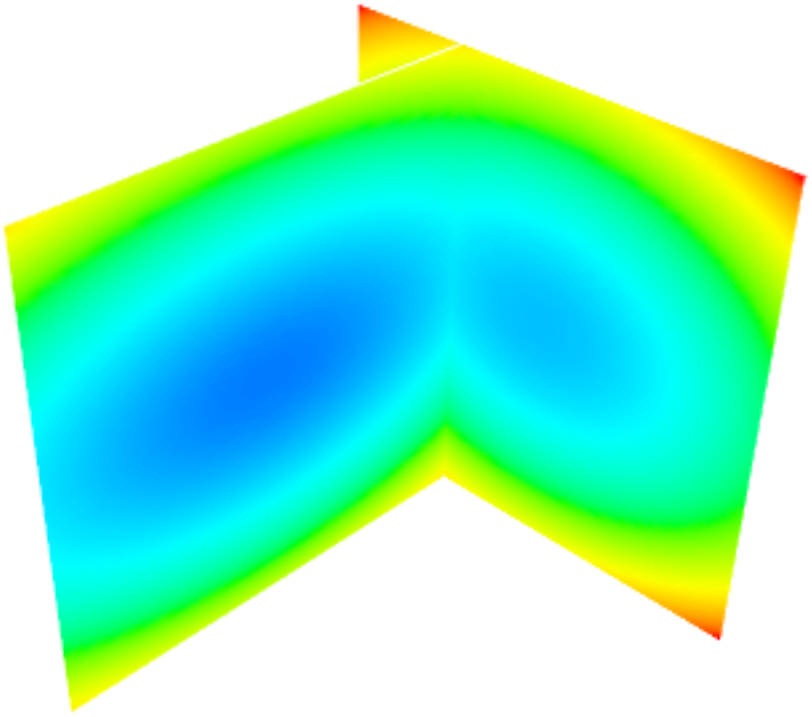
```
In [20]: mlab.clf()

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.

14.3 Figures and decorations

14.3.1 Figure management

Here is a list of functions useful to control the current figure

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

14.3.2 Changing plot properties

In general, many properties of the various objects on the figure can be changed. If these visualization 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, ...)
```

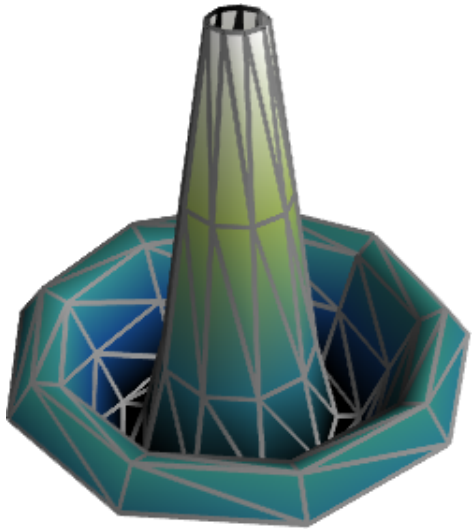
x, y, z are 2D arrays, all of the same shape, giving the positions of the vertices of the surface. The connectivity between these points is implied by the connectivity on the arrays.
For simple structures (such as orthogonal grids) prefer the surf function, as it will create more efficient data structures.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

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

Example:

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

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

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

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

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

In [6]: from enthought.mayavi import mlab

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

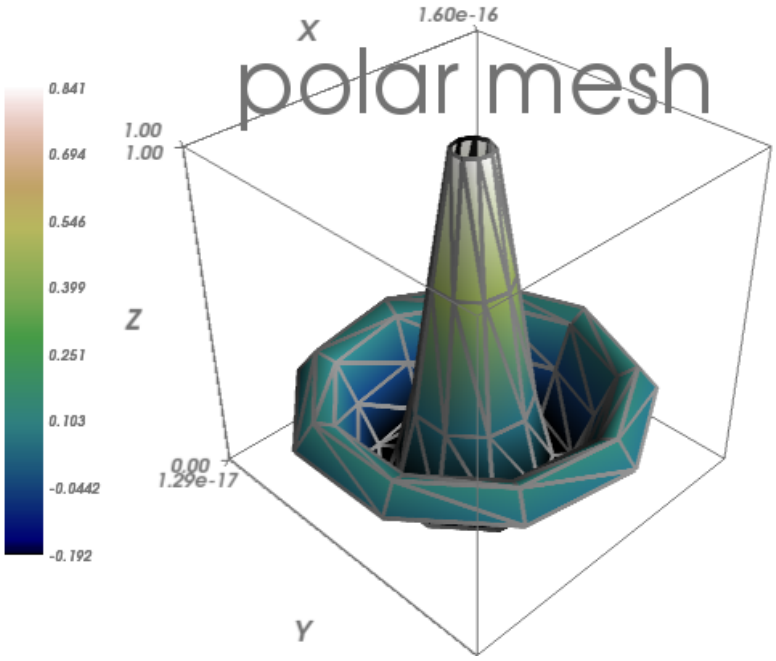
```
In [8]: mlab.mesh(x, y, z, extent=[0, 1, 0, 1, 0, 1],
   ...: representation='wireframe', line_width=1, color=(0.5, 0.5, 0.5))
Out[8]: <enthought.mayavi.modules.surface.Surface object at 0xdd6a71c>
```



14.3.3 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>
```

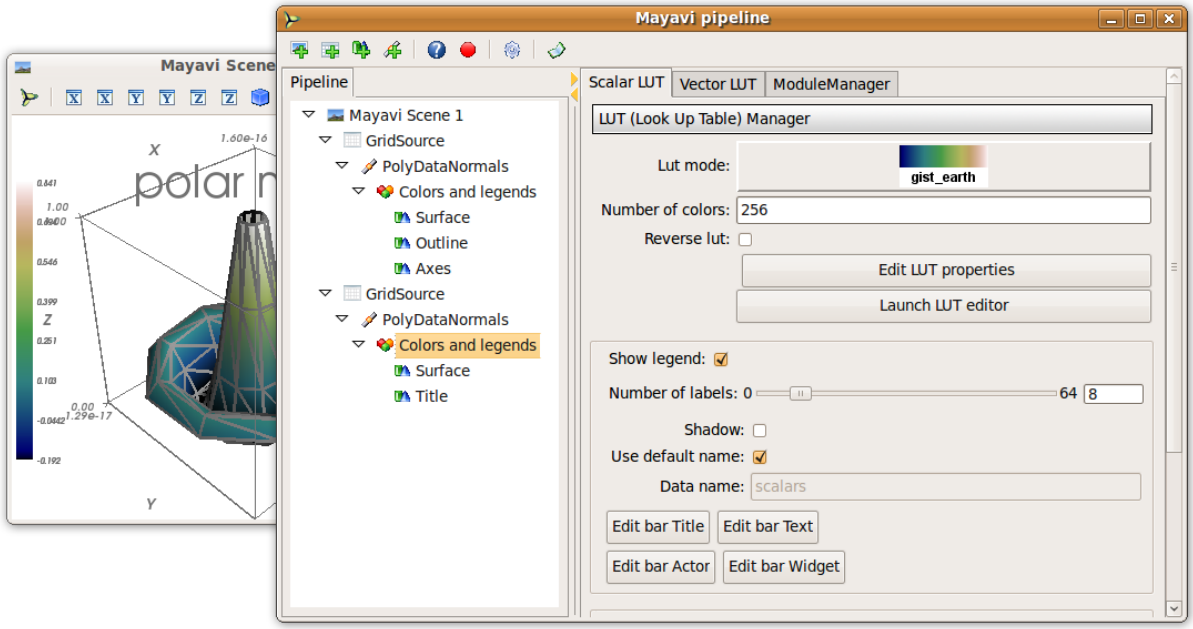


Warning: **extent:** If we specified extents for a plotting object, *mlab.outline' and 'mlab.axes* don't get them by default.

14.4 Interaction

The quicket way to create beautiful visualization with Mayavi is probably to interactivly 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 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 263)
  - Using SymPy as a calculator (page 263)
  - Exercises (page 264)
  - Symbols (page 264)
- Algebraic manipulations (page 264)
  - Expand (page 264)
  - Simplify (page 264)
  - Exercises (page 265)
- Calculus (page 265)
  - Limits (page 265)
  - Differentiation (page 265)
  - Series expansion (page 266)
  - Exercises (page 266)
  - Integration (page 266)
  - Exercises (page 266)
- Equation solving (page 266)
  - Exercises (page 267)
- Linear Algebra (page 267)
  - Matrices (page 267)
  - Differential Equations (page 268)
  - Exercises (page 268)

15.1 First Steps with SymPy

15.1.1 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
```

15.1.2 Exercises

1. Calculate $\sqrt{2}$ with 100 decimals.
2. Calculate $1/2 + 1/3$ in rational arithmetic.

15.1.3 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).

15.2 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.

15.2.1 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)
```

15.2.2 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
```

Simplification is a somewhat vague term, and more precises alternatives to simplify exists: powsimp (simplification of exponents), trigsimp (for trigonometric expressions) , logcombine, radsimp, together.

15.2.3 Exercises

1. Calculate the expanded form of $(x + y)^6$.
2. Simplify the trigonometric expression sin(x) / cos(x)

15.3 Calculus

15.3.1 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 -> 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
```

15.3.2 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)
```

15.3.3 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)
```

15.3.4 Exercises

1. Calculate $\lim x- > 0, sin(x)/x$
2. Calulate the derivative of log(x) for x.

15.3.5 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)
```

15.3.6 Exercises

15.4 Equation solving

SymPy is able to solve algebraic equations, in one and several variables:

```
In [7]: solve(x**4 - 1, x)
Out[7]: [I, 1, -1, -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
```

15.4.1 Exercises

1. Solve the system of equations $x + y = 2, 2 \cdot x + y = 0$
2. Are there boolean values `x`, `y` that make `(~x | y) & (~y | x)` true?

15.5 Linear Algebra

15.5.1 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]
```

15.5.2 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

15.5.3 Exercises

1. Solve the Bernoulli differential equation x*f(x).diff(x) + f(x) - f(x)**2

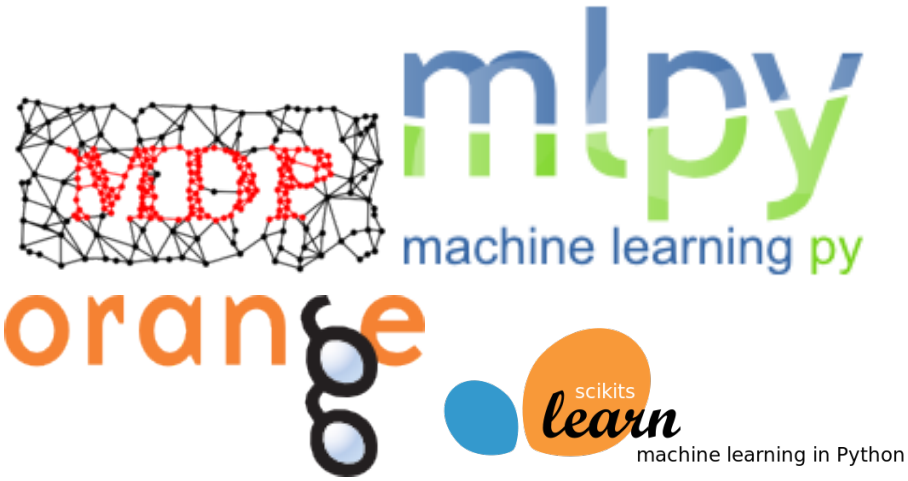
> **Warning:** TODO: correct this equation and convert to math directive!

2. Solve the same equation using hint='Bernoulli'. What do you observe ?

scikit-learn: machine learning in Python

author Fabian Pedregosa, Gael Varoquaux

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.org)

Chapters contents

- Loading an example dataset (page 270)
  - Learning and Predicting (page 271)
- Classification (page 271)
  - k-Nearest neighbors classifier (page 271)
  - Support vector machines (SVMs) for classification (page 272)
- Clustering: grouping observations together (page 274)
  - K-means clustering (page 274)
- Dimension Reduction with Principal Component Analysis (page 275)
- Putting it all together: face recognition (page 276)
- Linear model: from regression to sparsity (page 277)
  - Sparse models (page 277)
- Model selection: choosing estimators and their parameters (page 278)
  - Grid-search and cross-validated estimators (page 278)

Warning: As of version 0.9 (released in September 2011), the import path for scikit-learn has changed from `scikits.learn` to `sklearn`

16.1 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 measurements: sepal length, sepal width, petal length and petal width together with its subtype: *Iris setosa*, *Iris versicolor*, *Iris virginica*.

To load the dataset into a Python object:

```
>>> from sklearn import datasets
>>> iris = datasets.load_iris()
```

This data is stored in the `.data` member, which is a `(n_samples, n_features)` array.

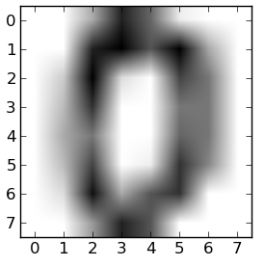
```
>>> iris.data.shape
(150, 4)
```

The class of each observation is stored in the `.target` attribute of the dataset. This is an integer 1D array of length `n_samples`:

```
>>> iris.target.shape
(150,)
>>> import numpy as np
```

```
>>> np.unique(iris.target)
array([0, 1, 2])
```

An example of reshaping data: the digits dataset



The digits dataset consists of 1797 images, where each one is an 8x8 pixel image representing a hand-written digit

```
>>> 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 into a vector of length 64

```
>>> data = digits.images.reshape((digits.images.shape[0], -1))
```

16.1.1 Learning and Predicting

Now that we've got some data, we would like to learn from it 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 sklearn import svm
>>> clf = svm.LinearSVC()
>>> clf.fit(iris.data, iris.target) # learn from the data
LinearSVC(...)
```

Once we have learned from the data, we can use our model to predict the most likely outcome on unseen data:

```
>>> clf.predict([[ 5.0,  3.6,  1.3,  0.25]])
array([0], dtype=int32)
```

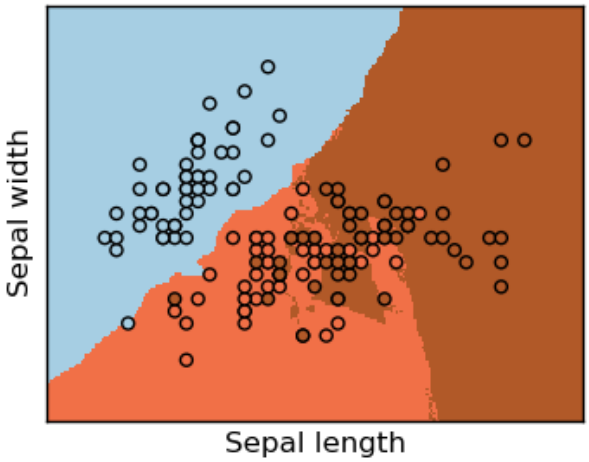
Note: We can access the parameters of the model via its attributes ending with an underscore:

```
>>> clf.coef_
array([[ 0...]])
```

16.2 Classification

16.2.1 k-Nearest neighbors classifier

The simplest possible classifier is the nearest neighbor: given a new observation, take the label of the training samples closest to it in *n*-dimensional space, where *n* is the number of *features* in each sample.



The k-nearest neighbors classifier internally uses an algorithm based on ball trees to represent the samples it is trained on.

KNN (k-nearest neighbors) classification example:

```
>>> # Create and fit a nearest-neighbor classifier
>>> from sklearn import neighbors
>>> knn = neighbors.KNeighborsClassifier()
>>> knn.fit(iris.data, iris.target)
KNeighborsClassifier(...)
>>> knn.predict([[0.1, 0.2, 0.3, 0.4]])
array([0])
```

Training set and testing set

When experimenting with learning algorithms, it is important not to test the prediction of an estimator on the data used to fit the estimator. Indeed, with the kNN estimator, we would always get perfect prediction on the training set.

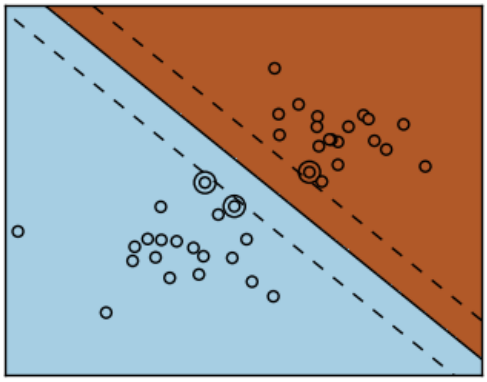
```
>>> perm = np.random.permutation(iris.target.size)
>>> iris.data = iris.data[perm]
>>> iris.target = iris.target[perm]
>>> knn.fit(iris.data[:100], iris.target[:100])
KNeighborsClassifier(...)
>>> knn.score(iris.data[100:], iris.target[100:])
0.95999...
```

Bonus question: why did we use a random permutation?

16.2.2 Support vector machines (SVMs) for classification

Linear Support Vector Machines

SVMs try to construct a hyperplane 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 hyperplane.



```
>>> from sklearn import svm
>>> svc = svm.SVC(kernel='linear')
>>> svc.fit(iris.data, iris.target)
SVC(...)
```

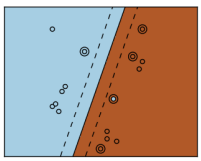
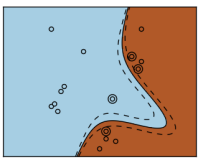
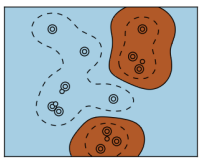
There are several support vector machine implementations in `scikit-learn`. The most commonly used ones are `svm.SVC`, `svm.NuSVC` and `svm.LinearSVC`; "SVC" stands for Support Vector Classifier (there also exist SVMs for regression, which are called "SVR" in `scikit-learn`).

Excercise

Train an `svm.SVC` on the digits dataset. Leave out the last 10% and test prediction performance on these observations.

Using kernels

Classes are not always separable by a hyperplane, so it would be desirable to have a decision function that is not linear but that may be for instance polynomial or exponential:

Linear kernel	Polynomial kernel	RBF kernel (Radial Basis Function)
		
`>>> svc = svm.SVC(kernel='linear')`	`>>> svc = svm.SVC(kernel='poly', ... degree=3) >>> # degree: polynomial degree`	`>>> svc = svm.SVC(kernel='rbf') >>> # gamma: inverse of size of radial kernel`

Exercise

Which of the kernels noted above has a better prediction performance on the digits dataset?

16.3 Clustering: grouping observations together

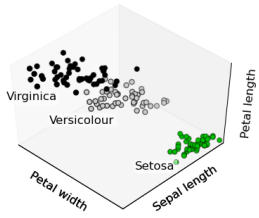
Given the iris dataset, if we knew that there were 3 types of iris, but did not have access to their labels, we could try **unsupervised learning**: we could **cluster** the observations into several groups by some criterion.

16.3.1 K-means clustering

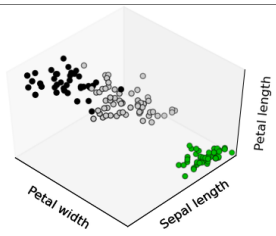
The simplest clustering algorithm is k-means. This divides a set into *k* clusters, assigning each observation to a cluster so as to minimize the distance of that observation (in *n*-dimensional space) to the cluster's mean; the means are then recomputed. This operation is run iteratively until the clusters converge, for a maximum for `max_iter` rounds.

(An alternative implementation of k-means is available in SciPy's `cluster` package. The `scikit-learn` implementation differs from that by offering an object API and several additional features, including smart initialization.)

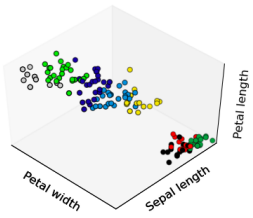
```
>>> from sklearn import cluster, datasets
>>> iris = datasets.load_iris()
>>> k_means = cluster.KMeans(k=3)
>>> k_means.fit(iris.data)
KMeans(copy_x=True, init='k-means++', k=3, ...
>>> print k_means.labels_[::10]
[1 1 1 1 1 0 0 0 0 0 2 2 2 2 2]
>>> print iris.target[::10]
[0 0 0 0 0 1 1 1 1 1 2 2 2 2 2]
```



Ground truth



K-means (3 clusters)



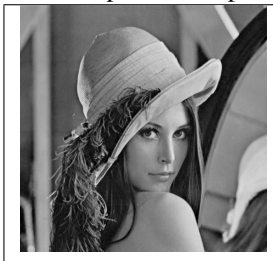
K-means (8 clusters)

Application to Image Compression

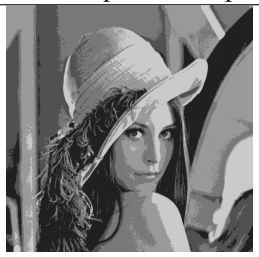
Clustering can be seen as a way of choosing a small number of observations from the information. For instance, this can be used to posterize an image (conversion of a continuous gradation of tone to several regions of fewer tones):

```
>>> from scipy import misc
>>> lena = misc.lena().astype(np.float32)
>>> X = lena.reshape((-1, 1)) # We need an (n_sample, n_feature) array
>>> k_means = cluster.KMeans(n_clusters=5)
>>> k_means.fit(X)
```

KMeans(...) >>> values = **k_means.cluster_centers_**.squeeze() >>> labels = **k_means.labels_** >>> lena_compressed = np.choose(labels, values) >>> lena_compressed.shape = lena.shape

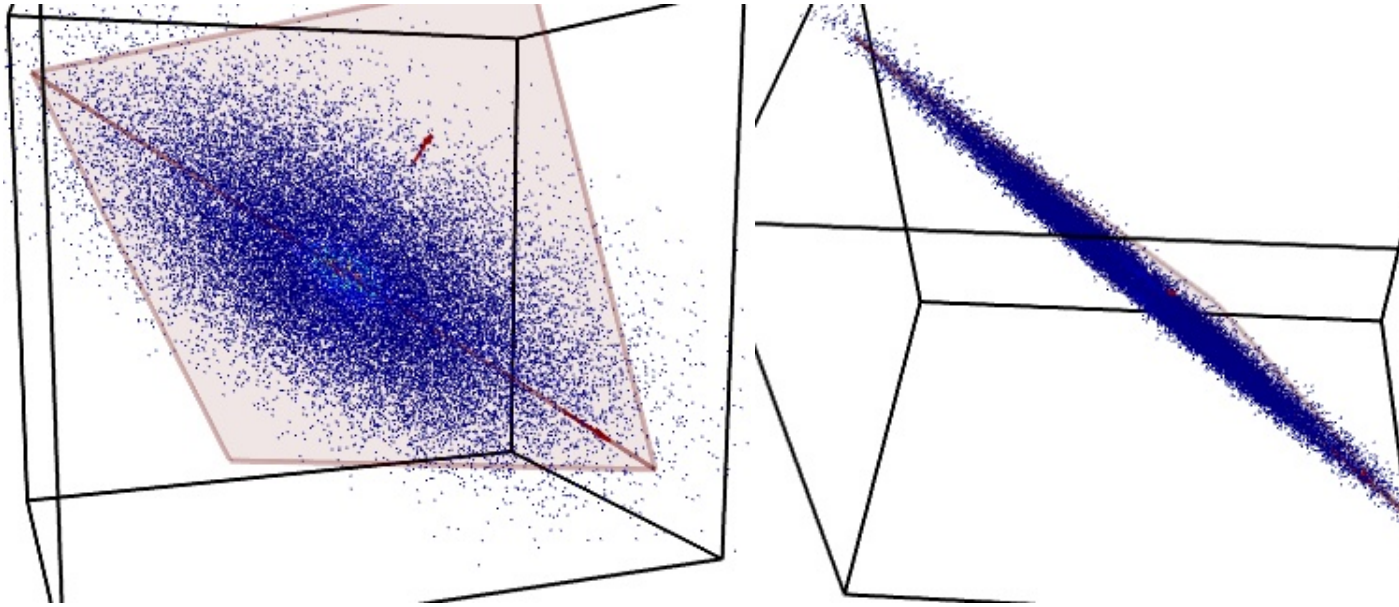


Raw image



K-means quantization

16.4 Dimension Reduction with Principal Component Analysis



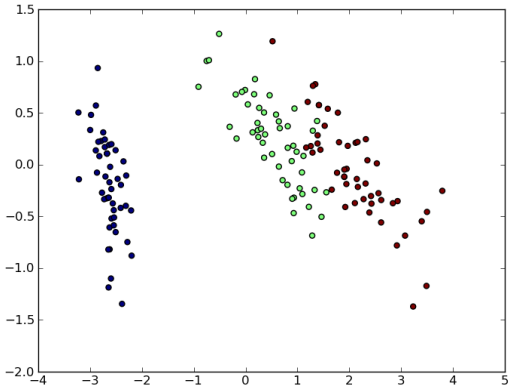
The cloud of points spanned by the observations above is very flat in one direction, so that one feature can almost be exactly computed using the 2 other. PCA finds the directions in which the data is not *flat* and it can reduce the dimensionality of the data by projecting on a subspace.

Warning: Depending on your version of scikit-learn PCA will be in module `decomposition` or `pca`.

```
>>> from sklearn 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)
<matplotlib.collections...Collection object at ...>
```



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 efficient with high dimensions.

16.5 Putting it all together: face recognition

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.org/dev/auto_examples/applications/face_recognition.html

## original shape of images: 50, 37
"""
import numpy as np
import pylab as pl
from sklearn import cross_val, datasets, decomposition, svm

# ..
# .. load data ..
lfw_people = datasets.fetch_lfw_people(min_faces_per_person=70, resize=0.4)
perm = np.random.permutation(lfw_people.target.size)
lfw_people.data = lfw_people.data[perm]
lfw_people.target = lfw_people.target[perm]
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(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()
```

16.6 Linear model: from regression to sparsity

Diabetes dataset

The diabetes dataset consists of 10 physiological variables (age, sex, weight, blood pressure) measure on 442 patients, and an indication of disease progression after one year:

```
>>> diabetes = datasets.load_diabetes()
>>> diabetes_X_train = diabetes.data[:-20]
>>> diabetes_X_test  = diabetes.data[-20:]
>>> diabetes_y_train = diabetes.target[:-20]
>>> diabetes_y_test  = diabetes.target[-20:]
```

The task at hand is to predict disease prediction from physiological variables.

16.6.1 Sparse models

To improve the conditioning of the problem (uninformative variables, mitigate the curse of dimensionality, as a feature selection preprocessing, etc.), it would be interesting to select only the informative features and set non-informative ones to 0. This penalization approach, called **Lasso**, can set some coefficients to zero. Such methods are called **sparse method**, and sparsity can be seen as an application of Occam's razor: prefer simpler models to complex ones.

```
>>> from sklearn import linear_model
>>> regr = linear_model.Lasso(alpha=.3)
>>> regr.fit(diabetes_X_train, diabetes_y_train)
Lasso(...)
>>> regr.coef_ # very sparse coefficients
array([   0.        ,   -0.        ,  497.34075682,  199.17441034,
         -0.        ,   -0.        , -118.89291545,    0.        ,
        430.9379595 ,    0.        ])
>>> regr.score(diabetes_X_test, diabetes_y_test)
0.5510835453...
```

being the score very similar to linear regression (Least Squares):

```
>>> lin = linear_model.LinearRegression()
>>> lin.fit(diabetes_X_train, diabetes_y_train)
LinearRegression(...)
>>> lin.score(diabetes_X_test, diabetes_y_test)
0.5850753022...
```

Different algorithms for a same problem

Different algorithms can be used to solve the same mathematical problem. For instance the `Lasso` object in the `sklearn` solves the lasso regression using a *coordinate descent* method, that is efficient on large datasets. However, the `sklearn` also provides the `LassoLARS` object, using the *LARS* which is very efficient for problems in which the weight vector estimated is very sparse, that is problems with very few observations.

16.7 Model selection: choosing estimators and their parameters

16.7.1 Grid-search and cross-validated estimators

Grid-search

The scikit-learn provides an object that, given data, computes the score during the fit of an estimator on a parameter grid and chooses the parameters to maximize the cross-validation score. This object takes an estimator during the construction and exposes an estimator API:

```
>>> from sklearn import svm, grid_search
>>> gammas = np.logspace(-6, -1, 10)
>>> svc = svm.SVC()
>>> clf = grid_search.GridSearchCV(estimator=svc, param_grid=dict(gamma=gammas),
...                    n_jobs=-1)
>>> clf.fit(digits.data[:1000], digits.target[:1000])
GridSearchCV(cv=None,
       estimator=SVC(C=1.0, ...
>>> clf.best_score
0.98899798001594419
>>> clf.best_estimator.gamma
0.00059948425031894088
```

By default the `GridSearchCV` uses a 3-fold cross-validation. However, if it detects that a classifier is passed, rather than a regressor, it uses a stratified 3-fold.

Cross-validated estimators

Cross-validation to set a parameter can be done more efficiently on an algorithm-by-algorithm basis. This is why, for certain estimators, the scikit-learn exposes "CV" estimators, that set their parameter automatically by cross-validation:

```
>>> from sklearn import linear_model, datasets
>>> lasso = linear_model.LassoCV()
>>> diabetes = datasets.load_diabetes()
>>> X_diabetes = diabetes.data
>>> y_diabetes = diabetes.target
>>> lasso.fit(X_diabetes, y_diabetes)
LassoCV(alphas=array([ 2.14804,  2.00327, ...,  0.0023 ,  0.00215]),
    copy_X=True, cv=None, eps=0.001, fit_intercept=True, max_iter=1000,
    n_alphas=100, normalize=False, precompute='auto', tol=0.0001,
    verbose=False)
>>> # The estimator chose automatically its lambda:
>>> lasso.alpha
0.013...
```

These estimators are called similarly to their counterparts, with 'CV' appended to their name.

Exercise

On the diabetes dataset, find the optimal regularization parameter alpha.

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