# Using Python for Interactive Data Analysis

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# Contents

## Purpose

This is intended to show how Python can be used to interactively analyze data much in the same way IDL$^{TM}$ or Matlab$^{TM}$ can. The approach taken is to illustrate as quickly as possible how one can perform common data analysis tasks. This is not a tutorial on how to program in Python (many good tutorials are available—targeting various levels of programming experience—, either as books or on-line material; many are free). As with IDL, one can write programs and applications also rather than just execute interactive commands. (Appendix A lists useful books, tutorials and on-line resources for learning the Python language itself as well as the specific modules addressed here.) Nevertheless, the focus will initially be almost entirely on interactive use. Later, as use becomes more sophisticated, more attention will be given to elements that are useful in writing scripts or applications (which themselves may be used as interactive commands).

The examples shown are mostly drawn from astronomy. Most of them should be understandable to those in other fields. There are some sections that should be skipped by those not interested in astronomical data analysis. These sections are noted in the text. Since all the data used by the examples is in the standard astronomical data format called FITS, it is necessary to use the PyFITS module to access these data to follow along.

This document is not intended as a reference, but it is unconventional in that it does serve as a light reference in that in many sections lists of functions or methods are given. The reasons are twofold: first, to give a quick overview of what capabilities are available. Generally these tables are limited to one line descriptions; generally enough to give a good idea of what can be done, but not necessarily enough information to use it (though often it is). Secondly, since the brief descriptions often sufficient to use the functions without resort to more detailed documentation, thus reducing the need to continually refer to other documentation if the user is using this document as a primary tool for learning how to use Python.

For those with IDL experience, Appendix B compares Python and IDL to aid those trying to decide whether they should use Python; and Appendix C provides a mapping between IDL and Python array capabilities to help IDL users find corresponding ways to carry out the same actions. Appendix D compares IDL plotting with matplotlib. Appendix E has some brief comments about editors and IDEs (Integrated Development Environments). Appendix F discusses the current situation regarding the different array packages available within Python.

## Prerequisites

Previous experience with Python of course is helpful, but is not assumed. Likewise, previous experience in using an array manipulation language such as IDL or matlab is helpful, but not required. Some familiarity with programming of some sort is necessary.

## Practicalities

This tutorial series assumes that Python (v2.4 or later), numpy (v1.0 or later), matplotlib (v0.87.7 or later), pyfits (v1.1 or later), numdisplay (v1.1 or later), and ipython (v0.6.12 or later) are installed (Google to find the downloads if not already installed). All these modules will run on all standard Unix, Linux, Mac OS X and MS Windows platforms (PyRAF is not supported on MS Windows since IRAF does not run on that platform). The initial image display examples assume that DS9 (or ximtool) is installed. A few examples require modules from scipy.stsci. These modules are also included with the stsci_python distribution. The tutorial web page has links to all of the software.

At STScI these are all available on Science cluster machines and the following describes how to set up your environment to access Python and these modules.

For the moment the PyFITS functions are available only on IRAFDEV. To make this version available either place IRAFDEV in your .envrc file or type `irafdev` at the shell level. Eventually this will be available for IRAFX as well.

If you have a Mac, and do not have all these items installed, follow the instructions on this web page: http://pyraf.stsci.edu/pyssg/macosx.html. At the very least you will need to do an update to get the latest PyFITS.

# 1 Reading and manipulating image data

## 1.1 Example session to read and display an image from a FITS file

The following illustrates how one can get data from a simple FITS file and display the data to DS9 or similar image display program. It presumes one has already started the image display program before starting Python. A short example of an interactive Python session is shown below (just the input commands, not what is printed out in return). The individual steps will be explained in detail in following sections.

```
>>> import pyfits                    # load FITS module
>>> from numpy import *              # load array module
>>> pyfits.info('pix.fits')          # show info about file
>>> im = pyfits.getdata('pix.fits') # read image data from file
>>> import numdisplay                # load image display module
>>> numdisplay.display(im)           # display to DS9
>>> numdisplay.display(im,z1=0,z2=300)  # repeat with new cuts
>>> fim = 1.*im                      # make float array
>>> bigvals = where(fim > 10)        # find pixels above threshold
                                    # log scale above threshold
>>> fim[bigvals] = 10*log(fim[bigvals]-10) + 10
>>> numdisplay.display(fim)
>>> hdr = pyfits.getheader('pix.fits')
>>> print hdr
>>> date = hdr['date']               # print header keyword value
>>> date
>>> hdr['date'] = '4th of July'      # modify value
>>> hdr.update('flatfile','flat17.fits') # add new keyword flatfile
>>> pyfits.writeto('newfile.fits',fim,hdr) # create new fits file
>>> pyfits.append('existingfile.fits',fim, hdr)
>>> pyfits.update('existingfile.fits',fim, hdr, ext=3)
```

## 1.2 Starting the Python interpreter

The first step is to start the Python interpreter. There are several variants one can use. The plain Python interpreter is standard with every Python installation, but lacks many features that you will find in PyRAF or IPython. We recommend that you use one of those as an interactive environment (ultimately PyRAF will use IPython itself). For basic use they all pretty much do the same thing. IPython special features will be covered later. The examples will show all typed lines starting the line with the standard prompt of the Python interpreter (>>>) unless it is IPython (numbered prompt) or PyRAF (prompt: -->) being discussed. (Note that comments begin with #.) At the shell command line you type one of the following

```
python  # starts standard Python interpreter
ipython # starts ipython (enhanced interactive features)
pyraf   # starts PyRAF
```

## 1.3 Loading modules

After starting an interpreter, we need to load the necessary libraries. One can do this explicitly, as in this example, or do it within a start-up file. For now we'll do it explicitly. There is more than one way to load a library; each has its advantages. The first is the most common found in scripts:

```
>>> import pyfits
```

This loads the FITS I/O module. When modules or packages are loaded this way, all the items they contain (functions, variables, etc.) are in the "namespace" of the module and to use or access them, one must preface the item with the module name and a period, e.g., `pyfits.getdata()` to call the pyfits module `getdata` function.

For convenience, particularly in interactive sessions, it is possible to import the module's contents directly into the working namespace so prefacing the functions with the name of the module is not necessary. The following shows how to import the array module directly into the namespace:

```
>>> from numpy import *
```

There are other variants on importing that will be mentioned later.

## 1.4 Reading data from FITS files

One can see what a FITS file contains by typing:

```
>>> pyfits.info('pix.fits')
Filename: pix.fits
No.    Name         Type      Cards   Dimensions    Format
0    PRIMARY     PrimaryHDU      71  (512, 512)    Int16
```

The simplest way to access FITS files is to use the function getdata.

```
>>> im = pyfits.getdata('pix.fits')
```

If the fits file contains multiple extensions, this function will default to reading the data part of the primary Header Data Unit, if it has data, and if not, the data from the first extension. What is returned is, in this case, an image array (how tables are handled will be described in the next tutorial).

## 1.5 Displaying images

Much like IDL and Matlab, many things can be done with the array. For example, it is easy to find out information about the array: `im.shape` tells you about the dimensions of this array. The image can be displayed on a standard image display program such as DS9 (ximtool and SAOIMAGE will work too, so long as an 8-bit display is supported) using numdisplay (the following examples presume that the image display program has already been started):

```
>>> import numdisplay
>>> numdisplay.display(im)
```

As one would expect, one can adjust the image cuts:

```
>>> numdisplay.display(im,z1=0,z2=300)
```

Note that Python functions accept both positional style arguments or keyword arguments.

There are other ways to display images that will be covered in subsequent tutorials.

## 1.6 Array expressions

The next operations show that applying simple operations to the whole or part of arrays is possible.

```
>>> fim = im*1.
```

creates a floating point version of the image.

```
>>> bigvals = where(fim > 10)
```

returns arrays indicating where in the `fim` array the values are larger than 10 (exactly what is being returned is glossed over for the moment). This information can be used to index the corresponding values in the array to use only those values for manipulation or modification as the following expression does:

```
>>> fim[bigvals] = 10*log(fim[bigvals]-10) + 10
```

This replaces all of the values that are larger than 10 in the array with a scaled log value added to 10

```
>>> numdisplay.display(fim)
```

The details on how to manipulate arrays will be the primary focus of this tutorial.

## 1.7 FITS headers

Looking at information in the FITS header is easy. To get the header one can use `pyfits.getheader`:

```
>>> hdr = pyfits.getheader('pix.fits')
```

Both header and data can be obtained at the same time using getdata with an optional header keyword argument (the ability to assign to two variables at once will be explained a bit more in a later tutorial; it's particularly useful when functions return more than one thing):

```
>>> data, hdr = pyfits.getdata('pix.fits', header=True)
```

To print out the whole header:

```
>>> print hdr
SIMPLE  =                    T / Fits standard
BITPIX  =                   16 / Bits per pixel
NAXIS   =                    2 / Number of axes
NAXIS1  =                  512 / Axis length
NAXIS2  =                  512 / Axis length
EXTEND  =                    F / File may contain extensions
```

[...]

```
CCDPROC = 'Apr 22 14:11 CCD processing done'
AIRMASS =    1.08015632629395   / AIRMASS
HISTORY 'KPNO-IRAF'
HISTORY '24-04-87'
HISTORY 'KPNO-IRAF'           /
HISTORY '08-04-92'            /
```

To get the value of a particular keyword:

```
>>> date = hdr['date']
>>> date
'2004-06-05T15:33:51'
```

To change an existing keyword:

```
>>> hdr['date'] = '4th of July'
```

To change an existing keyword or add it if it doesn't exist:

```
>>> hdr.update('flatfile','flat17.fits')
```

Where `flatfile` is the keyword name and `flat17.fits` is its value.

Special methods are available to add history, comment or blank cards (see Tutorial 3 for examples). When

## 1.8 Writing data to FITS files

```
>>> pyfits.writeto('newfile.fits',fim,hdr) # User supplied header
```

or

```
>>> pyfits.append('existingfile.fits',fim, hdr)
```

or

```
>>> pyfits.update('existingfile.fits',fim, hdr, ext=3)
```

There are alternative ways of accessing FITS files that will be explained in a later tutorial that allow more control over how files are written and updated.

## 1.9 Some Python basics

It's time to gain some understanding of what is going on when using Python tools to do data analysis this way. Those familiar with IDL or matlab will see much similarity in the approach used. It may seem a bit more alien to those used to running programs or tasks in IRAF or similar systems.

### 1.9.1 Memory vs. data files

First it is important to understand that the results of what one does usually reside in memory rather than in a data file. With IRAF, most tasks that process data produce a new or updated data file (if the result is a small number of values it may appear in the printout or as a task parameter). In IDL, matlab, or Python, one usually must explicitly write the results from memory to a data file. So results are volatile in the sense that they will be lost if the session is ended. The advantage of doing things this way is that applying a sequence of many operations to the data does not require vast amount of I/O (and the consequent cluttering of directories). The disadvantage is that very large data sets, where the size approaches the memory available, tend to need special handling (these situations will be addressed in a subsequent tutorial).

### 1.9.2 Python variables

Python is what is classified as a dynamically typed language (as is IDL). It is not necessary to specify what kind of value a variable is permitted to hold in advance. It holds whatever you want it to hold. To illustrate:

```
>>> value = 3
>>> print value
3
>>> value = “hello”
```

Here we see the integer value of 3 assigned to the variable `value`. Then the string `'hello'` is assigned to the same variable. To Python that is just fine. You are permitted to create new variables on the fly and assign whatever you please to them (and change them later). Python provides many tools (other than just `print`) to find out what kind of value the variable contains. Variables can contain simple types such as integers, floats, and strings, or much more complex objects such as arrays. Variable names contain letters, digits and '_'s and cannot begin with a digit. Variable names are case sensitive: `name`, `Name`, and `NAME` are all different variables.

Another important aspect to understand about Python variables is that they don't actually contain values, they refer to them (i.e., point), unlike IDL or matlab. So where one does:

```
>>> x = im # the image we read in
```

creates a new variable `x` but not a copy of the image. If one were to change a part of the image:

```
>>> im[5,5] = -999
```

The very same change would appear in the image referred to by `x`. This point can be confusing to some and everyone not used to this style will eventually stub their toes on it a few times. Generally speaking, when you want to copy data one must explicitly ask for a copy by some means. For example:

```
>>> x = im.copy()
```

(The odd style of this–for those not used to object oriented languages–will be explained next)

### 1.9.3 How does object oriented programming affect you?

While Python does support object-oriented programming very well, it does not require it to be used to write scripts or programs at all (indeed, there are many kinds of problems best not approached that way). It is quite simple to write Python scripts and programs without having to use object-oriented techniques (unlike Java and some other languages). In other words, just because Python supports object-oriented programming doesn't mean you have to use it that way or even that you should. That's good because the mere mention of object-oriented programming will give many astronomers the heebie-jeebies. That being said, there is a certain aspect of object oriented programming all users need to know about. While you are not required to write object-oriented programs, you will be required to use objects. Many Python libraries were written with the use of certain core objects in mind. Once you learn some simple rules, using these objects is quite simple. It's writing code that defines new kinds of objects that is what can be difficult to understand for newbies; not so for using them.

If one is familiar with structures (e.g., from C or IDL) one can think of objects as structures with bundled functions. Instead of functions, they are called methods. These methods in effect define what things are proper to do with the structure. For those not familiar with structures, they are essentially sets of variables that belong to one entity. Typically these variables can contain references to yet other structures (or for objects, other objects). An example illustrates much better than abstract descriptions.

```
>>> f = open('myfile.txt')
```

This opens a file and returns a file object. The object has attributes, things that describe it, and it has methods, things you can do with it. File objects have few attributes but several methods. Examples of attributes are:

```
>>> f.name
'myfile.txt'
>>> f.mode
'r'
```

These are the name of the file associated with the file object and the read/write mode it was opened in. Note that attributes are identified by appending the name of the attribute to the object with a period. So one always uses `.name` for the file object's name. Here it is appended to the specific file object one wants the name for, that is `f`. If I had a different file object `bigfile`, then the name of that would be represented by `bigfile.name`.

Methods essentially work the same way except they are used with typical function syntax. One of a file object's methods is `readline`, which reads the next line of the file and returns it as a string. That is:

```
>>> f.readline()
'a line from the text file'
```

In this case, no arguments are needed for the method. The `seek` method is called with an argument to move the file pointer to a new place in the file. It doesn't return anything but instead performs an action to change the state of file object:

```
f.seek(1024) # move 1024 bytes from the file beginning.
```

Note the difference in style from the usual functional programming. A corresponding kind of call for seeking a file would be `seek(f,1024)`. Methods are implicitly supposed to work for the object they belong to. The method style of functions also means that it is possible to use the same method names for very different objects (particularly nice if they do the same basic action, like `close`). While the use of methods looks odd to those that haven't seen them before, they are pretty easy to get used to.

### 1.9.4 Errors and dealing with them

People make mistakes and so will you. Generally when mistakes are made with Python that the program did not expect to handle, an "Exception" is "raised". This essentially means the program has crashed and returned to the interpreter (it is not considered normal for a Python program to segfault or otherwise crash the Python interpreter; it can happen with bugs in C extensions–especially ones you may write–but it is very unusual for it to happen in standard Python libraries or Python code). When this happens you will see what is called a "traceback" which usually shows where in all the levels of the program, it failed. While this can be lengthy and alarming looking, there is no need to get frightened. The most immediate cause of the failure will be displayed at the bottom (depending on the code and it's checking of user input, the original cause may or may not be as apparent). Unless you are interested in the programming details, it's usually safe to ignore the rest. To see your first traceback, let's intentionally make an error:

```
>>> f = pyfits.open(3)
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
  File "/usr/stsci/pyssg/py/pyfits.py", line 3483, in open
    ffo = _File(name, mode=mode, memmap=memmap)
  File "/usr/stsci/pyssg/py/pyfits.py", line 2962, in __init__
    self.__file = __builtin__.open(name, python_mode[mode])
TypeError: coercing to Unicode: need string or buffer, int found
```

The message indicates that a string (or suitable alternative) was expected and that an integer was found instead. The open function expects a filename, hence the exception.

The great majority of exceptions you will see will be due to usage errors. Nevertheless, some may be due to errors in the libraries or applications though, and should be reported if encountered (after ruling out usage errors).

Unlike IDL, exceptions do not leave you at the level of the program that caused them. Enabling that behavior is possible, and will be discussed in tutorial 4.

## 1.10 Array basics

Arrays come with extremely rich functionality. A tutorial can only scratch the surface of the capabilities available. More details will be provided in later tutorials; the details can be found in the numpy documentation listed in Appendix A.

### 1.10.1 Creating arrays

There are a few different ways to create arrays besides modules that obtain arrays from data files such as PyFITS.

```
>>> from numpy import *
>>> x = zeros((20,30))
```

creates a 20x30 array of zeros (default integer type; details on how to specify other types will follow). Note that the dimensions ("shape" in numpy parlance) are specified by giving the dimensions as a comma-separated list within parentheses. The parentheses aren't necessary for a single dimension. As an aside, the parentheses used this way are being used to specify a Python tuple; more will be said about those in a later tutorial. For now you only need to imitate this usage.

Likewise one can create an array of 1's using the `ones()` function.

The `arange()` function can be used to create arrays with sequential values. E.g.,

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

Note that that the array defaults to starting with a 0 value and does not include the value specified (though the array does have a length that corresponds to the argument)

Other variants:

```
>>> arange(10.)
array([ 0., 1., 2., 3., 4., 5., 6., 7., 8., 9])
>>> arange(3,10)
array([3, 4, 5, 6, 7, 8, 9])
>>> arange(1., 10., 1.1) # note trickiness
array([1. , 2.1, 3.2, 4.3, 5.4, 6.5, 7.6, 8.7, 9.8])
```

Finally, one can create arrays from literal arguments:

```
>>> print array([3,1,7])
[3 1 7]
>>> print array([[2,3],[4,4]])
[[2 3]
 [4 4]]
```

The brackets, like the parentheses in the zeros example above have a special meaning in Python which will be covered later (Python lists). For now, just mimic the syntax used here.

### 1.10.2 Array numeric types

numpy supports all standard numeric types. The default integer matches what Python uses for integers, usually 32-bit integers or what numpy calls `int32`. The same is true for floats, i.e., generally 64-bit doubles called `float64` in numarray. The default complex type is `complex64`. Many of the functions accept a `dtype` argument. For example

```
>>> zeros(3, int8) # Signed byte
>>> zeros(3, dtype=uint8) # Unsigned byte
>>> array([2,3], dtype=float32)
>>> arange(4, dtype=complex64)
```

The possible types are `int8, uint8, int16, uint16, int32, uint32, int64, uint64, float32, float64, complex64, complex128.` If one uses `int`, `float`, or `complex`, one gets the default precision for that type on the platform you are using. There are a number of other aliases for these types, as well as a few other possibilities, but won't be discussed here. To find out the type of an array use the `dtype` attribute. E.g.,

```
>>> arr = arange(4.)
>>> arr.dtype
dtype('float64')
```

To convert an array to a different type use the `astype()` method, e.g,

```
>>> a = arr.astype(float32)
```

### 1.10.3 Printing arrays

Interactively, there are two common ways to see the value of an array. Like many Python objects, just typing the name of the variable itself will print its contents (this only works in interactive mode). You can also explicitly print it. The following illustrates both approaches:

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

By default the array module limits the amount of an array that is printed out (to spare you the effects of printing out millions of values). For example:

```
>>> x = arange(1000000)
print x
[    0     1     2 ..., 999997 999998 999999]
```

If you really want to print out lots of array values, you can disable this feature or change the size of the threshold.

```
>>> set_printoptions(threshold=1000000) # prints entire array if not
                                        # more than a million elements
>>> set_printoptions(threshold=1000) # reset default
```

Can also use this function to alter the number of digits printed, how many elements at the beginning and end for oversize arrays, number of characters per line, and whether to suppress scientific notation for small floats.

### 1.10.4 Indexing 1-D arrays

As with IDL and matlab, there are many options for indexing arrays.

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

Simple indexing:

```
>>> x[2] # 3rd element
2
```

Indexing is 0-based. The first value in the array is `x[0]`

Indexing from end:

```
>>> x[-2] # -1 represents the last element, -2 next to last...
8
```

Slices

To select a subset of an array:

```
>>> x[2:5]
array([2, 3, 4])
```

Note that the upper limit of the slice is not included as part of the subset! This is viewed as unexpected by newcomers and a defect. Most find this behavior very useful after getting used to it (the reasons won't be given here). Also important to understand is that slices are views into the original array in the same sense that references view the same array. The following demonstrates:

```
>>> y = x[2:5]
>>> y[0] = 99
>>> y
array([99, 3, 4])
>>> x
array([0, 1, 99, 3, 4, 5, 6, 7, 8, 9])
```

Changes to a slice will show up in the original. If a copy is needed use `x[2:5].copy()`

Short hand notation

```
>>> x[:5] # presumes start from beginning
array([ 0, 1, 99, 3, 4])
>>> x[2:] # presumes goes until end
array([99, 3, 4, 5, 6, 7, 8, 9])
>>> x[:] # selects whole dimension
array([0, 1, 99, 3, 4, 5, 6, 7, 8, 9])
```

Strides:

```
>>> x[2:8:3] # "Stride" every third element
array([99, 5])
```

Index arrays:

```
>>> x[[4,2,4,1]]
array([4, 99, 4, 1])
```

Using results of `where` function (which behaves somewhat differently than for IDL; covered in tutorial 3):

```
>>> x[where(x>5)]
array([99, 6, 7, 8, 9])
```

Mask arrays:

```
>>> m = x > 5
>>> m
array([False, False, True, False, False, False, True, True, True, True], dtype=Bool)
>>> x[m]
array([99, 6, 7, 8, 9])
```

### 1.10.5 Indexing multidimensional arrays

Before describing this in detail it is very important to note an item regarding multidimensional indexing that will certainly cause you grief until you become accustomed to it. BY DEFAULT ARRAY INDICES USE THE OPPOSITE CONVENTION AS FORTRAN, IDL AND IRAF REGARDING ORDER OF INDICES FOR MULTIDIMENSIONAL ARRAYS! There are long standing reasons for this and there are good reasons why this cannot be changed. It is possible to define arrays so that the traditional index ordering applies (details will not be given here). Nevertheless, if you are working with large images you are strongly encouraged to avoid this; it will only cause you problems later and you will eventually go insane as a result. Well, perhaps we exaggerate. But don't do it. (For those using multidimensional arrays in a non-image context, this advice may not be appropriate. See Appendix G for a more in-depth discussion of the pros and cons of the alternate approach) Yes, we realize this is viewed by most as a tremendous defect. (If that prevents you from using or considering Python, so be it, but do weigh this against all the other factors before dismissing Python as a numerical tool out of hand).

```
>>> im = arange(24)
>>> im.shape=(4,6)
>>> im
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]])
```

To emphasize the point made in the previous paragraph, the index that represents the most rapidly varying dimension in memory is the 2nd index, not the first. We are used to that being the first dimension. Thus for most images read from a FITS file, what we have typically treated as the "x" index will be the second index. For this particular example, the location that has the value 8 in the array is `im[1, 2]`.

```
>>> im[1, 2]
8
```

Partial indexing:

```
>>> im[1]
array([6, 7, 8, 9, 10, 11])
```

If only some of the indices for a multidimensional array are specified, then the result is an array with the shape of the "leftover" dimensions, in this case, 1-dimensional. The 2nd row is selected, and since there is no index for the column, the whole row is selected.

All of the indexing tools available for 1-D arrays apply to $n$-dimensional arrays as well. To understand all the indexing options in their full detail, read section 3.4 in the Guide to Numpy (see Appendix A for links to this book).

### 1.10.6 Compatibility of dimensions

In operations involving combining (e.g., adding) arrays or assigning them there are rules regarding the compatibility of the dimensions involved. For example the following is permitted:

```
>>> x[:5] = 0
```

since a single value is considered "broadcastable" over a 5 element array. But this is not permitted:

```
>>> x[:5] = array([0,1,2,3])
```

since a 4 element array does not match a 5 element array.

*The following explanation can probably be skipped by most on the first reading;* it is only important to know that rules for combining arrays of different shapes are quite general. It is hard to precisely specify the rules without getting a bit confusing, but it doesn't take long to get a good intuitive feeling for what is and isn't permitted. Here's an attempt anyway: The shapes of the two involved arrays when aligned on their trailing part must be equal in value or one must have the value one for that dimension. The following pairs of shapes are compatible:

```
(5,4):(4,) -> (5,4)
(5,1):(4,) -> (5,4)
(15,3,5):(15,1,5) -> (15,3,5)
(15,3,5):(3,5) -> (15,3,5)
(15,1,5):(3,1) -> (15,3,5)
```

so that one can add arrays of these shapes or assign one to the other (in which case the one being assigned must be the smaller shape of the two). For the dimensions that have a 1 value that are matched against a larger number, the values in that dimension are simply repeated. For dimensions that are missing, the sub-array is simply repeated for those. The following shapes are not compatible:

```
(3,4):(4,3)
(1,3):(4,)
```

Examples:

```
>>> x = zeros((5,4))
>>> x[:,:] = [2,3,2,3]
>>> x
array([[2, 3, 2, 3],
       [2, 3, 2, 3],
       [2, 3, 2, 3],
       [2, 3, 2, 3],
       [2, 3, 2, 3]])
>>> a = arange(3)
>>> b = a[:] # different array, same data (huh?)
>>> b.shape = (3,1)
>>> b
array([[0],
       [1],
       [2]])
>>> a*b # outer product
array([[0, 0, 0],
       [0, 1, 2],
       [0, 2, 4]])
```

### 1.10.7 ufuncs

A ufunc (short for Universal Function) applies the same operation or function to all the elements of an array independently. When two arrays are added together, the `add` ufunc is used to perform the array addition. There are ufuncs for all the common operations and mathematical functions. More specialized ufuncs can be obtained from add-on libraries. All the operators have corresponding ufuncs that can be used by name (e.g., `add` for +). These are all listed in table below. Ufuncs also have a few very handy methods for binary operators and functions whose use are demonstrated here.

```
>>> x = arange(9)
>>> x.shape = (3,3)
>>> x
array([0, 1, 2],
      [3, 4, 5],
      [6, 7, 8]])
>>> add.reduce(x) # sums along the first index
array([9, 12, 15])
>>> add.reduce(x, axis=1) # sums along the 2nd index
array([3, 12, 21])
>>> add.accumulate(x) # cumulative sum along the first index
array([[0,  1,  2],
       [3,  5,  7],
       [9, 12, 15]])
>>> multiply.outer(arange(3),arange(3))
array([[0, 0, 0],
       [0, 1, 2],
       [0, 2, 4]])
```

Standard Ufuncs (with corresponding symbolic operators, when they exist, shown in parentheses)

| | | |
|---|---|---|
| add (+) | log | greater (>) |
| subtract (-) | log10 | greater_equal (>=) |
| multiply (*) | cos | less (<) |
| divide (/) | arcos | less_equal (<=) |
| remainder (%) | sin | logical_and |
| absolute, abs | arcsin | logical_or |
| floor | tan | logical_xor |
| ceil | arctan | bitwise_and (&) |
| fmod | cosh | bitwise_or (\|) |
| conjugate | sinh | bitwise_xor (^) |
| minimum | tanh | bitwise_not (~) |
| maximum | sqrt | rshift (>>) |
| power (**) | equal (==) | lshift (<<) |
| exp | not_equal (!=) | |

*Note that there are no corresponding Python operators for* `logical_and` *and* `logical_or`*. The Python* `and` *and* `or` *operators are NOT equivalent to these respective ufuncs!* (Try them on arrays and see what happens.)

### 1.10.8 Array functions

There are many array utility functions. The following lists the more useful ones with a one line description. See the numarray manual for details on how they are used. Arguments shown with argument=value indicate what the default value is if called without a value for that argument. Those functions that are identical to array methods are so noted.

`all`(*a*, *axis=None*): are all elements of array nonzero? [also method], identical to `alltrue()`

`allclose`(*a1, a2, rtol=1.e-5, atol=1.e-8*): true if all elements within specified amount (between two arrays)

`alltrue`(*a, axis=0*): are all elements nonzero along specified axis true.

`any`(*a*, *axis= None*): are any elements of an array nonzero [also method], identical to `sometrue()`

`argmax`(*a, axis=-1*), argmin(*a,axis=-1*): return array with min/max locations for selected axis

`argsort`(*a, axis=-1*): returns indices of results of sort on an array

`choose`(*selector, population, clipmode=CLIP*): fills specified array by selecting corresponding values from a set of arrays using integer selection array (population is a tuple of arrays; see tutorial 2)

`clip`(*a, amin, amax*): clip values of array *a* at values *amin*, *amax*

`dot`(*a1, a2*): dot product of arrays *`a1`* & *`a2`*

`compress`(*condition, a ,axis=0*): selects elements from array *a* based on Boolean array condition

`concatenate`(*arrays, axis=0*): concatenate arrays contained in sequence of arrays arrays

`cumproduct`(*a, axis=0*): net cumulative product along specified axis. Note: see caution after this list regarding cumulative operations.

`cumsum`(*a, axis=0*): accumulate array along specified axis. Note: see caution after this list regarding cumulative operations.

`diagonal`(*a, offset=0, axis1=0, axis2=1*): returns diagonal of 2-d matrix with optional offsets.

`fromfile`(*file, type, shape=None*): Use binary data in file to form new array of specified type.

`fromstring`(*datastring, type, shape=None*): Use binary data in *datastring* to form new array of specified shape and type `identity`(*n, type=None*): returns identity matrix of size nxn.

`indices`(*shape, type=None*): generate array with values corresponding to position of selected index of the array

`innerproduct`(*a1, a2*): guess

`matrixmultiply`(*a1, a2*): guess

`outerproduct`(*a1, a2*): guess

`product`(*a, axis=0*): net product of elements along specified axis. Note: see caution after this list regarding cumulative operations.

`ravel`(*a*): creates a 1-d version of an array

`repeat`(*a, repeats, axis=0*): generates new array with repeated copies of input array *a*

`resize`(*a, shape*): replicate or truncate array to new shape

`searchsorted`(*bin, a*): return indices of mapping values of an array *a* into a monotonic array *bin*

`sometrue`(*a, axis=0*): are any elements along specified axis true

`sort`(*a, axis=-1*): sort array elements along selected axis

`sum`(*a, axis=0*): sum array along specified axis. Note: see caution after this list regarding cumulative operations.

`swapaxes`(*a, axis1, axis2*): switch indices for axis of array (doesn't actually move data, just maps indices differently)

`trace`(*a, offset=0, axis1=0, axis2=1*): compute trace of matrix *a* with optional offset.

`transpose`(*a, axes=None*): transpose indices of array (doesn't actually move data, just maps indices differently)

`where`(*a*): find "true" locations in array *a*

**Caution:** The cumulative class of operations that either sum or multiply elements of an array (sum, product, cumsum, cumproduct) use the input array type as the type to perform the cumulative sum or product. If you are not using the largest type for the array (i.e., int64, float64, etc.) you are asking for trouble. One is likely to run into integer overflows or floating point precision problems if you don't specifcally ask for a higher precision result, especially for large array. One should get into the habit of specifying the keyword argument dtype to a highest precision type when using these functions, e.g. sum(arr, dtype=float64)).

### 1.10.9 Array methods

Arrays have several methods. They are used as methods are with any object. For example (using the array from the previous example):

```
>>> # sum all array elements
>>> x.sum() # the L indicates a Python Long integer
36L
```

The following lists all the array methods that exist for an array object `a` (a number are equivalent to array functions; these have no summary description shown):

`a.all`(*axis=None, out=None*)

`a.any`(*axis=None, out=None*)

*a* .`argmax`(axis=*None, out=None*)

*a* .`argmin`(*axis=None, out=None*)

*a* .`argsort`(*axis=None, kind='quick', order=None*)

*a* .`astype`(*dtype*): copy array to specified numeric type

`a.byteswap(`*inplace=False*`):` swap bytes in place

`a.choose(`*c0, c1,...cn, out=None, clip='raise'*)

`a.clip(`*min, max, out=None*)

`a.compress(`*condition, axis=None, out=None*)

`a.conj(`*out=None*`):` same as a.conjugate()

*a* .`conjugate`(*out=None*): complex conjugate. Same as a.conj()

*a* .`copy`(): produce copied version of array (instead of view)

`a.cumprod(`*axis=None, dtype=None, out=None*). Note caution from previous section about cumulative operations.

`a.cumsum(`*axis=None, dtype=None, out=None*). Note caution from previous section about cumulative operations.

*a* .`diagonal`(*offset=0, axis1=0, axis2=1*)

`a.dtype()`

`a.dump(`*file*`)`

`a.dumps()`

`a.fill(`*scalar*`)`

`a.flatten(`*order='C'*`)`

`a.getfield(`*dtype, offset=0*)

`a.item(`**args*`)`

`a.itemset(`**args*`)`

*a* .`max`(*axis=None*): maximum value in array

`a.mean(`*axis=None, dtype=None, out=None*). Note caution from previous section about cumulative operations.

*a* .`min`(*axis=None*): minimum value in array

`a.newbyteorder()`

`a.nonzero():` True when array is not zero.

`a.prod(`*axis=None, dtype=None, out=None*). Note caution from previous section about cumulative operations.

`a.ptp(`*axis=None, out=None*)

`a.put(`*indices, values, mode='raise'*) `a.ravel(`*order='C'*`)`

*a* `.repeat(`*a,repeats,axis=0*`)`:

*a* `.resize(`*d1, d2, ..., dn, refcheck=1, order='C'*`)`:

`a.round(`*decimals=0, out=None*`)`

`a.searchsorted(`*values*`)`

`a.setfield(`*value, dtype, offset*`)`

`a.setflags(`*write=None, align=None, uic=None*`)`

`a.sort(`*axis=None, kind='quick'*`)`

`a.squeeze()`

`a.std(`*axis=None, dtype=None, out=None*`)`

`a.sum(`*axis=None, dtype=None, out=None*`)`. Note caution from previous section about cumulative operations.

`a.swapaxes(`*axis1, axis2*`)`

`a.take(`*indices, axis=None, out=None, mode='raise'*`)`

`a.type()`: returns type of array

`a.tofile(`*file, sep=", format="*`)`: write binary data to file

`a.tolist()`: convert data to Python list format

`a.tostring(`*order='C'*`)`: copy binary data to Python string

`a.trace(`*offset=0, axis1=0, axis2=1, dtype=None, out=None*`)`

`a.transpose(`*permute*`)`: transpose array

`a.std(`*axis=None, dtype=None*`)`: standard deviation

`a.sum(`*axis=None, dtype=None*`)`: sum of all elements

`a.swapaxes(`*axis1, axis2*`)`

`a.trace(`*offset, axis1=0, axis2=0, dtype=None*`)`

`a.var(`*axis=None, dtype=None, out=None*`)`

`a.view(`*obj*`)`: generate a view of the data based on the type of the supplied object

#### 1.10.10 Array attributes:

The following lists all the array attributes. Some can be modified by assignment (e.g., arr.attribue = newvalue) and some cannot directly be assigned to. These are indicated by "Modifiable" and "Not Modifiable" respectively. Note that attributes marked as "Not modifiable" doesn't mean they can't change. For example, if one assigns a new shape to the shape attribue, the ndim value may change as a result.

`a.base:` Object array is using for its data buffer, or None if it doesn't own the memory for the data. Not Modifiable.

`a.ctypes:` Object to simplify interaction with the ctypes module (see *Guide to Numpy* book, section 3.1.4, for details). Not modifiable.

`a.data`: The buffer object that holds the array data. Modifiable

`a.dtype`: data type object for the array. Modifiable.

`a.flags`: Information on the internal data representation. Not modifiable (though some attribues of the flags object can be changed).

`a.flat`: returns view of array treating it as 1-dimensional (actually an iterator object, see *Guide to Numpy* book. section 8.8, for details)

`a.itemsize`: Size in bytes of each element of the array. Not modifiable

`a.nbytes`: Total number of bytes used. Not modifiable.

`a.ndim`: Number of dimensions in the array. Not modifiable.

`a.shape`: returns shape of array. Modifiable.

`a.size`: Total number of elements. Not modifiable.

`a.strides`: Tuple containing information on the spacing of elements in each dimension (see *Guide to Numpy* book, section 3.1.1, for details). Modifiable.

`a.real`: return real component of array (exists for all types). Modifiable

`a.imag`: return imaginary component (exists only for complex types). Modifiable

`__array_interface__,__array_struct__,__array_priority__`: For advanced users only, see *Guide to Numpy* book, section 3.1.4, for details.

## 1.11 Example

The following example shows how to use some of these tools. The idea is to select only data within a given radius of the center of the galaxy displayed and compute the total flux within that radius using the built-in array facilities.

First we will create a mask for all the pixels within 50 pixels of the center. We begin by creating x and y arrays that whose respective values indicate the x and y locations of pixels in the arrays:

```
# first find location of maximum in image
y, x = indices(im.shape, dtype=float32) # note order of x, y!
# after finding peak at 257,258 using ds9
x = x-257 # make peak have 0 value
y = y-258
radius = sqrt(x**2+y**2)
mask = radius < 50
display mask*im
(mask*im).sum() # sum total of masked image
# or
im[where(mask)].sum() # sum those points within the radius
# look Ma, no loops!
```

## 1.12 Exercises

The needed data for these exercises can be downloaded from stsdas.stsci.edu/python.

1. Start up Python (Python, PyRAF, or IPython). Type `print 'hello world'`. Don't go further until you master this completely.

2. Read pix.fits, find the value of the OBJECT keyword, and print all the image values in the 10th column of the image.

3. Scale all the values in the image by 2.3 and store in a new variable. Determine the mean value of the scaled image

4. Save the center 128x128 section of the scaled image to a new FITS file using the same header. It won't be necessary to update the NAXIS keywords of the header; that will be handled automatically by PyFITS.

5. Extra credit: Create an image (500x500) where the value of the pixels is a Gaussian-weighted sinusoid expressed by the following expression:

   $\sin(x/\pi)e^{-((x-250)^2+(y-250)^2)/2500.}$

   where x represents the x pixel location and likewise for y. Display it. Looking at the numarray manual, find out how to perform a 2-D FFT and display the absolute value of the result.

# 2 Reading and plotting spectral data

In this tutorial we will cover some simple plotting commands using `matplotlib`, a Python plotting package developed by John Hunter of the University of Chicago. We will also talk about reading FITS tables, delve a little deeper into some of Python's data structures, and use a few more of Python's features that make coding in Python so straightforward.

## 2.1 Example session to read spectrum and plot it

The sequence of commands below represent reading a spectrum from a FITS table and using matplotlib to plot it. Each step will be explained in more detail in following subsections.

```
>>> import pyfits
>>> from pylab import *              # import plotting module
>>> pyfits.info('fuse.fits')
>>> tab = pyfits.getdata('fuse.fits') # read table
>>> tab.names                        # names of columns
>>> tab.formats                      # formats of columns
>>> flux = tab.field('flux').flat    # reference flux column
>>> wave = tab.field('wave').flat
>>> flux.copy().shape                # show shape of flux column array
>>> plot(wave, flux)                 # plot flux vs wavelength
    # add xlabel using symbols for lambda/angstrom
>>> xlabel(r'$\lambda (\angstrom)$', size=13)
>>> ylabel('Flux')
# Overplot smoothed spectrum as dashed line
>>> from convolve import boxcar
>>> sflux = boxcar(flux.copy(), (100,)) # smooth flux array
>>> plot(wave, sflux, '--r', hold=True) # overplot red dashed line
>>> subwave = wave[::100]            # sample every 100 wavelengths
>>> subflux = flux.flat[::100]
>>> plot(subwave,subflat,'og')       # overplot points as green circles
>>> errorbar(subwave, subflux, yerr=0.05*subflux, fmt='.k')
>>> legend(('unsmoothed', 'smoothed', 'every 100'))
>>> text(1007, 0.5, 'Hi There')
    # save to png and postscript files
>>> savefig('fuse.png')
>>> savefig('fuse.ps')
```

## 2.2 An aside on how Python finds modules

When you import a module, how does Python know where to look for it? When you start up Python, there is a search path defined that you can access using the `path` attribute of the `sys` module. So:

```
>>> import sys
>>> sys.path
['', 'C:\\WINNT\\system32\\python23.zip',
'C:\\Documents and Settings\\rij\\SSB\\demo',
'C:\\Python23\\DLLs', 'C:\\Python23\\lib',
'C:\\Python23\\lib\\plat-win',
'C:\\Python23\\lib\\lib-tk',
'C:\\Python23',
'C:\\Python23\\lib\\site-packages ',
'C:\\Python23\\lib\\site-packages\\numpy',
'C:\\Python23\\lib\\site-package s\\gtk-2.0',
'C:\\Python23\\lib\\site-packages\\win32',
'C:\\Python23\\lib\\site -packages\\win32\\lib',
'C:\\Python23\\lib\\site-packages\\Pythonwin']
```

This is a list of the directories that Python will search when you import a module. If you want to find out where Python actually found your imported module, the `__file__` attribute shows the location:

```
>>> pyfits.__file__
'C:\\Python23\\lib\\site-packages\\pyfits.pyc'
```

Note the double '\' characters in the file specifications; Python uses \ as its escape character (which means that the following character is interpreted in a special way. For example, `\n` means "newline", `\t` means "tab" and `\a` means "ring the terminal bell"). So if you really *want* a backslash, you have to escape it with another backslash. Also note that the extension of the `pyfits` module is `.pyc` instead of `.py`; the `.pyc` file is the bytecode compiled version of the `.py` file that is automatically generated whenever a new version of the module is executed.

## 2.3 Reading FITS table data (record arrays)

As well as reading regular FITS images, PyFITS also reads tables as arrays of records. These record arrays may be indexed just like numeric arrays though numeric operations cannot be performed on the record arrays themselves. All the columns in a table may be accessed as arrays as well.

```
>>> import pyfits
```

Assuming a FITS table of FUSE data in the current directory with the imaginative name of `'fuse.fits'`

```
>>> pyfits.info('fuse.fits')
Filename: fuse.fits
No.    Name         Type      Cards   Dimensions   Format
0    PRIMARY     PrimaryHDU     365  ()            int16
1    SPECTRUM    BinTableHDU     35  1R x 7C       [10001E,
10001E, 10001E, 10001J, 10001E, 10001E, 10001I]
>>> tab = pyfits.getdata('fuse.fits') # returns table as record array
```

PyFITS record arrays have a `names` attribute that contains the names of the different columns of the array (there is also a `format` attribute that describes the type and contents of each column).

```
>>> tab.names
['WAVE', 'FLUX', 'ERROR', 'COUNTS', 'WEIGHTS', 'BKGD', 'QUALITY']
>>> tab.formats
['10001E', '10001E', '10001E', '10001J','10001E', '10001E', '10001I']
```

The latter indicates that each column element contains a 10001 element array of the types indicated.

```
>>> tab.shape
(1,)
```

The table only has one row. Each of the columns may be accessed as it own array by using the field method. Note that the shape of these column arrays is the combination of the number of rows and the size of the columns. Since in this case the columns contain arrays, the result will be two-dimensional (albeit with one of the dimensions only having length one). For example:

```
>>> wave = tab.field('wave')
>>> wave.shape
(1, 10001)
```

To facilitate further operations on the arrays, the .flat attribute is used is to turn these into 1-D arrays. Well, not exactly. The .flat attribute is not exactly an array; it behaves like a 1-D equivalent most times, but in some respects it isn't (it's actually an iterator object, but discussion of that point will be deferred). Hence the use of the .copy() method so that one can get the shape.

```
>>> wave = tab.field('wave').flat
>>> flux = tab.field('flux').flat
>>> flux.copy().shape
(10001, )
```

The arrays obtained by the field method are not copies of the table data, but instead are views into the record array. If one modifies the contents of the array, then the table itself has changed. Likewise, if a record (i.e., row) of the record array is modified, the corresponding column array will change. This is best shown with a different table:

```
>>> tab2 = pyfits.getdata('table2.fits')
>>> tab2.shape # how many rows?
(3,)
>>> print tab2
[('M51', 13.5, 2) ('NGC4151', 5.8, 5) ('Crab Nebula', 11.12, 3)]
>>> col3 = tab2.field('nobs')
>>> col3
array([2, 5, 3], dtype=int16)
>>> col3[2] = 99
>>> print tab2
[('M51', 13.5, 2) ('NGC4151', 5.8, 5) ('Crab Nebula', 11.12, 3)]
```

Numeric column arrays may be treated just like any other numpy array. Columns that contain character fields are returned as character arrays (with their own methods, described in the PyFITS User Manual)

Updated or modified tables can be written to FITS files using the same functions as for image or array data.

## 2.4 Quick introduction to plotting

The package `matplotlib` is used to plot arrays and display image data. This section gives a few examples of how to make quick plots. More examples will appear later in the tutorial (these plots assume that the `.matplotlibrc` file has been properly configured; the default version at STScI has been set up that way. There will be more information about the `.matplotlibrc` file later in the tutorial).

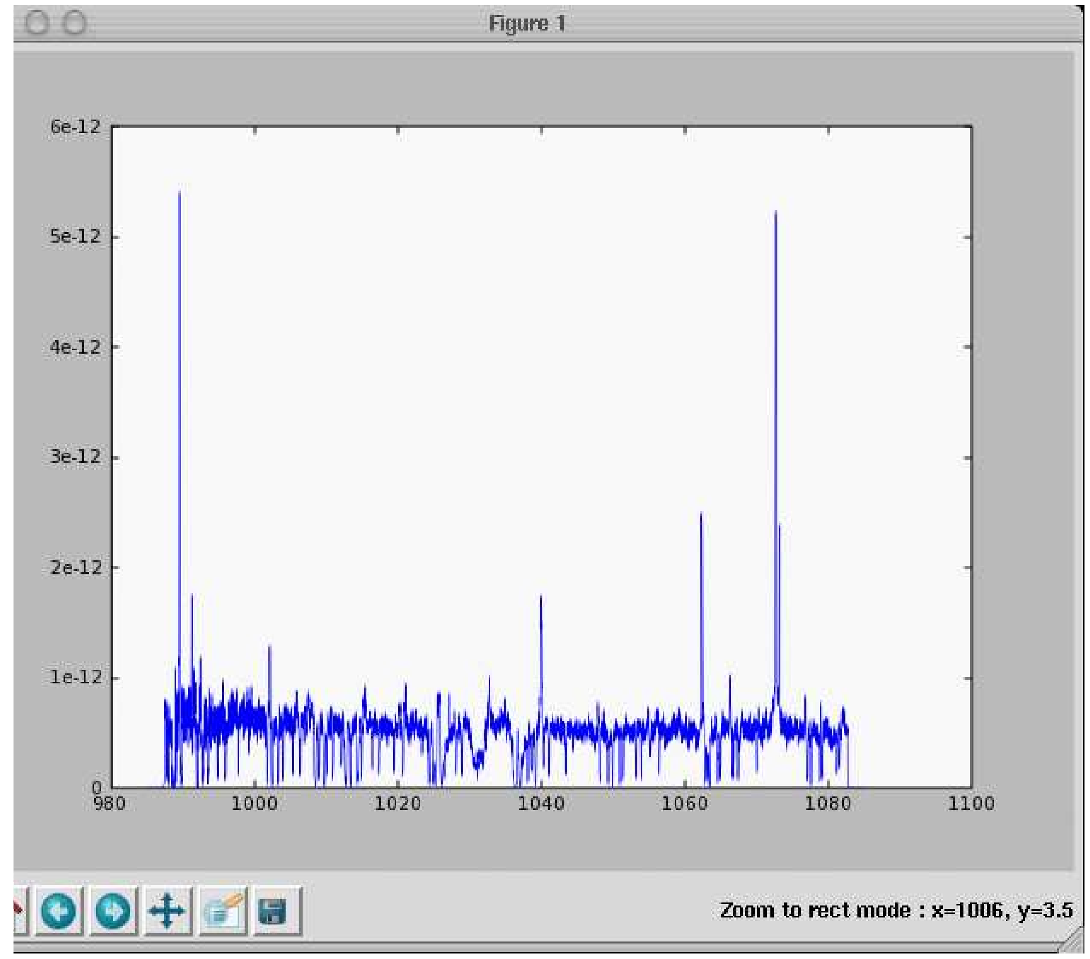
First, we must import the functional interface to matplotlib

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

### 2.4.1 Simple x-y plots

To plot flux vs wavelength:

```
>>> plot(wave, flux)
[<matplotlib.lines.Line2D instance at 0x02A07440>]
```



Note that the resulting plot is interactive. The toolbar at the bottom is used for a number of actions. The button with arrows arranged in a cross pattern is used for panning or zooming the plot. In this mode the zooming is accomplished by using the middle mouse button; dragging it in the x direction affects the zoom in that direction and likewise for the y direction. The button with a magnifying glass and rectangle is used for the familiar zoom to rectangle (use the left mouse button to drag define a rectangle that will be the new view region for the plot. The left and right arrow buttons can be used to restore different views of the plot (a history is kept of every zoom and pan). The button with a house will return it the the original view. The button with a diskette allows one to save the plot to a `.png` or postscript file. You can resize the window and the plot will re-adjust to the new window size.

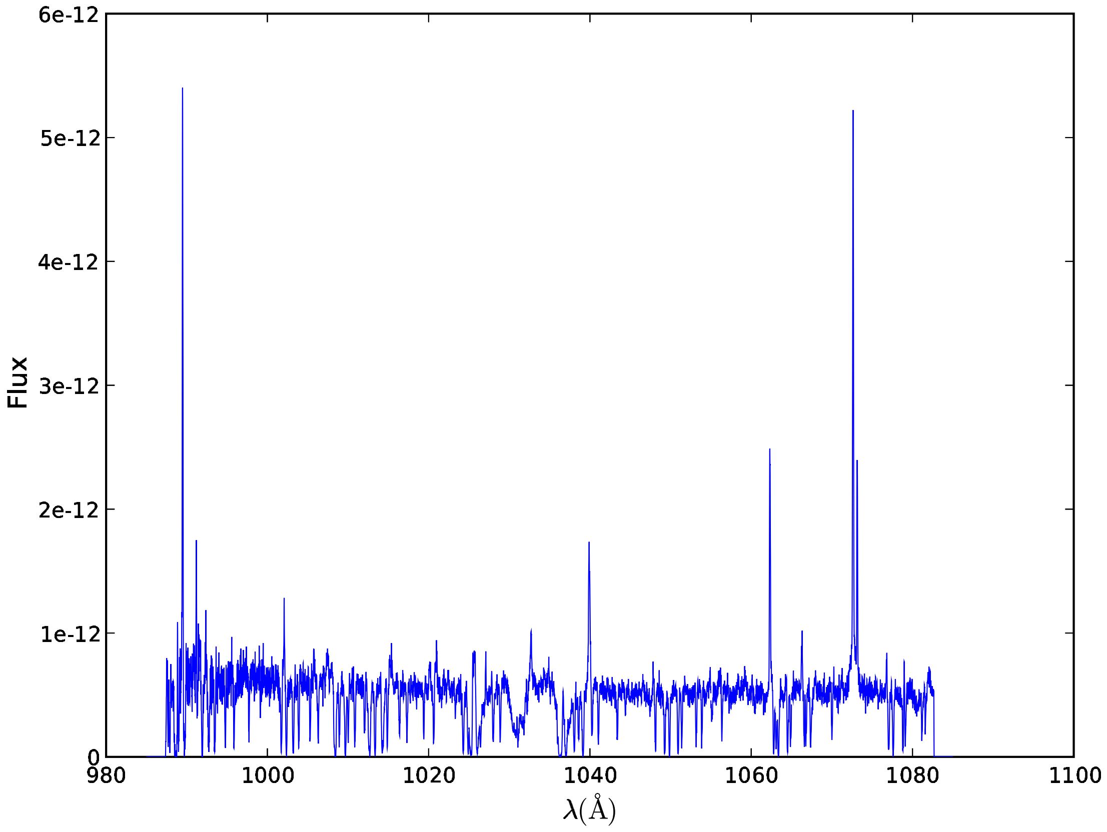
Also note that this and many of the other pylab commands result in a cryptic printout. That's because these function calls return a value. In Python when you are in an interactive mode, the act of entering a value at the command line, whether it is a literal value, evaluated expression, or return value of a function, Python attempts to print out some information on it. Sometimes that shows you the value of the object (if it is simple enough) like for numeric values or strings, or sometimes it just shows the type of the object, which is what is being shown here. The functions return a value so that you can assign it to a variable to manipulate the plot later (it's not necessary to do that, though for now it does help keep the screen uncluttered). We are likely to change the behavior of the object so that nothing is printed (even though it is still returned) so your session screen will not be cluttered with these messages.

### 2.4.2 Labeling plot axes

It is possible to customize plots in many ways. This section will just illustrate a few possibilities

```
>>> xlabel(r'$\lambda (\angstrom)$', size=13)
<matplotlib.text.Text instance at 0x029A9F30>
```

```
>>> ylabel('Flux')
<matplotlib.text.Text instance at 0x02A07BC0>
```



One can add standard axis labels. This example shows that it is possible to use special symbols using TEX notation.

### 2.4.3 Overplotting

Overplots are possible. First we make a smoothed spectrum to overplot.

```
>>> from convolve import boxcar # yet another way to import functions
>>> sflux = boxcar(flux, (100,)) # smooth flux array using size 100 box
>>> plot(wave, sflux, '--r', hold=True) # overplot red dashed line
[<matplotlib.lines.Line2D instance at 0x0461FC60>]
```

This example shows that one can use the `hold` keyword to overplot, and how to use different colors and linestyles. This case uses a terse representation (`--` for dashed and `r` for red) to set the values, but there are more verbose ways to set these attributes. As an aside, the function that matplotlib uses are closely patterned after Matlab. Next we subsample the array to overplot circles and error bars for just those points.

```
>>> subwave = wave[::100] # sample every 100 wavelengths
>>> subflux = flux[::100]
>>> plot(subwave,subflat,'og', hold=True) # overplot points as green circles
[<matplotlib.lines.Line2D instance at 0x046EBE40>]
>>> error = tab.field('error')
>>> suberror = error.flat[::100]
>>> errorbar(subwave, subflux, suberror, fmt='.k', hold=True)
(<matplotlib.lines.Line2D instance at 0x046EBEE0>, <a list of 204 Line2D errorbar objects>)
```

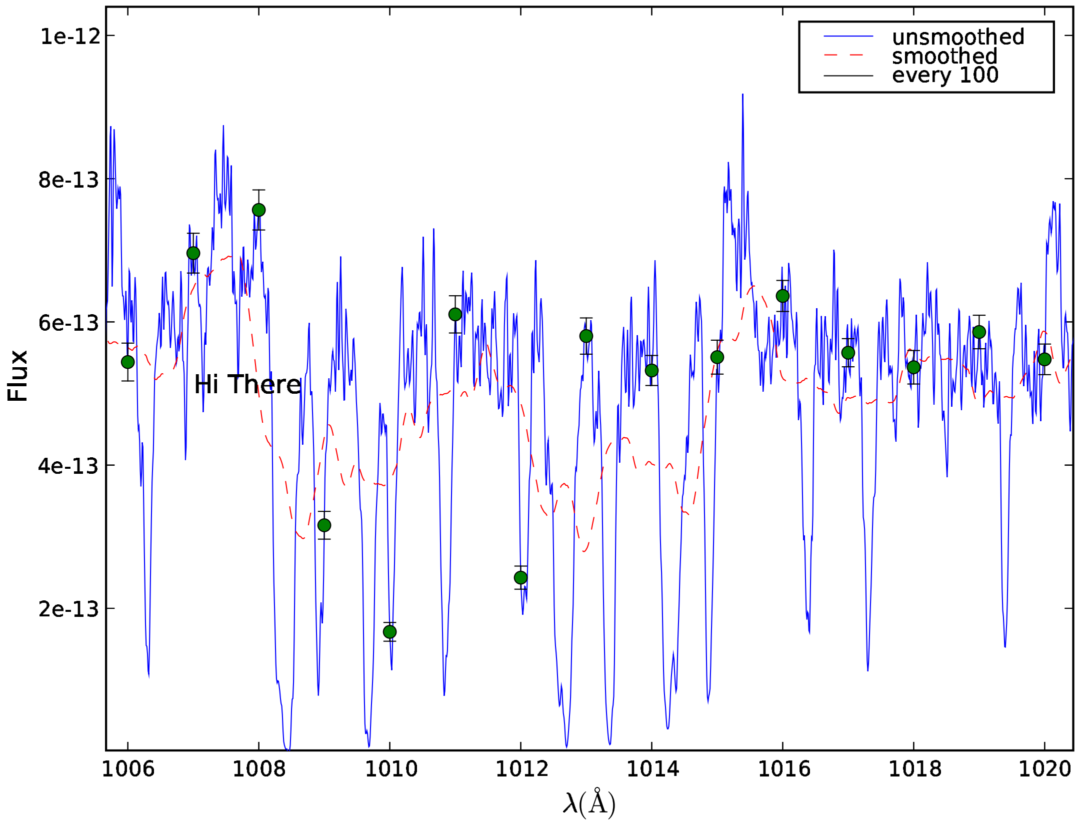
### 2.4.4 Legends and annotation

Adding legends is simple:

```
>>> legend(('unsmoothed', 'smoothed', 'every 100'))
<matplotlib.legend.Legend instance at 0x04978D28>
```

As is adding arbitrary text.

```
>>> text(1007., 0.5e-12, 'Hi There')
<matplotlib.text.Text instance at 0x04B27328>
```



### 2.4.5 Saving and printing plots

Matplotlib uses a very different style from IDL regarding how different devices are handled. Underneath the hood, matplotlib saves all the information to make the plot; as a result, it is simple to regenerate the plot for other devices without having to regenerate the plotting commands themselves (it's also why the figures can be interactive). The following saves the figure to a .png and postscript file respectively.

```
>>> savefig('fuse.png')
>>> savefig('fuse.ps')
```

## 2.5 A little background on Python sequences

Python has a few, powerful built-in "sequence" data types that are widely used. You have already encountered 3 of them: strings, lists and tuples.

### 2.5.1 Strings

Strings are so ubiquitous, that it may seem strange treating them as a special data structure. That they share much with the other two (and arrays) will be come clearer soon. First we'll note here that there are several ways to define literal strings. One can define them in the ordinary sense using either single quotes (') or double quotes ("). Furthermore, one can define multi-line strings using triple single or double quotes to start and end the string. For example:

```
>>> s = '''This is an example
of a multi-line string that
goes on and on and on.'''
>>> s
'This is an example\nof a string that\ngoes on and on\nand on'
>>> print s
This is an example
of a string that
goes on and on
and on
```

As with C, one uses the backslash character in combination with others to denote special characters. The most common is `\n` for new line (which means one uses `\\` to indicate a single `\` is desired). See the Python documentation for the full set. For certain cases (like regular expressions or MS Windows path names), it is more desirable to avoid special interpretation of backslashes. This is accomplished by prefacing the string with an `r` (for 'raw' mode):

```
>>> print 'two lines \n in this example'
two lines
in this example
>>> print r'but not \n this one'
but not \n this one
```

Strings are full fledged Python objects with many useful methods for manipulating them. The following is a brief list of all those available with a few examples illustrating their use. Details on their use can be found in the Python library documentation, the references in Appendix A or any introductory Python book. Note that optional arguments are enclosed in square brackets. For a given string *s*:

*s*`.capitalize()`: capitalize first character

*s*`.center(`*width [,fillchar]*`)`: return string centered in string of width specified with optional fill char

*s*`.count(`*sub [,start[,end]]*`)`: return number of occurrences of substring

*s*`.decode(`*[encoding [,errors]]*`)`: see documentation

*s*`.encode(`*[encoding [,errors]]*`)`: see documentation

*s*`.endswith(`*suffix [,start [,end]]*`)`: True if string ends with suffix

*s*`.expandtabs(`*[tabsize]*`)`: defaults to 8 spaces

*s*`.find(`*substring[,start [,end]]*`)`: returns position of substring found

*s*`.index(`*substring[,start [,end]]*`)`: like find but raises exception on failure *s*`.isalnum()`: true if all characters are alphanumeric

*s*`.isdigit()`: true if all characters are digits

*s*`.islower()`: true if all characters are lowercase

*s*`.isspace()`: true if all characters are whitespace

*s*`.istitle()`: true if titlecased

*s*`.isupper()`: true if all characters are uppercase

*s*`.join(`*seq*`)`: use string to join strings in the seq (note, this is a method of the string used to join the strings in seq, not the sequence of strings!)

*s*`.ljust(`*width [,fillchar]*`)`: return string left justified within string of specified width

*s*`.lower()`: convert to lower case

*s*`.lstrip(`*[chars]*`)`: strip leading whitespace (and optional characters specified)

**s.partition(sep):** Split a string at the first occurance of sep and return a 3-tuple containing the first part, sep, and the last part of the string. If sep isn't found, returns string followed by two empty strings. (new in Python 2.5)

*s*`.replace(`*old, new [,count]*`)`: substitute old substring with new string

*s*`.rfind(`*substring [,start [,end]]*`)`: return position of rightmost match of substring

*s*`.rindex(`*substring [,start [,end]]*`)`: like rfind but raises exception on failure

*s*`.rjust(`*width [,fillchar]*`)`: like ljust but right justified instead

`s.rpartition`**(sep):** same as partition, excepts finds last occurance of sep.(new in Python 2.5)

*s*`.rsplit(`*[sep [,maxsplit]]*`)`: similar to split, see documentation

*s*`.split(`*[sep [,maxsplit]*`)`: return list of words delimited by whitespace (or optional sep string)

*s*`.splitlines(`*[keepends]*`)`: returns list of lines within string

*s*`.startswith(`*prefix [.start [,end]]*`)`: true if string begins with prefix

*s*`.strip(`*[chars]*`)`: strip leading and trailing whitespace

*s*`.swapcase()`: switch lower to upper case and visa versa

*s*`.title()`: return title-cased version

*s*`.translate(`*table [,deletechars]*`)`: maps characters using table

*s*`.upper()`: convert to upper case

*s*`.zfill(`*width*`)`: left fill string with zeros to given width

```
>>> “hello world”.upper()
“HELLO WORLD”
>>> s = “hello world”
>>> s.find(“world”)
6
>>> s.endwith(“ld”)
True
>>> s.split()
['hello', 'world]
```

### 2.5.2 Lists

Think of lists as one-dimensional arrays that can contain anything for its elements. Unlike arrays, the elements of a list can be different kinds of objects (including other lists) and the list can change in size. Lists are created using simple brackets, e.g.:

```
>>> mylist = [1, 'hello', [2,3]]
```

This particular list contains 3 objects, the integer value `1`, the string `'hello'` and the list `[2, 3]`.

Empty lists are permitted:

```
>>> mylist = []
```

Lists also have several methods:

*l*`.append`(*x*): adds *x* to the end of the list

*l*`.extend`(*x*): concatenate the list *x* to the list

*l*`.count`(*x*): return number of elements equal to *x*

*l*`.index`(*x [,i [,j]]*): return location of first item equal to x

*l*`.insert`(*i, x*): insert *x* at $i^{\text{th}}$ position

*l*`.pop`(*[i]*): return last item [or $i^{\text{th}}$ item] and remove it from the list

*l*`.remove`(*x*): remove first occurrence of *x* from list

*l*`.reverse`(): reverse elements in place

*l*`.sort`(*[cmp [,key [,reverse]]]*): sort the list in place (how sorts on disparate types are handled are described in the documentation)

### 2.5.3 Tuples

One can view tuples as just like lists in some respects. They are created from lists of items within a pair of parentheses. For example:

```
>>> mytuple = (1, "hello", [2,3])
```

Because parentheses are also used in expressions, there is the odd case of creating a tuple with only one element:

```
>>> mytuple = (2) # not a tuple!
```

doesn't work since (2) is evaluated as the integer 2 instead of a tuple. For single element tuples it is necessary to follow the element with a comma:

```
>>> mytuple = (2,) # this is a tuple
```

Likewise, empty tuples are permitted:

```
>>> mytuple = ()
```

If tuples are a lot like lists why are they needed? They differ in one important characteristic (why this is needed won't be explained here, just take our word for it). They cannot be changed once created; they are called immutable. Once that "list" of items is identified, that list remains unchanged (if the list contains mutable things like lists, it is possible to change the contents of mutable things within a tuple, but you can't remove that mutable item from the tuple). Tuples have no standard methods.

### 2.5.4 Standard operations on sequences

Sequences may be indexed and sliced just like arrays:

```
>>> s[0]
'h'
>>> mylist2 = mylist[1:]
>>> mylist2
[“hello”, [2, 3]]
```

Note that unlike arrays, slices produce a new copy.

Likewise, index and slice assignment are permitted for lists (but not for tuples or strings, which are also immutable)

```
>>> mylist[0] = 99
>>> mylist
[99, “hello”, [2, 3]]
>>> mylist2
[1, “hello”, [2,3]] # note change doesn't appear on copy
>>> mylist[1:2] = [2,3,4]
>>> mylist
[1, 2, 3, 4, [2, 3]]
```

Note that unlike arrays, slices may be assigned a different sized element. The list is suitably resized.

There are many built-in functions that work with sequences. An important one is `len()` which returns the length of the sequence. E.g,

```
>>> len(s)
11
```

This function works on arrays as well (arrays are also sequences), but it will only return the length of the next dimension, not the total size:

```
>>> x = array([[1,2],[3,4]])
>>> print x
[[1 2]
[3 4]]
>>> len(x)
2
```

For strings, lists and tuples, adding them concatenates them, multiplying them by an integer is equivalent to adding them that many times. All these operations result in new strings, lists, and tuples.

```
>>> 'hello '+'world'
'hello world'
>>> [1,2,3]+[4,5]
[1,2,3,4,5]
>>> 5*'hello '
'hello hello hello hello hello '
```

### 2.5.5 Dictionaries

Lists, strings and tuples are probably somewhat familiar to most of you. They look a bit like arrays, in that they have a certain number of elements in a sequence, and you can refer to each element of the sequence by using its index. Lists and tuples behave very much like arrays of pointers, where the pointers can point to integers, floating point values, strings, lists, etc. The methods allow one to do the kinds of things you need to do to arrays; insert/delete elements, replace elements of one type with another, count them, iterate over them, access them sequentially or directly, etc.

Dictionaries are different. Dictionaries define a mapping between a key and a value. The key can be either a string, an integer, a floating point number or a tuple (technically, it must be immutable, or unchangeable), but not a list, dictionary, array or other mutable objects, while the value has no limitations. So, here's a dictionary:

```
>>> thisdict = {'a':26.7, 1:['random string', 66.4], -6.3:”}
```

As dictionaries go, this one is pretty useless. There's a key whose name is the string 'a', with the floating point value of 26.7. The second key is the integer 1, and its value is the list containing a string and a floating point value. The third key is the floating point number -6.3, with the empty string as its value. Dictionaries are examples of a mapping data type, or associative array. The order of the key/value pairs in the dictionary is not related to the order in which the entries were accumulated; the only thing that matters is the association between the key and the value. So dictionaries are great for, for example, holding IRAF parameter/value sets, associating numbers with filter names, and passing keyword/value pairs to functions. Like lists, they have a number of built-in methods:

***d*.copy()**: Returns a shallow copy of the dictionary (subtleties of copies will be addressed in tutorial 4)

***d*.has_key(*k*)**: Returns True if key *k* is in *d*, otherwise False

***d*.items()**: Returns a list of all the key/value pairs

***d*.keys()**: Returns a list of all the keys

***d*.values()**: Returns a list of all the values

***d*.fromkeys(*seq[,value]*)**: Creates new dictionary with keys from seq and values set to value.

***d*.iteritems()**: Returns an iterator on all items

***d*.iterkeys()**: Returns an iterator an all keys

***d*.itervalues()**: Returns an iterator on all keys

***d*.get(*k [,x]*)**: Returns *d[k]* if *k* is in *d*, otherwise *x*

***d*.clear()**: Removes all items

***d*.update(*D*)**: For each *k* in dictionary *D*, sets (or adds) *k* of dictionary = *D[k]*

***d*.setdefault(*k [,x]*)**: Returns value of *k* if *k* is in dictionary, otherwise creates key *k*, sets value to *x*, and returns x

***d*.popitem()**: Removes and returns an arbitrary item

So, for example, we could store the ACS photometric zeropoints in a dictionary where the key is the name of the filter:

```
>>> zeropoints = {'F435W':25.779, 'F475W':26.168, 'F502N':22.352, 'F550M':24.867,
'F555W':25.724, 'F606W':26.398, 'F625W':25.731, 'F658N':22.365, 'F660N':21.389,
'F775W':25.256, 'F814W':25.501, 'F850LP':24.326, 'F892N':21.865}
>>> filter = hdr['filter1']
>>> if filter.find('CLEAR') != -1: filter = hdr['filter2']
>>> zp = zeropoints[filter]
```

Dictionaries are very powerful; if your programs do not use them regularly, you are likely doing something very wrong.

The power afforded by dictionaries, lists, tuples and strings and their built-in methods is one of the great strengths of Python.

### 2.5.6 A section about nothing

Python uses a special value to represent a null value called `None`. Functions that don't return a value actually return `None`. At the interactive prompt, a `None` value is not printed (but a `print None` will show its presence).

## 2.6 More on plotting

It is impossible in a short tutorial to cover all the aspects of plotting. The following will attempt to give a broad brush outline of matplotlib terminology, what functionality is available, and show a few examples.

### 2.6.1 `matplotlib` terminology, configuration and modes of usage

The "whole" area that matplotlib uses for plotting is called a figure. Matplotlib supports multiple figures at the same time. Interactively, a figure corresponds to a window. A plot (a box area with axes and data points, ticks, title, and labels...) is called an axes object. There may be many of these in a figure. Underneath, matplotlib has a very object-oriented framework. It's possible to do quite a bit without knowing the details of it, but the most intricate or elaborate plots most likely will require some direct manipulation of these objects. For the most part this tutorial will avoid these but a few examples will be shown of this usage.

While there may be many figures, and many axes on a figure, the matplotlib functional interface (i.e, `pylab`) has the concept of current figures, axes and images. It is to these that commands that operate on figures, axes, or images apply to. Typically most plots generate each in turn and so it usually isn't necessary to change the current figure, axes, or image except by the usual method of creating a new one. There are ways to change the current figure, axes, or image to a previous one. These will be covered in a later tutorial.

Matplotlib works with many "backends" which is another term for windowing systems or plotting formats. We recommend (for now anyway) using the standard, if not quite as snazzy, Tkinter windows. These are compatible with PyRAF graphics so that matplotlib can be used in the same session as PyRAF if you use the TkAgg backend.

Matplotlib has a very large number of configuration options. Some of these deal with backend defaults, some with display conventions, and default plotting styles (linewidth, color, background, etc.). The configuration file, `.matplotlibrc,` is a simple ascii file and for the most part, most of the settings are obvious in how they are to be set. Note that usage for interactive plotting requires a few changes to the standard `.matplotlibrc` file as downloaded (we have changed the defaults for our standard installation at STScI). A copy of this modified file may be obtained from `http://stsdas.stsci.edu/python/.matplotlibrc`. Matplotlib looks for this file in a number of locations including the current directory. There is an environmental variable that may be set to indicate where the file may be found if yours is not in a standard location.

Some of the complexity of matplotlib reflects the many kinds of usages it can be applied to. Plots generated in script mode generally have interactive mode disabled to prevent needless regenerations of plots. In such usage, one must explicitly ask for a plot to be rendered with the `show()` command. In interactive mode, one must avoid the `show` command otherwise it starts up a GUI window that will prevent input from being typed at the interactive command line. Using the standard Python interpreter, the only backend that supports interactive mode is TkAgg. This is due to the fact most windowing systems require an event loop to be running that conflicts with the Python interpreter input loop (Tkinter is special in that the Python interpreter makes special provisions for checking Tk events thus no event loop must be run). IPython has been developed to support running all the backends while accepting commands. Do not expect to be able to use a matplotlib backend while using a different windowing system within Python. Generally speaking, different windowing frameworks cannot coexist within the same process.

Since matplotlib takes its heritage from Matlab, it tends toward using more functions to build a plot rather than many keyword arguments. Nevertheless, there are many plot parameters that may be set through keyword arguments.

The `axes` command allows arbitrary placement of plots within a figure (even allowing plots to be inset within others). For cases where one has a regular grid of plots (say 2x2) the `subplot` command is used to place these within the figure in a convenient way. See one of the examples later for its use.

Generally, matplotlib doesn't try to be too clever about layout. It has general rules for how much spaces is needed for tick labels and other plot titles and labels. If you have text that requires more space than that, It's up to you to replot with suitable adjustments to the parameters.

Because of the way that matplotlib renders interactive graphics (by drawing to internal memory and then moving to a display window), it is slow to display over networks (impossible over dial-ups, slow over broadband; gigabit networks are quite usable however)

### 2.6.2 matplot functions

The following lists most of the functions available within pylab for quick perusal followed by several examples.

***basic plot types*** *(with associated modifying functions)*

`acorr: plot autocorrelation function`

`bar:` bar charts

`barh:` horizontal bar charts

`broken_barh:` a set of horizontal bars with gaps

`boxplot:` box and whisker plots

`cohere:` plot of coherence

`contour:`

`contourf:` filled contours

`csd:` plot of cross spectral density

`errorbar:` errorbar plot

`hist:` histogram plot

`implot:` display image within axes boundaries (resamples image)

`loglog:` log log plot

`matshow:` display a matrix in a new figure preserving aspect

`pcolor:` make a pseudocolor plot

`pcolormesh:` make a pseudocolor plot using a quadrilateral mesh

`pie`

`plot:` x, y plots

`plot_date:` plot using x or y argument as date values and label axis accordingly

`polar`

`psd:` power spectral density

`quiver:` vector field plot

`scatter`

`semilogx:` log x, linear y, x y plot

`semilogy:` linear x, log y, x y plot

`specgram:` spectrogram plot

`stem`

`spy:` plot sparsity pattern using markers

`spy2:` plot sparsity pattern using image

`xcorr:` plot the autocorrelation function of x and y

***plot decorators and modifiers***

`annotate: annotate something in figure`

`arrow: add arrow to plot`

`axhline`: plot horizontal line across axes

`axvline`: plot vertical line across axes

`axhspan`: plot horizontal bar across axes

`axvspan`: plot vertical bar across axes

`clabel`: label contour lines

`clim`: adjust color limits of current image

`fill`: make filled polygons

`grid`: set whether grids are visible

`legend`: add legend to current axes

`rgrids`: customize the radial grids and labels for polar plots

`table`: add table to axes

`text`: add text to axes

`thetagrids`: for polar plots

`title`: add title to axes

`xlabel`: add x axes label

`ylabel`: add y axes label

`xlim`: set/get x axes limits

`ylim`: set/get y axes limits

`xticks`: set/get x ticks

`yticks`: set/get y ticks

***figure functions***

`colorbar`: add colorbar to current figure

`figimage`: display unresampled image in figure

`figlegend`: display legend for figure

`figtext`: add text to figure

***object creation/modification/mode/info functions***

`axes`: create axes object on current figure

`box`: set axis frame state on or off

`cla`: clear current axes

`clf`: clear current figure

`close`: close a figure window

`delaxes`: delete axes object from the current figure

`draw`: force a redraw of the current figure

`figure`: create or change active figure

`gca`: get the current axes object

`gcf`: get the current figure

`gci`: get the current image

`getp`: get a handle graphics property

`hold`: set the hold state (overdraw or clear?)

`ioff`: set interactive mode off

`ion:` set interactive mode on

`isinteractive:` test for interactive mode

`ishold:` test for hold mode

`plotting:` list plotting commands

`rc:` control the default parameters

`savefig:` save the current figure

`setp:` set a handle graphics property

`show:` show the current figures (for non-interactive mode)

`subplot:` create an axes within a grid of axes

`subplot_adjust:` change the params controlling the subplot positions

`subplot_tool:` launch the subplot configuration tool

***color table functions***

`autumn, bone, cool, copper, flag, gray, hot, hsv, pink, prism, spring, summer, winter` spectral

## 2.7 Plotting mini-Cookbook

### 2.7.1 customizing standard plots

The two tables below list the properties of data and text properties and information about what values they can take. The variants shown in parentheses indicate acceptable abbreviations when used as keywords.

**Data properties**

| Property | Value |
|---|---|
| alpha | Alpha transparency (between 0. and 1., inclusive) |
| animated | True or False, facilitates faster animations (see wiki animation link for details) |
| antialiased (aa) | Use antialiased rendering (True or False) |
| color (c) | Style 1:<br>'b' -> blue<br>'g' -> green<br>'r' -> red<br>'c' -> cyan<br>'m' -> magenta<br>'y' -> yellow<br>'k' -> black<br>'w' -> white<br>Style 2: standard color string, eg. 'yellow', 'wheat'<br>Style 3: grayscale intensity (between 0. and 1., inclusive)<br>Style 4: RGB hex color triple, eg. #2F4F4F<br>Style 5: RGB tuple, e.g., (0.18, 0.31, 0.31), all values between 0. and 1.) |
| dash_capstyle | one of 'butt', 'round', or 'projecting' |
| dash_joinstyle | one of 'miter', 'round', or 'bevel' |
| data_clipping | Clip data before plotting (if the great majority of points will fall outside the plot window this may be much faster); True or False |
| figure | figure instance (to direct specifically to a existing figure) |
| label | A string optionally used for legend |
| linestyle (ls) | One of '–' (dashed), ':' (dotted), '-.' (dashed dot), '-' solid |
| linewidth (lw) | width of line in points (nonzero float value) |
| marker | symbol:<br>'o' -> circle<br>'^','v','<','>' triangles: up, down, left, right respectively<br>'s' -> square<br>'+' -> plus<br>'x' -> cross<br>'D' -> diamond<br>'d' -> thin diamond<br>'1','2','3','4' tripods: down, up, left, right<br>'h' -> hexagon<br>'p' -> pentagon<br>'\|' -> vertical line<br>'_' -> horizontal line<br>'steps' (keyword arg only) |
| markeredgewidth (mew) | width in points (nonzero float value) |
| markeredgecolor (mec) | color value |
| markerfacecolor (mef) | color value |
| markersize (ms) | size in points (nonzero float value) |
| solid_capstyle | one of 'butt', 'round', or 'bevel' |
| solid_joinstyle | one of 'miter', 'round', or 'bevel' |
| visible | True or False |
| xdata | array (for x coordinates of data points) |
| ydata | array (for y coordinates of data points) |
| zorder | any floating number; used to determine layering order of plot data |

The following describes text attributes (those shared with lines are not detailed)

| Property | Value |
|---|---|
| alpha, color | As with Lines |
| family | font family, eg 'sans-serif','cursive','fantasy' |
| fontangle | the font slant, 'normal', 'italic', 'oblique' |
| horizontalalignment | 'left', 'right', 'center' |
| verticalalignment | 'top', 'bottom', 'center' |
| multialignment | 'left', 'right', 'center' (only for multiline strings) |
| name | font name, eg. 'Sans', 'Courier', 'Helvetica' |
| position | x, y position |
| variant | font variant, eg. 'normal', 'small-caps' |
| rotation | angle in degrees for text orientation |
| size | size in points |
| style | 'normal', 'italic', or 'oblique' |
| text | the text string itself |
| weight | e.g 'normal', 'bold', 'heavy', 'light' |

These two sets of properties are the most ubiquitous. Others tend to be specialized to a specific task or function. The following illustrates with some examples (plots are not shown) starting with the ways of specifying red for a plotline

```
>>> x = arange(100.)
>>> y = (x/100.)**2
>>> plot(x,y,'r')
>>> plot(x,y, c='red')
>>> plot(x,y, color='#ff0000')
>>> lines = plot(x,y)                  # lines is a list of objects, each has set methods
                                        for each property
>>> setp(lines, 'color', (1.,0,0)) # or
>>> lines[0].set_color('red') ; draw()  # object manipulation example
>>> plot(y[::10], 'g>:',markersize=20') # every 10 points with large green triangles and
                                        dotted line
```

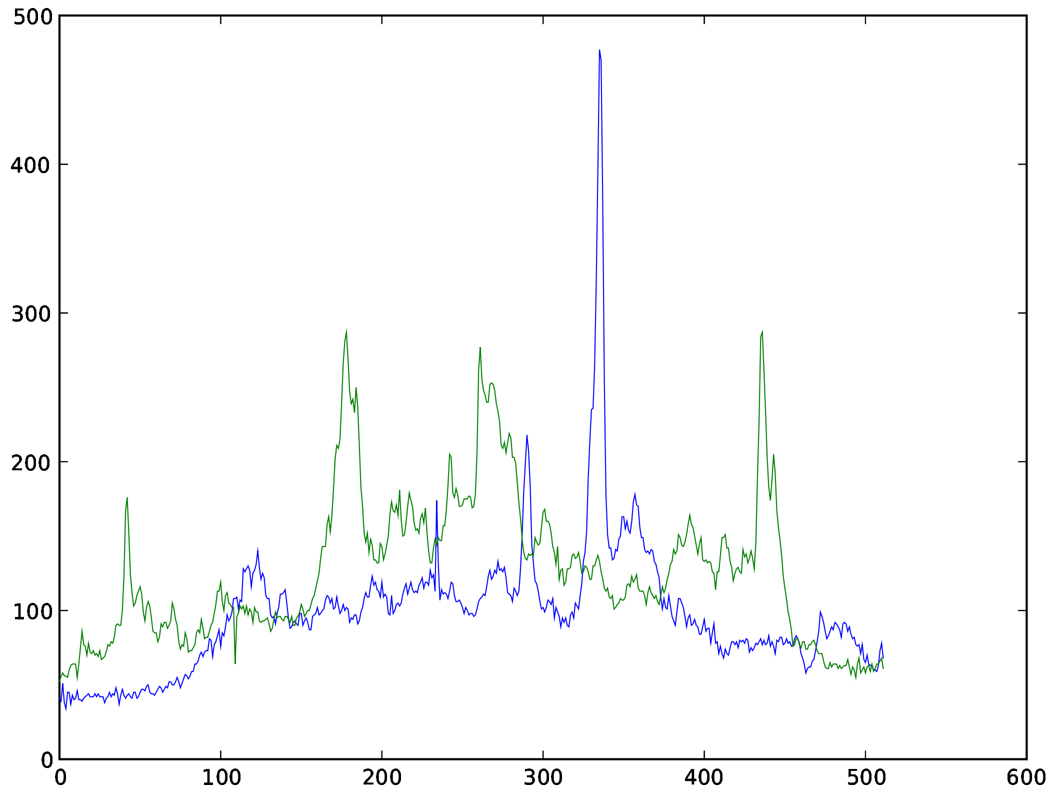
And more examples specifying text:

```
>>> textobj = xlabel('hello', color='red',ha='right')
>>> setp(textobj, 'color', 'wheat') # change color
>>> setp(textobj, 'size', 5) # change size
```

### 2.7.2 implot example

You can duplicate simple use of the IRAF task `implot` like this:

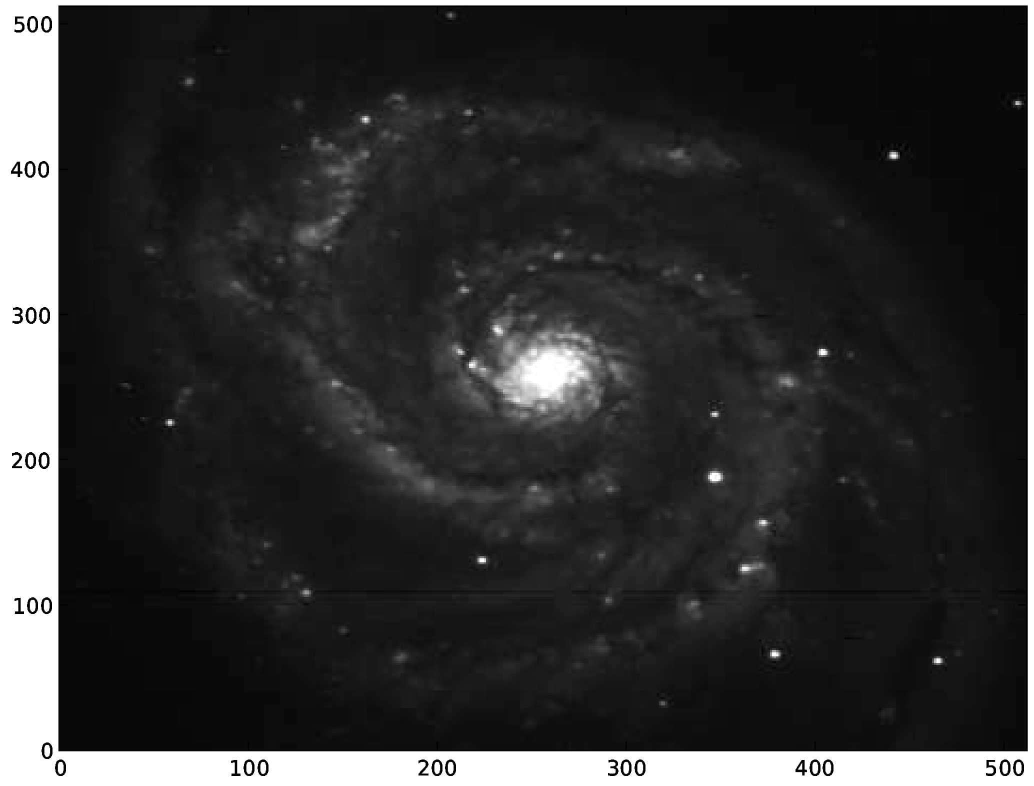
```
>>> pixdata = pyfits.getdata('pix.fits')
>>> plot(pixdata[100], hold=False)                # plots row 101
>>> plot(pixdata[:,200],hold=True)                #overplots col 201
```



### 2.7.3 imshow example

Images can be displayed both using `numdisplay`, which was introduced in the last tutorial and the `matplotlib` `imshow` command:

```
>>> import numdisplay
>>> numdisplay.open()
>>> numdisplay.display(pixdata,z1=0,z2=1000)
>>> clf()                                        # clears the current figure
>>> imshow(pixdata,vmin=0,vmax=1000)
>>> gray()                                       # loads a greyscale color table
```



The default type of display in Matplotlib "out of the box" has the Y coordinate increasing from top to bottom. This behavior can be overridden by changing a line in the .matplotlibrc file:

```
image.origin : lower
```

The `.matplotlibrc` that is the default on STScI unix systems (Solaris, Linux and Mac) has this already set up. If you are using Windows, you will need to get the STScI default .matplotlibrc from one of the Unix systems, or from the web.

`imshow` will resample the data to fit into the figure using a defined interpolation scheme. The default is set by the `image.interpolation` parameter in the `.matplotlibrc` file (`bilinear` on STScI systems), but this can be set to one of `bicubic, bilinear, blackman100, blackman256, blackman64, nearest, sinc144, sinc256, sinc64, spline16` and `spline36`. Most astronomers are used to blocky pixels that come from using the nearest pixel; so we can get this at run-time by doing

```
>>> imshow(pixdata, vmin=0, vmax=1000, interpolation='nearest')
```

### 2.7.4 figimage

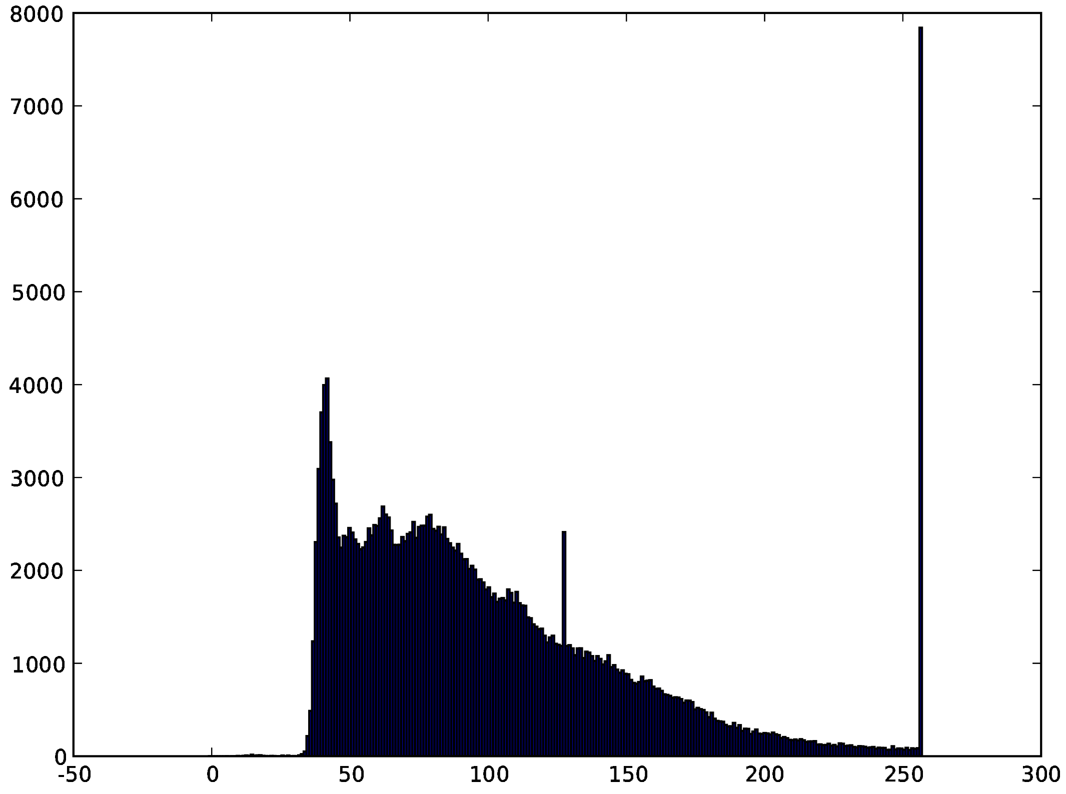
`figimage` is like `imshow`, except no spatial resampling is performed. It also allows displaying RGB or RGB-alpha images. This function behaves more like the IDL `TVSCL` command. See the manual for more details.

### 2.7.5 histogram example

Histograms can be plotted using the `hist` command.

```
>>> pixdata[pixdata>256] = 256
>>> hist(pixdata,bins=256)
```

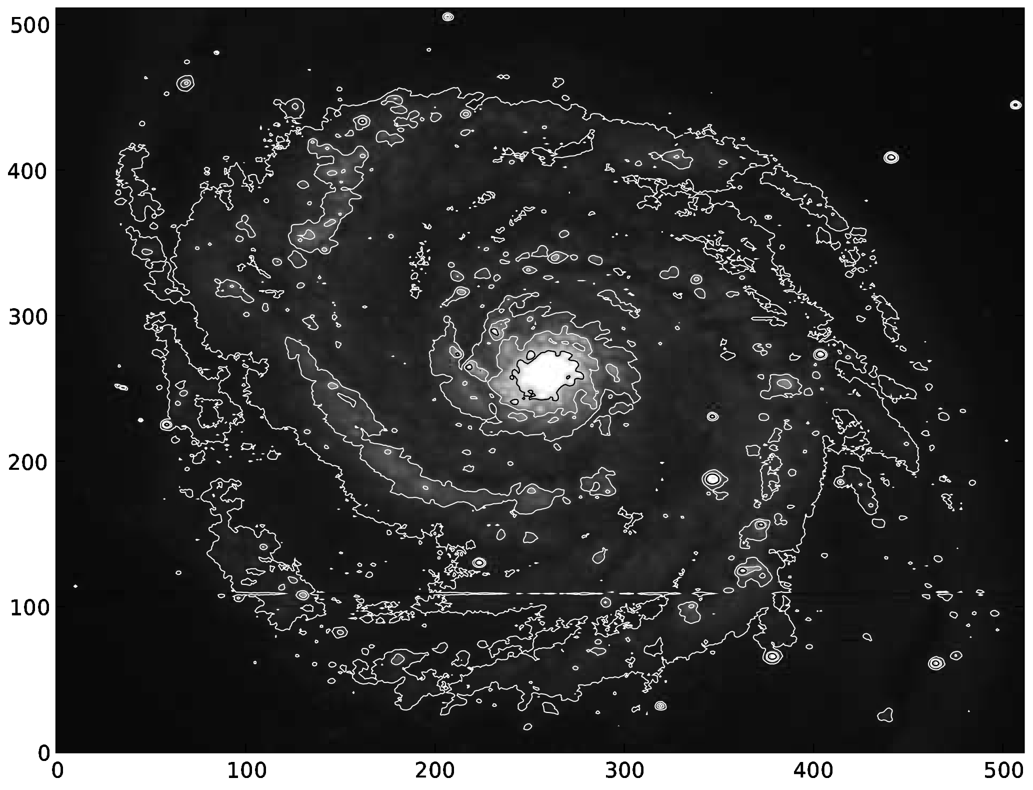
Duplicating the functionality of, for example, the IRAF `imhistogram` task will take a bit more work.



### 2.7.6 contour example

To overplot green contours at levels of 100, 200, 400 and 800, we can do:

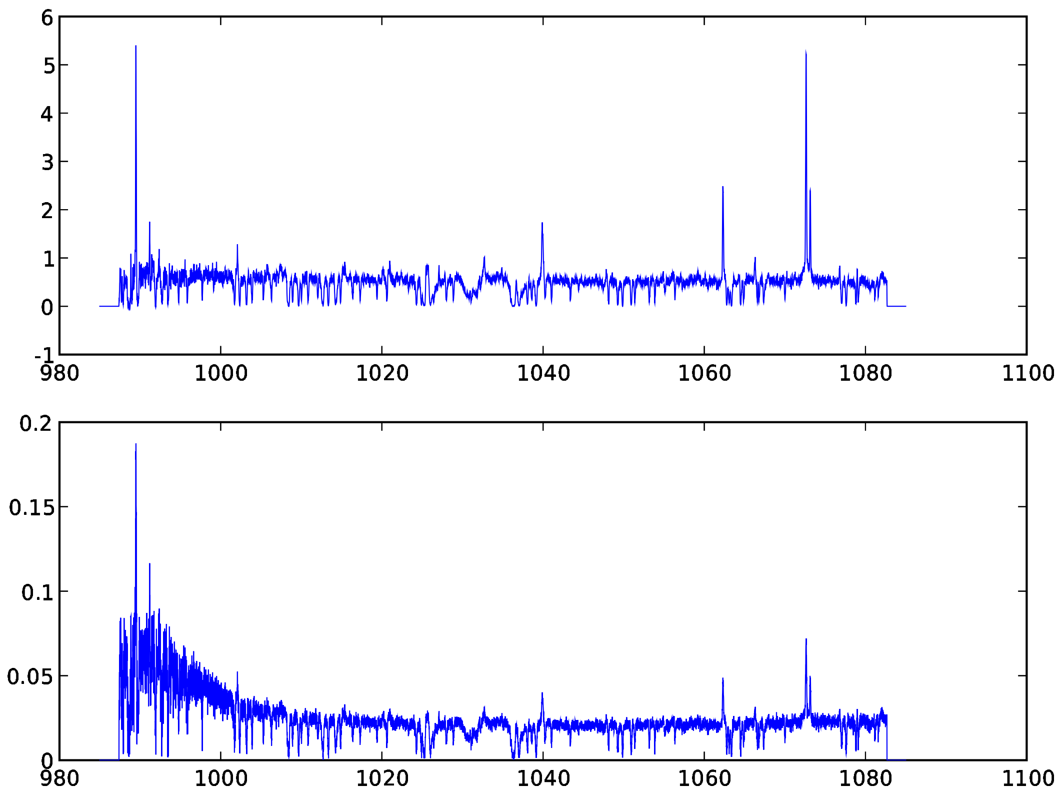
```
>>> levels = [100,200,400,800]
>>> imshow(pixdata,vmin=0,vmax=1000,origin='lower')
>>> contour(pixdata,levels,colors='1.0')
```



### 2.7.7 subplot example

You aren't limited to having one plot per page. The `subplot` command will divide the page into a user-specified number of plot.

```
>>> subplot(211)                   # Divide area into 2 vertically, 1
                                     horizontally and select the first plot
>>> plot(wave,flux)
>>> subplot(212)                   # Select second plot
>>> plot(wave,error.flat)
```



### 2.7.8 readcursor example

Finally, it is possible to set up functions to interact with a plot using the event handling capabilities of `Matplotlib`. Like many other GUIs, `Matplotlib` provides an interface to the underlying GUI event handling mechanism. This is achieved using a callback function that is activated when a certain prescribed action is performed. The prescribed action could be a mouse button click, key press or mouse movement. You can set up a handler function to handle the event by registering the event you want to detect, and connecting your callback function with the required event. This is getting a little bit ahead of ourselves here, since we weren't going to explain functions until the fourth tutorial, but it's impossible to explain event handling without it....

This is best explained using an example. Say you want to print the X and Y coordinates when you click the mouse in an image. Start by displaying the image in an `imshow()` window:

```
>>> imshow(pixdata, vmin=0, vmax=200)
```

Then set up a handler to print out the X and Y coordinates. This will be run every time the mouse button is clicked, until the "listener" function is killed (this actually defines a function, which will covered in more detail later; don't worry about the details yet).

```
>>> def clicker(event):
...     if event.inaxes:
...         print event.xdata, event.ydata
...
>>>
```

This is a very simple handler: it just checks whether the cursor is inside the figure (`if event.inaxes`), and if it it, it prints out the X and Y coordinates in data coordinates (i.e. in the coordinates as specified by the axes). If the cursor is outside the figure, nothing is done.

Now we set up a "listener" by connecting the event we are looking for (`'button_press_event'`) with the function we will call (`clicker`).

```
>>> cid = connect('button_press_event', clicker)
```

The connect function returns a "connect id", which we will use when we want to kill the listener.

Now, when we press the mouse button when we are in the figure, we get the coordinates printed out on our screen. This works even if we zoom the image, since we have requested the coordinates in data space, so matplotlib takes care of determining the X and Y coordinates correctly for us. When we're done, we can just do the following:

```
>>> disconnect(cid)
```

and we are no longer listening for button presses.

There are more details in the `matplotlib` manual.

## 2.8 Exercises

1. Using only Python tools, open the FITS file `fuse.fits`, extract the flux and error columns from the table, and plot these against each other using `plot()`. Scale the flux and error by 1.0e12 before plotting.

2. Smooth `pix.fits` with a 31x31 boxcar filter (see first tutorial) and make a contour plot at 90, 70, 50, and 30, and 10% of the peak value of the smoothed image.

3. Repeat 2, except before generating a contour plot display the unsmoothed image underneath.

4. Change the colortable to gray and label your favorite feature with a mathematical expression

5. Save the result as a postscript file and view it in your favorite postscript viewer

6. Extra credit: parroting the readcursor example, write a short callback function to display a cross cut plot of a displayed image on a left mouse button click, and a vertical cut plot on a right button click (overplotting the image). [Hint: this needs use of subplot(111, Frameon=False) to get overplotting on images to work]

# 3 More advanced topics in PyFITS, numarray and IPython

## 3.1 IPython

IPython is a souped up interactive environment for Python. It adds many special features to make interactive analysis sessions easier and more productive. These features include:

- easy invocation of common shell commands with shell-like syntax (e.g., `ls`, `cd`, etc.)
- Alias facility for defining system aliases
- Complete system shell access (through `!` and `!!` prefixes)
- TAB completion
- Easy ways to find out information about modules, functions and objects.
- Numbered input/output prompts with command history
- User-extensible magic commands
- Session logging and restoring (through playback of logged commands)
- Background execution of Python commands in a separate thread
- Automatic indentation
- Macro system
- Auto parenthesis and auto quoting
- Flexible configuration system allowing for multiple configurations
- Easy reimportation (useful for script and module development)
- Easy debugger access
- Syntax highlighting and editor invocation, easier to interpret tracebacks
- Profiler support

This tutorial will only touch a subset of its extensive features (IPython has its own, very complete manual: see Appendix A for instructions on how to obtain it). When started (simply by typing `ipython`) the most apparent difference from the standard Python interpreter is the prompt. Each line entered by the user is numbered. Commands can be recalled through the standard up and down arrow keystrokes (if the readline library is installed) as well as by number (shown later).

### 3.1.1 Obtaining information about Python objects and functions

IPython provides a few very handy ways of finding out information about modules, functions, and objects. Some examples:

```
In [10]: x = [1, 2] # create a short list
```

Typing `?` before or after a name (module, variable, etc.) gives information about that module or object including documentation included in the source code for that module or object (the "docstring", discussed later).

```
In [11]: x?
Type:          list
Base Class:    <type 'list'>
String Form:   [1, 2]
Namespace?:    Interactive
Length:        2
Docstring:
    list() -> new list
    list(sequence) -> new list initialized from sequence's items
```

This shows a little info about the object.

If one types a TAB character after the object or module name with a period, IPython will list all the possible contents of that module or object (i.e., its attributes or methods). One can then look at any documentation available for these items using the ? feature. E.g.,

```
In [12]: x.<TAB>
x.__add__          x.__iadd__          x.__setattr__
x.__class__        x.__imul__          x.__setitem__
x.__contains__     x.__init__          x.__setslice__
x.__delattr__      x.__iter__          x.__str__
x.__delitem__      x.__le__            x.append
x.__delslice__     x.__len__           x.count
x.__doc__          x.__lt__            x.extend
x.__eq__           x.__mul__           x.index
x.__ge__           x.__ne__            x.insert
x.__getattribute__ x.__new__           x.pop
x.__getitem__      x.__reduce__        x.remove
x.__getslice__     x.__reduce_ex__     x.reverse
x.__gt__           x.__repr__          x.sort
x.__hash__         x.__rmul__
In [13]: x.append?
Type:             builtin_function_or_method
Base Class:       <type 'builtin_function_or_method'>
String Form:      <built-in method append of list object at 0x15bcff0>
Namespace:        Interactive
Docstring:
    L.append(object) -- append object to end
```

This lists all the attributes and methods for lists. Generally you should ignore any names that begin with underscore (the meaning of all these will be explained in the next tutorial). The next inquiry shows the docstring info for the list append method.

These techniques can be used to inspect what's available within any Python object or module. One caution: objects that use more sophisticated means of handling attributes and methods will generally not show these by these inspection tools. So just because you don't see something doesn't mean it doesn't exist. A good example is the data attribute for pyfits objects (something that will be covered in this tutorial). There is such an attribute, but it won't be seen through the TAB completion mechanism here.

### 3.1.2 Access to the OS shell

Any system shell command may be executed by prepending it with '!' E.g.,

```
In [14]: !ls
newfile.fits   seq.fits  pix.fits
```

### 3.1.3 Magic commands

IPython has what it calls magic commands. These are special commands not normally part of Python. The following lists the default set. Users may define their own magic commands.

| Magic Command | Action |
|---|---|
| Exit | Exit IPython without confirmation |
| Pprint | Toggle pretty printing on/off |
| Quit | same as Exit |
| alias | Define an alias for a system command |
| autocall | Make functions callable without typing parenthesis (default) |
| autoindent | Toggle autoindent on/off (default on) |
| automagic | Make magic functions callable without having to type '%' (default) |
| bg | Run a job in the background, in a separate thread |
| bookmark | Manage bookmark system (for directories) |
| cd | Change directories |
| color_info | Toggle color syntax highlighting (default on) |
| colors | switch color scheme |
| config | Show IPython's internal configuration |
| dhist | Print history of visited directories |
| dirs | Return current directory stack |
| ed | Alias to edit |
| edit | Bring up editor and execute the resulting code |
| env | List environmental variables |
| hist | Print input history, most recent last |
| logoff | Stop logging |
| logon | Restart logging |
| logstart | Start logging |
| logstate | Print the status of the logging system |
| lsmagic | List currently available magic functions |
| macro | Define set of input lines as macro |
| magic | Print info about magic function system |
| p | Alias for Python print function |
| page | Pretty print the object and display it through a pager |
| pdb | Control the calling of the pdb interactive debugger |
| pdef | Print the definition header of any callable object |
| pdoc | Print the docstring for an object |
| pfile | Print the file where an object is defined |
| pinfo | Provide detailed information about an object |
| popd | Change to a directory popped off the directory stack |
| profile | Print currently active IPython profile |
| prun | Run a statement through the Python code profiler |
| psource | Print source code for object |
| pushd | Push current directory on stack and change directory |
| pwd | Return current working directory |
| r | Repeat previous input |
| rehash | Update the alias table with all entries in $PATH |
| rehashx | Update the alias table with all executables in $PATH |
| reset | Reset the namespace by removing all names defined by user |
| run | Run the named file inside IPython as a program |

| | |
|---|---|
| runlog | Run files as logs |
| save | Save a set of lines to a given filename |
| sc | Execute a shell command and capture its output |
| sx | Run a shell command and capture its output |
| system_verbose | Toggle verbose printing of system commands on and off |
| time | Time execution of a Python statement or expression |
| unalias | Remove alias |
| who | Print all interactive variables with minimal formatting |
| who_ls | Return sorted list of all interactive variables |
| whos | Like who but with extra info about each variable |
| xmode | Switch modes for exception handlers |

The use of many of these is fairly obvious; for others consult the IPython documentation on their use.

IPython has default aliases for the following system commands: `cat, clear, cp, less, mkdir, mv, rm, rmdir,` and many variants on `ls` (`lc, ldir, lf, lk, ll` and lx). The magic `alias` command allows one to change or add to the list.

IPython saves the history of previous commands from one session to the next (the manual describes how to keep different session histories).

### 3.1.4 Syntax shortcuts

With autocall mode on, it means that it is not necessary to provide parentheses for functions that aren't being assigned:

```
In [15]: pyfits.info 'pix.fits' # instead of pyfits.info('pix.fits')
------->pyfits.info('pix.fits')
Filename: pix.fits
No.    Name         Type      Cards   Dimensions  Format
0    PRIMARY     PrimaryHDU      71  (512, 512)   Int16
```

but note that this doesn't work:

```
In [16]: im = pyfits.getdata 'pix.fits'
------------------------------------------------------------
   File "<console>", line 1
     im = pyfits.getdata 'pix.data'

SyntaxError: invalid syntax
```

If one starts a line with a comma, every argument of a function is assumed to be auto quoted. E.g.:

```
In [17]:,pyfits.info pix.fits
------->pyfits.info('pix.fits')
Filename: pix.fits
No.    Name         Type      Cards   Dimensions  Format
0    PRIMARY     PrimaryHDU      71  (512, 512)   Int16
```

Note also that when IPython does this sort of autotransformation, it prints the command actually executed. What is saved in the log files is the proper Python syntax, not what you typed. For functions that expect strings only, this allows near shell-like syntax to be used.

### 3.1.5 IPython history features

Typing `Control-p` (or `Control-n`) after you typed something at the command line will match the closest previous (or next) command in the history that matches what you've typed.

Previous input commands are available for re-execution (or other manipulation) by accessing special variables. The variable `In` is effectively a list of the previous commands that can be indexed with the number that matches the prompt. Slicing works as well. The following example show how to select a set of previous lines for re-execution:

```
In[18]: print 1
1

In[19]: print 2
2

In[20]: print 3
3

In[21]: print 4
4
In [22]: exec In[18:20]+In[21]
1
2
4
```

The previous lines are also accessible through variables `_i`<*n*> and `_ih`<*n*>. E.g.,

```
In [23]: print _i21
print 4
```

The return value of statements that return a value (and thus often print or display something to the output) are stored in similar variables. The most recent is in a variable `_`, the next most recent in `__`, and likewise for `___`. For example:

```
In[24]: 6+9
15
In[25]: print _
15
```

Since assignments don't return anything, they are not saved this way. Like input commands, output values are saved in Out and can be indexed, or the variables `_o`<*n*> or _oh<*n*>. This feature may use extra memory since it is saving references to things that normally would be deleted so the feature can be turned off (see the later discussion on memory usage for a better understanding of what happens).

By defining a `.ipythonrc` file in each working directory, one can customize what IPython does for a session started in that directory. Additional IPython features will be illustrated throughout the rest of the tutorials.

## 3.2 Python Introspection

Snake navel gazing? No, not quite. This term refers to the capabilities that Python provides for finding out information about Python objects from the objects themselves (IPython makes use of these facilities). Python has very extensive tools for doing this. Only a couple of the simplest will be mentioned here. By using the Python `dir()` function, one can examine the "contents" of various Python entities including modules, objects and classes. For example using `dir()` on a module will list variables, functions, and classes defined within the module (but not indicate what they are; in the list there is no visual way of distinguishing a function from a variable–except by use of standard naming conventions in some cases). As an example dir(pyfits) lists over a hundred such items. This can be useful if you can't quite remember the name of a method or attribute. By itself, don't expect to understand everything you see (or even most). One can use dir() on these items in turn to find out about them.

The Python function type() can be used on any object to tell you what type it is. From its use you can tell if something is an integer, string, list, function, or specific object.

Every Python module, function, class and method has a provision for a special string that is available for inspection. This string is called the "docstring". If it exists, it is the __doc__ attribute of the object. Here are a few examples:

```
>>> x = [1,2] # a simple python list
>>> print x.__doc__
list() -> new list
list(sequence) -> new list initialized from sequence's items
```

This shows the docstring for the list creator function.

```
>>> print pyfits.__doc__ # print the pyfits module docstring
A module for reading ....
....
>>> print pyfits.getdata.__doc__
...
```

With these few features it is usually possible to find out quite a bit about any object.

## 3.3 Saving your data

At the moment, there are no comparable functions to the IDL save and restore commands. There are ways of saving and restoring Python objects (which goes by the odd name of pickling) but its use is far from being convenient as the IDL save command. We are working on a command to make saving and restoring data much easier (and similar to how it is done in IDL), but given the richness of the forms that Python objects can be generated, it is not possible to ensure that all objects can be saved. The future command will allow saving of all reasonably saveable objects (for example, open files objects cannot be saved).

## 3.4 Python loops and conditionals

### 3.4.1 The for statement

Like many other languages Python has a for statement. Its use is a little different than most are likely used to seeing. Here is an example:

```
>>> pets = ['dog','cat','gerbil','canary','goldfish','rock']
>>> for pet in pets: print 'I have a pet', pet
I have a pet dog
I have a pet cat
I have a pet gerbil
I have a pet canary
I have a pet goldfish
I have a pet rock
```

The for pet in pets syntax means that a loop will be performed for each item in the list pets. In order, the item is taken from the list pets, assigned to the variable pet, which can be used within the loop. Anything that is considered a Python sequence can be used after the in. This includes lists, strings, tuples, arrays and anything else (including user-defined objects) that satisfy certain sequence requirements (actually, it's more general than that, iterator objects, not described here can be use used as well). In fact, the exact same approach is used for performing "counted" loops:

```
>>> for i in range(3): print i
0
1
2
```

The function range(n) effectively generates a list of n integers starting at 0 (it's the analog of arange(n)). It turns out that it doesn't actually generate a list that long (so worries about using up lots of memory for performing a large number of loops are unfounded).

### 3.4.2 Blocks of code, and indentation

The form of having the code looped over on the same line as the for statement is atypical. Normally the statements being looped over follow on separate lines. So what is used to delimit these blocks? Begin/end statements like IDL? Curly braces ({}) like C and Java? No, nothing other than simple indentation. When code following a statement that expect a block of code (such as for) is consistently indented more than the statement starting the block, it is considered to identify the block of code. For example:

```
>>> for i in range(3):
...     x = i*i
...     print x
...
0
1
4
```

Note that when one is in interactive mode, that using a statement that starts a block causes the interpreter to prompt with ... and typing an empty line terminates the block (that's not necessary within scripts or programs, returning to a previous level of indentation or ending the file is sufficient). The amount of indentation is entirely up to you. It can be 1 space or 40, so long as it is consistent. Tabs may be used, but their use is not recommended. If you do use them, use only tabs for indentation. A mixture of tabs and spaces is bound to cause confusion since different tools show tabs with varying amounts of equivalent spaced. Most sensible editors allow tabs to be automatically converted to spaces with the appropriate configuration (the next tutorial will provide information about editors and available features for Python).

This aspect of Python astonishes some, but most that actually try it find it refreshing. The structure that you see is the real structure of the program. Cutting and pasting such code into different levels of indentation is not usually a problem if you use an editor that supports changing indentation for multiple lines of code.

### 3.4.3 Python if statements

Python if statements are simple:

```
>>> x = 0
>>> if x==0:
...     print "x equals 0"
...
x equals 0
```

The if statement allows optional elif (short for "else if") and else clauses:

```
>>> if x==1:
...     print "x equals 1"
... elif x==0:
...     print "x equals 0"
... else:
...     print "x equals something other than 1 or 0"
...
x equals 0
```

### 3.4.4 What's True and what's False

Python now has explicit `True` and `False` values. But it also has standard rules for determining what is considered true and false for other data types. Numeric data types are considered false if equal to 0 and true for all other values. The Python value `None` is always considered false. Empty sequences and dictionaries are considered false (e.g., the empty string).

```
>>> if '': print 'True' # nothing will be printed
...
>>> if '0': print 'True'
...
True
```

As for user-defined objects, Python permits the code to define what is true or not. Or whether a test for truth is even permitted; numpy arrays may not be used as truth values in most cases:

```
>>> from numpy import *
>>> x = arange(9)
>>> if x: print 'True'
[...]
ValueError: The truth value of an array with more than one element is ambiguous. Use a.any() or a.a
```

Error!

### 3.4.5 The in crowd

Another use for the in operator encountered in the for statement is as a test of whether an object is a member of a sequence. This can considerably simplify logical tests as the following example shows.

```
>>> if x in ['dog', 'cat', 'goldfish', 'gerbil', 'canary']: print x
```

## 3.5 Advanced PyFITS Topics

[This section can be skipped by non-astronomers]

The PyFITS functions introduced in the first tutorial are sufficient for simple manipulation of FITS files, but if you need to have more control over the handling of the FITS file, you will need to use some of the more advanced features of the module.

### 3.5.1 Header manipulations

Normally most people will find the means of using and updating headers described in the first tutorial sufficient for most tasks. There are more methods available for header objects that allow adding commentary keywords (HISTORY, COMMENT, or 'blank' keywords). The following show their use.

```
>>> hdr = pyfits.getheader('pix.fits')
>>> hdr.add_history('This is a test history card')
>>> hdr.add_comment('A test comment card',after='date')
>>> hdr.add_blank('',before='comment')
# To delete a keyword just use the del statement
>>> del hdr['date']
```

Note that while headers behave in a number of respects like dictionaries, they aren't dictionaries and don't support all dictionary methods.

To have complete control over header cards and their placement of header cards it is necessary to access the header as a "cardlist" object. With this representation one can use list manipulations to place each card as desired, and use card methods to control the exact contents of any card. By this interface it is possible to make the card use any string desired, even if it is not legal FITS or one of the standard conventions (to write such illegal cards into an output file requires specifically instructing the `writeto` method or function to force illegal cards into the file; see the following section on noncompliant FITS data).

See the PyFITS documentation for the full set of methods and examples of use.

### 3.5.2 PyFITS Object Oriented Interface

The object oriented interface permits more flexible handling of FITS files. The object functionality mirrors that available from the functions. The chief advantages are:

- Files are not repeatedly opened and closed for each data access (but the objects should be explicitly closed now with the close() method).
- Allows creating FITS headers from scratch (i.e., not having to use an existing file's header).
- There is more flexibility in how data are accessed. One can easily determine how many extensions exist and access all the headers directly without making many `getheader` function calls.

As for the latter, it is possible to read just portions of an image from disk (rather than reading the whole image), and it is possible to open files using memory mapping as a data access mode. Consult the *PyFITS User's Guide* for details on how to do both of these.

Simple example:

```
>>> hdus = pyfits.open('fuse.fits') # returns an HDUList object
>>> tabhdu = hdus[1] # the table extension
>>> hdr = tabhdu.header # getting the header from the HDU
>>> tab = tabhdu.data   # and the table
```

The data attribute of the HDU object contains the data regardless of the type of extension (a record array for tables, a simple array for image extensions). The `HDUList` may be indexed by number or by extension name (and optionally EXTVER). For example:

```
>>> hdus = pyfits.open('acs.fits')
>>> sci = hdus['sci',1] # EXTNAME=SCI, EXTVER=1
```

HDULists can be written to a new file, or updated if the file was opened in update mode.

```
>>> hdus.writeto('temp.fits') # write current form to new file
>>> hdus.flush() # update opened file with current form
```

### 3.5.3 Controlling memory usage

Offhand, it sounds convenient to read a whole FITS file into memory as an `HDUlist` in one step, but some may wonder about the demands this puts on memory. If the file is memory mapped, then that isn't a problem. However, if the default mode of using regular I/O to read FITS files is being used it turns out that only the headers are loaded. Until one actually refers to the `data` attribute the data are not read into memory (it's done with smoke and mirrors). By using this, it is possible to control what is in memory. The following illustrates how (the next tutorial unveils some of the details of how memory is handled in general in Python).

```
>>> ff = pyfits.open('nicmos.fits')
>>> sum = 0.  # plan is to sum all SCI extension images
>>> for hdu in ff[1:]: # skip primary
...     if hdu.header['extname'].startswith('SCI'):
...         sum = sum + hdu.data # now data is read in
...         hdu.data = None # done with it, delete it from memory
>>> ff.close()
```

If the images are too large to comfortably process in memory, the `section` attribute can be used to read subsets of the image. An example that sums all the values in sections of an image without loading it all in memory at once:

```
>>> ff = pyfits.open('pix.fits') # returns an HDUList object
>>> hdu = ff[0] # Get first (and only) HDU
>>> sum = 0L # for keeping a running sum of all image values
>>> # now read data 64 lines at a time (although small, it illustrates the principle)
>>> for i in range(8):
...     subim = hdu.section[i*64:(i+1)*64,:]
...     sum = sum + subim.sum()
...
>>> print sum
>>> ff.close()
```

This can be done more elegantly using image iterators described later.

`HDULists` can be created and manipulated entirely in memory without any reference to any input or output files.

PyFITS is also capable of handling variable-length table entries, random groups, and ascii table extensions.

### 3.5.4 Support for common FITS conventions

PyFITS supports the CONTINUE convention automatically on reading files that use it (this permits the use of string values longer than permitted in a standard card). To enable its usage in a header just provide string values to keywords that are longer than standard FITS allows. The HIERARCH convention is now supported. The INHERIT convention is not supported. It is not planned to be in the base pyfits module but some convenience functions or objects may be provided in the future to support it.

### 3.5.5 Noncompliant FITS data

Normally PyFITS tries to handle FITS files that don't meet the FITS standard as best it can when reading them in (and make the most reasonable interpretations possible of any ambiguities). (If users encounter problems in this regard, particularly with FITS data that is widely used, please let us know so we can adjust PyFITS to handle it). In contrast, PyFITS normally takes a very strict view toward the FITS files it writes. By default, PyFITS will not permit non-compliant FITS files to be written. When the errors in the input file have obvious corrections, PyFITS will automatically make these corrections in writing the header to a new file with either of the fix options (e.g., `output_verify='fix'` or `output_verify='silentfix'`. When there is ambiguity about what should be done, PyFITS will raise an exception. It is possible to change this behavior, i.e., to warn or raise errors on bad input files, and to permit FITS non-compliant headers to be written. Some illustrations:

```
>>> hdu = pyfits.PrimaryHDU() # create an HDU from scratch
>>> hdu.header.update('P.I.','Hubble') # Try creating an illegal keyword
ValueError: Illegal keyword name 'P.I.'
# force into header an illegal keyword
>>> card = pyfits.Card().fromstring("P.I.      = 'Hubble'")
>>> hdu.header.ascardlist().append(card)
>>> hdu.writeto('pi.fits') # try writing to file
Output verification result:
HDU 0:
    Card 4:
        Unfixable error: Illegal keyword name 'P.I'
[...]
      raise VerifyError
```

```
VerifyError
# now force it to file
>>> hdu.writeto('pi.fits', output_verify='ignore')
>>> hdus = pyfits.open('pi.fits')
>>> print hdus[0].header.ascardlist()
[...]
P.I.      = 'Hubble'
>>> hdus[0].header['p.i.']
'Hubble'
>>> hdus.verify()
[repeat of previous error message]
```

The `verify()` method (and the `output_verify` keyword) has the possible values of: `'ignore'`, `'fix'`, `'silentfix'`,`' exception'` (default for output), and `'warn'`.

## 3.6 A quick tour of standard numpy packages

The standard numpy distribution comes with auxiliary modules that will be quickly outlined here (all these are described in considerably more detail in the numpy book). There are also a vast number of modules availble in the scipy package that will not be covered here.

### 3.6.1 random

The random module is used to generate arrays of random values with a variety of distributions as well as seed-related functions. The following lists the available functions with a couple examples at the end. Functions that return random values all take a shape argument for the desired array shape.

`set_state`(*state*): sets the state of the random number generator (as gotten from get_state). This allows one to repeat random sequences for testing purposes.

`get_state`(): return the current state used by the random number generator

`rand`(*d1,d2,...,dn*): returns Float array of uniformly distributed random numbers between 0. and 1 (not including) with shape (d1, d2,...,dn).

`random`(*shape*): variant on rand that takes a shape tuple.

`uniform`(*low=0., high=1., size*=None): returns uniformly-distributed Float values between specified low and high (which themselves may be arrays)

`randint`(*min, max, shape=[]*): like uniform, but returns int values.

`permutation`(*n*): returns all n values from 0 to *n*-1 with order randomly permuted

`shuffle`(*sequence*): Randomly permute the items of any sequence. Array argument must be 1-D.

Other supported distributions are: (Float) `beta, chi_square, exponential, f, gamma, gumbel, lapace, lognormal, logistic, multivariate_normal, noncentral_chisquare, noncentral_f, normal, pareto, power, randn, rayleigh, standard_cauchy, standard_exponential, standard_gamma, standard_normal, standard_t, triangular, vonmises, wald, weibull,` and (Int) `binomial, geometric, hypergeometric, logseries, multinomial, negative_binomial, poisson, zipf.` In general, the parameters for these distributions may be arrays.

Examples:

```
>>> import numpy.random as ran
>>> ran.rand(3,3) # trivial example
```

Example of generating a Poisson noise image of a Gaussian PSF

```
>>> y, x = indices((11,11))
>>> y -= 5 # example of “augmented operator, subtract 5 from y and place result in y
>>> x -= 5
>>> im = 1000*exp(-(x**2+y**2)/2**2) # noiseless gaussian
>>> nim = ran.poisson(im)
>>> print nim
```

### 3.6.2 fft

This provides the common FFT functions:

`fft`(*a, n=None, axis=-1*): Standard 1-d fft (applies fft only 1-dimension of multidimensional arrays)

`ifft`(*a, n=None, axis=-1*): Standard inverse 1-d fft

`rfft`(*a, n=None, axis=-1*): Only accepts real inputs and returns half of the symmetric complex transform.

`irfft`(*a, n=None, axis=-1*): Only accepts real inputs and returns half of the symmetric complex transform.

**`fftshift(`***x, axes=None*): Shift 0-frequency component to center of spectrum

**`ifftshift(`***x, axes=None*): Reverse of fftshift

**`fftfreq(`***n,d=1.0***):** Return the DFT sample frequencies

`fft2`(*a, s=None, axes=(-2,-1)*): 2-d fft.

**`ifft2(`***a, s=None, axes=(-2,-1)*): 2-d analog of ifft

`rfft2`(*a, s=None, axes=(-2,-1)*): 2-d analog of rfft

**`fftn(`***x, s=None, axes=None*): N-dimensional fft of x

**`ifftn(`***x, s= None, axes=None*): inverse of fftn

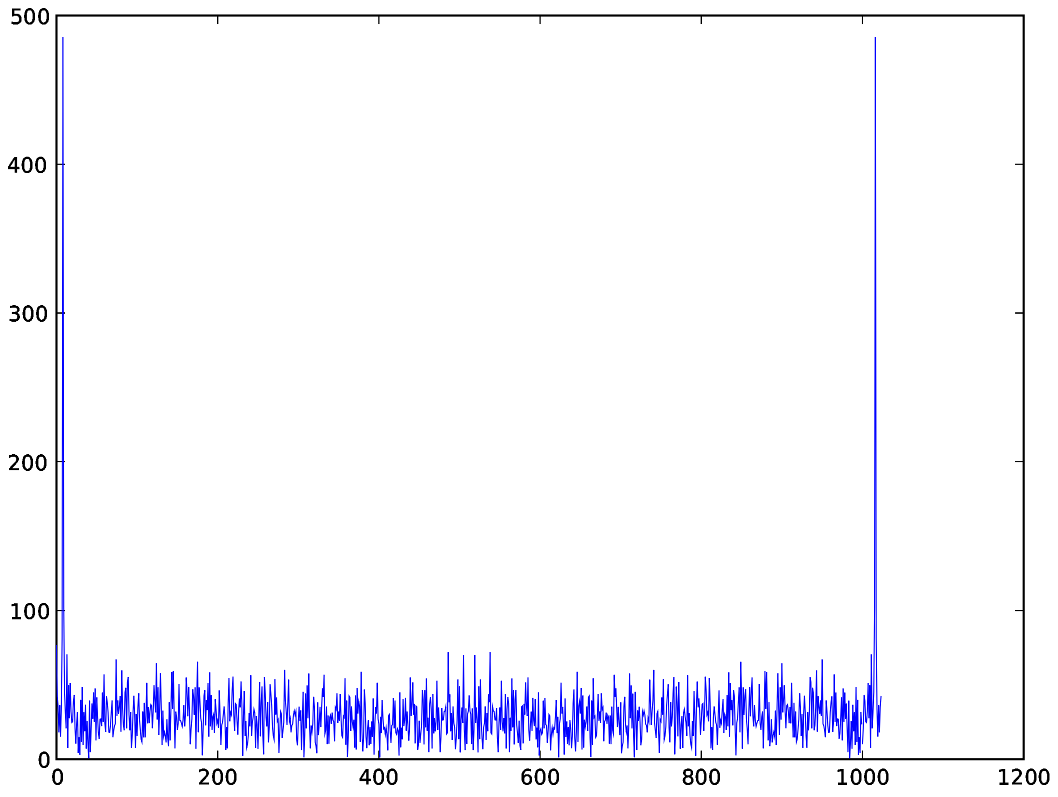
**`irfftn(`***x, x=None, axes=None*): N-dimensional analog of rfft

**`hfft(x,`** n=None, axis=-1): n-point real-valued fft from first half of Hermitian-symmetric data

**`ihfft(x,`** n=None, axis=-1): inverse of hfft

Example:

```
>>> from numpy.fft import fft
>>> x = sin(arange(1024)/20.) + ran.normal(0,1,size=1024)
>>> # sine wave with gaussian noise
>>> from pylab import *
>>> plot(abs(fft(x)))
```



### 3.6.3 convolve

The convolve package is not part of numpy but instead is part of scipy.stsci; since it contains operations frequently used by astronomers it is described here. This package is included with the stsci_python distribution so that it is not necessary to install scipy in order to use it. This includes the following smoothing and correlation functions:

`boxcar`(*data, boxshape, output=None, mode='nearest', cval=0.*): standard 1-d and 2-d boxcar smoothing.

`convolve`(*data, kernel, mode=FULL*): 1-d convolution function

`convolve2d`(*data, kernel, output=None, fft=0, mode='nearest', cval=0.*): 2-d convolution with option to use FFT.

`correlate`(*data, kernel, mode=FULL*): 1-d correlation function

`correlate2d`(*data, kernel, output=None, fft=0, mode='nearest', cval=0.*): 2-d correlation function with option to use FFT

These functions have various options that determine the size of the resulting array (`FULL, PASS, SAME, VALID`)

### 3.6.4 linear algebra

This includes the common linear algebra operations. The module is `numpy.linalg`. The functions available are (details and examples in numpy book):

`cholesky`(*a*): Cholesky decomposition

`det`(*a*): determinate

`eigvals`(*a*): return all eigenvalues of matrix a

`eig`(*a*): return all eigenvalues, eigenvectors of matrix a

`eigvalsh(`*u*`):` same as eigvals but expects hermitian matrix

`eigh(`*u*`):` same as eig but expects hermitian matrix

`generalized_inverse`(*a, rcond=1e-10*): aka pseudo-inverse or Moore-Penrose inverse

`Heigennvalues`(a): the real positive eigenvalues of a square, Hermitian positive definite matrix.

`Heigenvectors`(*a*): likewise, the eigenvalues and eigenvectors for Hermitian matrices

`inv`*a*): Inverse of a

`lstsq`(*a, b, rcond=1e-10*): Linear least squares.

`pinv(`*a*`):` psuedo inverse of a

`solve`(*a, b*): Find solution to linear equation defined by ax = b

`svd`(*a, full_ matrices=0*): Singular Value Decomposition of a

`tensorinv(`*a, ind=2*): Find tensor inverse of a

`tensorsolve(`*a, b, axes=None*): Find solution to multi-index linear equation

### 3.6.5 Masked Arrays

The masked array facility allows associating data masks with arrays that will be appropriately propagated when using ufuncs (though many of the add-on modules, e.g., `fft` or `matplotlib`, will not handle the masks implicitly). The use of masks impacts performance (and memory as well), but can be handy if systematic use of masks is required. Note that use of IEEE-754 special values (e.g., Inf, NaNs) can be a faster way of representing bad data values. See section 3.6.7.

The masked array facility is found in `numpy.ma`. The details of its use are too long to describe here. Only a simple example will be shown.

```
>>> from numpy import *
>>> x = arange(3) # regular array
>>> y = ma.array([1, 2, 3], mask = [0, 1, 0]) # masked array, 2nd element invalid
>>> x+y
array(data =
[      1 999999     5],
mask =
[False True False],
     fill_value=999999)
```

Details of its use can be found in the *Guide to Numpy* book (Section 8.6).

### 3.6.6 ieespecial values

This capabilities are now part of core numpy; there are several tools for handling IEEE-754 special floating point values (NaNs, Inf, etc.). You can test whether an array has any of these values (and generate a mask array showing the locations), and to set locations in an array to these values. See the *Guide to Numpy* book for details on these functions (Sections 9.1.4, 9.5.5) A brief overview is given here regarding special values. Note that one should not use typical equality tests for NaN values since the IEEE standard requires that two floats that have NaN values ***are not considered equal*** when compared. Thus you ***must*** use special functions to do such comparisons. For example:

```
>>> x = arange(3.)
>>> y = x / 0
Warning: divide by zero encountered in divide
Warning: invalid value encountered in double_scalars
>>> y
array([ nan, inf, inf])
>>> isinf(y)
array([False, True, True], dtype=bool)
>>> isnan(y)
array([ True, False, False], dtype=bool)
>>> isfinite(y)
array([False, False, False], dtype=bool)
```

But note that you should not do this to find NaN values:

```
>>> y == nan
array([False, False, False], dtype=bool)
```

To set special values, simply use assignment:

```
>>> x = arange(6.)
>>> x[[1,3]] = nan
>>> x[0] = inf
>>> x
array([ inf, nan, 2. , nan, 4. , 5. ])
```

### 3.6.7 Customizing numeric error handling

The default behavior of numpy is to print warnings when numerical errors are encountered in computations but not to stop or raise an exception. It is possible to change this, however. One can use the `seterr` function to do this as the following examples illustrate:

```
>>> x = arange(3.)
>>> y = x/0
Warning: divide by zero encountered in divide
Warning: invalid value encountered in double_scalar
>>> oldsettings = seterr(all='ignore')'
>>> y = x/0
```

The return value of seterr is a dictionary that holds the previous values. To reset them simply do:

```
>>> seterr(**oldsettings) # the odd syntax will be explained later
                          # when defining functions is covered
{'divide': 'ignore', 'invalid': 'ignore', 'over': 'ignore', 'under': 'ignore'}
>>> y = x/0
Warning: divide by zero encountered in divide
Warning: invalid value encountered in double_scalars
```

This example showed how to change the behavior for all error types. It is possible to set each error type behavior individually: divide (divide by 0 errors), invalid (computations that produce NaN), underflow, and overflow. The possible choices for each are: `'ignore'`, `'warn'` (print a warning), `'raise'` (raise an exception), or `'call'` (call a user-supplied function). For example:

```
>>> seterr(divide='warn', invalid='raise', underflow='ignore', overflow='call')
```

This will thus result in exceptions if any NaNs are produced, a warning if divide by 0 occurs, nothing if underflows are encountered, and finally, it will call the user supplied function that was set with `seterrcall()` if an overflow was encountered (see the *Guide to Numpy* for details, section 9.1.4). Note that this seterr also affects the behavior with integer computations with regard to divide by 0.

## 3.7 Intermediate numarray topics

### 3.7.1 The Zen of array programming

The trick to making Python data processing efficient for large data sets is the avoidance of loops over small amounts of data (or worse, individual array points). Not that you can't do it. By all means, go ahead. But don't be surprised if the program runs very slowly. Since Python is interpreted, there is a certain overhead to each interpreted Python statement. Efficiency is achieved by avoiding large number of repetitions of Python statements that do relatively little work and instead using operations that operate on the whole array. The following is a simple illustration using the data from `pix.fits`.

```
>>> im = pyfits.getdata('pix.fits')
>>> # Using the Fortran or C approach
>>> sum = 0L
>>> for j in range(512):
...     for i in range(512):
...         sum = sum + im[j, i] # remember that index order!!
print sum
28394234
>>> Using the array approach
>>> print im.sum()
28394234
```

The time taken by the first is over 30 times longer than the second.

Avoiding loops requires a different mindset. Some algorithms are relatively easy to code in an array formulation, others are not quite as easy, and some are very difficult. At some point the complexity of avoiding loops is not worth the trouble and consideration should be given to accepting the overhead of loops or writing the algorithm in C. The skill of avoiding loops is a somewhat acquired art and it helps to see lots of examples to learn all the tricks that are involved. Those experienced at using IDL are likely familiar with most of the techniques. Most of the existing array functions are there to facilitate the avoidance of loops. By far, the most useful function in this regard is `where()`. The solutions to more advanced examples will show examples of some of the techniques.

### 3.7.2 The power of mask arrays, index arrays, and where()

The simplest and usually the most efficient way of conditionally operating on a subset of points is to use mask arrays (i.e., Boolean arrays). One can use such mask arrays as an index into an array. For example, to set all points in `im` that are greater than 100 to 100:

```
>>> im[im>100] = 100
```

In a similar vein the following will select all those values greater than 100 and generate a new array of those values:

```
>>> bigvalues = im[im>100]
```

The following illustrates how to use mask arrays to do a crude cosmic ray rejection algorithm (i.e., for non-astronomers, rejecting pixels that have much higher values than are found in other exposures of the same target):

```
>>> bigdiffmask = abs(im1-im2) > nsigma*sqrt(min(im1, im2))
```

The mask can now be used to set the values of the image with the larger value to the value of the other image.

```
>>> im1mask = bigdiffmask & (im1>im2)
>>> im1[im1mask] = im2[im1mask]
>>> im2mask = bigdiffmask * (im2>im1)
>>> im2[im2mask] = im1[im2mask]
```

Some problems need use of explicit index arrays instead, either because some functions only return index arrays (E.g., `argsort()`) or the indices will be manipulated or processed in some way. As previously mentioned, index arrays can be used as indices as well (hence their name!). The `where()` function is used to turn a mask into index arrays.

Use with one-dimensional arrays is the most straightforward. What isn't quite so obvious is that `where()` does not return an array, but rather a tuple of arrays (the reasons for this are explained a little bit later). Thus to manipulate the array(s) returned by where, one needs to index the tuple with the appropriate index. This isn't necessary if the tuple is to be used as an index to another array. To take a very simple example:

```
>>> x = arange(10)
>>> ind = where(x > 5)
>>> x[ind] # this works
array([6, 7, 8, 9])
>>> ind.shape # this doesn't
[...]
AttributeError: 'tuple' object has no attribute 'shape'
>>> ind
(array([6, 7, 8, 9],)
>>> ind[0].shape # this does
(4,)
>>> len(ind) # this is effectively the number of dimensions
1
>>> len(ind[0]) # this is the number of points and is likely what was desired
4
```

Having `where()` return tuples of arrays is more awkward in the 1-d case, however, it is the most natural solution for multidimensional arrays, and there is the side benefit that 1-d and $n$-d arrays are handled the same way. No doubt that new users will bump into this issue at least a few times.

When multidimensional arrays are used, where() returns an index for each dimension as part of the tuple. So, using the standard M51 image data:

```
>>> indices = where(im > 300)
>>> indices
(array([ 31,  31,  32, ..., 505, 506, 506]),
 array([319, 320, 318, ..., 208, 206, 207]))
>>> im[indices[0], indices[1]]=300 # the explicit approach of using
                                   # the component index arrays
>>> im[indices] = 300 # the "magic" approach, exactly equivalent to the explicit form
```

The examples that follow will illustrate how mask and index arrays may be used to avoid explicitly looping over all elements in an array. You may note that in many cases one could use index or mask arrays. Generally speaking, if mask arrays will do, use them instead. Only when index arrays are much smaller than the original arrays will they be faster than using a mask array.

### 3.7.3 1-D polynomial interpolation example

We expect interpolation routines to soon become available so the following example should not be necessary to follow to do interpolation. But it remains a good illustration of how it is possible to avoid looping over array elements. Suppose one has a pair of arrays that represent x,y functional pairs. The `x` array represents x samples for some smooth function and the `y` array are the values of that function at those x values. We presume that the x values are in increasing order (if they weren't already, use of sort functions could easily reorder the x and y arrays to make that so). Given a third array, `xx`, of x values for which interpolated values of the function are desired, determine the interpolated values. To keep it reasonably simple, this example will use linear interpolation.

```
>>> x = arange(10.)* 2
>>> y = x**2
>>> import numpy.random as ran
>>> xx = ran.uniform(0., 18., size=(100,)) # 100 random numbers between 0 and 18
>>> xind = searchsorted(x, xx)-1 # indices where x is next value below that in xx
>>> xfract = (xx - x[xind])/(x[xind+1]-x[xind]) # fractional distance between x points
>>> yy = y[xind] + xfract*(y[xind+1]-y[xind]) # the interpolated values for xx
```

The same approach can be generalized to higher-order interpolation functions or multiple dimensions.

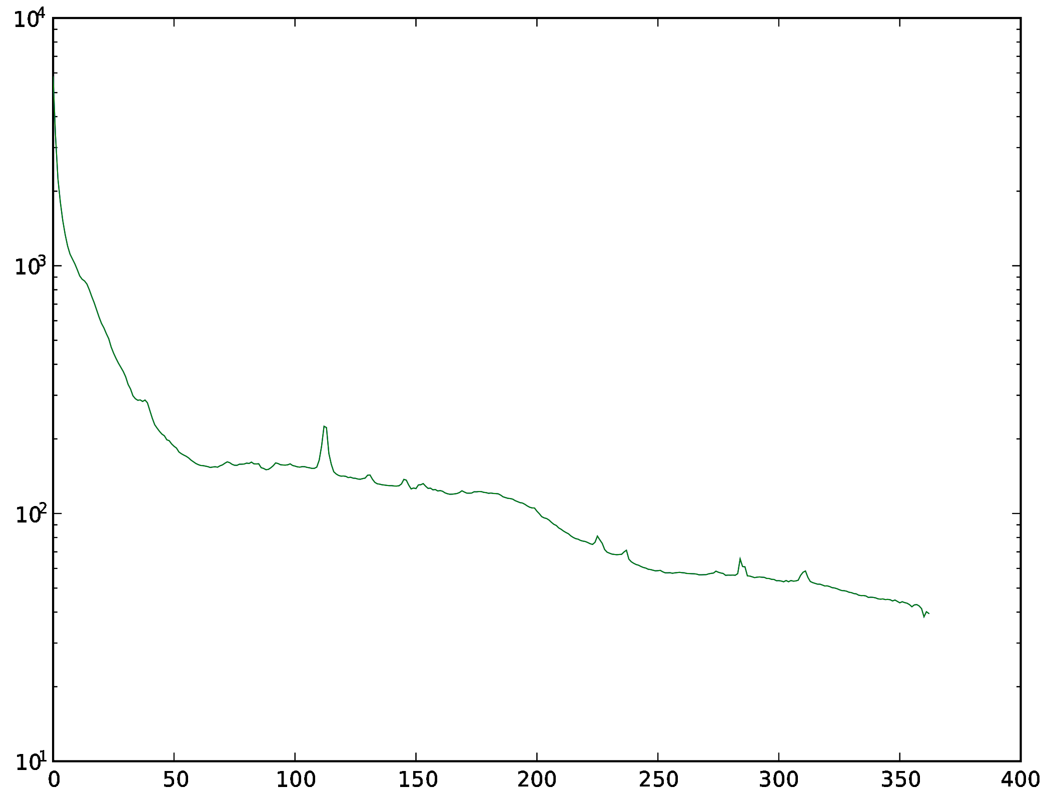
### 3.7.4 Radial profile example

Suppose one wants to compute the average radial profile for a galaxy (say, M51). The basic problem is to bin image values into radial distance bins and average all the values that fall into the same bin. How can one average all the values at the same radial bin without looping through all radial values? The following shows a way that is faster (but not as fast as one could do in C).

```
>>> y, x = indices((512,512)) # first determine radii of all pixels
>>> r = sqrt((x-257.)**2+(y-258)**2)
>>> ind = argsort(r.flat) # get sorted indices (could use sort
                          # if not needed to arange image values too
>>> sr = r.flat[ind] # sorted radii
>>> sim = im.flat[ind] # image values sorted by radii
>>> ri = sr.astype(int16) # integer part of radii (bin size = 1)
```

Things get trickier here; find numbers in same radius bin by looking for where radius change value and determining distance between changes

```
>>> deltar = ri[1:] - ri[:-1] # assume all radii represented
                              # (more work if not)
>>> rind = where(deltar)[0] # location of changed radius
>>> nr = rind[1:] - rind[:-1] # number in radius bin
>>> csim = cumsum(sim, dtype=float64) # cumulative sum to figure out sums for each radii bin
>>> tbin = csim[rind[1:]] - csim[rind[:-1]] # sum for image values in radius bins
>>> radialprofile = tbin/nr # the answer
>>> semilogy(radialprofile)
```



Well, almost. A careful look at what happens shows that the 0 pixel radius bin is excluded from the final array. It isn't hard to prepend the single value to radial profile.

This is a case where doing it with array operations isn't a great deal simpler than it would be in C. Performance isn't as good largely because of the cost of doing a sort on radius values (not necessary in C). On the other hand, you don't need to learn C, don't need to deal with the hassles of compiling and linking (particularly if you want to share the code), don't need to deal with pointer errors in C, and so forth. So it is often still desirable to solve problems this way.

### 3.7.5 Random ensemble simulation example

Given a coin, what are the odds of tossing 2 heads in a row before 2 tails given respective probabilities of p and q for heads and tails? This can be computed analytically, but serves as a reasonably simple example of a Monte-Carlo simulation that can be done with arrays. The general approach to solving this problem is to iterate over every coin toss, but to start with an ensemble of coins. As the iteration continues, some of the coins will hit one or the other termination condition and fewer cases will remain to iterate. For this case, it is necessary to keep the state of the previous coin toss.

```
>>> p = .4
>>> n = 1000000 # initial ensemble size
>>> n2heads = 0; n2tails = 0 # totals for each case
>>> import numpy.random as ran
>>> prev = ran.rand(n) < p # true if heads, false if not
>>> while n>0:
...     next = ran.rand(n) < p
...     notdone = (next != prev)
...     n2heads += sum(prev & next,dtype=int64) # careful about sums!
...     n2tails += sum(logical_not(prev | next),dtype=int64)
...     prev = next[notdone]
...     n = len(prev)
...     print n
...
480311
239661
[...]
1
1
0
>>> n2heads, n2tails
(336967, 663033)
```

This works efficiently so long as many points remain. For the last few iterations where there are few points, the overhead of doing array computations will increase inefficiency. So long as there are relatively few of these, this algorithm should have speeds comparable to those of C. (By the way, the analytically-derived probability is $p^2(1+q)/(1-pq)$.)

### 3.7.6 thermal diffusion solution example

The following shows how one can apply an iterative solution for Laplace's equation. We construct a 500x500 grid and set a 100x100 pixel boundary condition of 100 at the center and 0 at the edges.

```
>>> grid = zeros((500,500),float32)
>>> prevgrid = grid.copy()
>>> grid[200:300,200:300] = 100.
>>> done = False
>>> i = 0
>>> while not done:
...     i +=1
...     prevgrid[:,:] = grid # just reuse arrays
...     # new value is average of 4 neighboring values
...     grid[1:-1,1:-1] = 0.25*(
...         grid[:-2,1:-1]
...       + grid[2:, 1:-1]
...       + grid[1:-1,:-2]
...       + grid[1:-1,2:])
...     grid[200:300,200:300] = 100.
...     diffmax = abs(grid - prevgrid).max()
...     print i, diffmax
...     if diffmax < 0.1: done = True
1 25.0
2 12.5
[...]
243 0.0996131896973
```

### 3.7.7 Finding nearest neighbors

Suppose one has a list of coordinates (lets presume simple $x$,$y$ Cartesian) and we want to find the nearest coordinate to each of the coordinates in the list. If the coordinates are provided as $x$, $y$ arrays of equal length it is possible to use broadcasting to do this quite easily:

```
>>> x = array([1.1, 1.8, 7.3, 3.4])
>>> y = array([2.3, 9.3, 1.5, 5.7])
>>> deltax = x - reshape(x,(len(x),1)) # computes all possible combinations
>>> deltay = y - reshape(y,(len(y),1)) # could also use subtract.outer()
>>> dist = sqrt(deltax**2+deltay**2)
>>> dist = dist + identity(len(x))*dist.max() # eliminate self matching
>>> # dist is the matrix of distances from one coordinate to any other
>>> print argmin(dist, axis=0) # the closest points corresponding to each coordinate
[3 3 3 1]
```

This approach works well so long as there aren't too many points (since it creates arrays that have that number squared entries)

### 3.7.8 Cosmic ray detection in single image

This example uses a local STScI package and `ndimage` to identify cosmic rays (ndimage is part of scipy.stsci but is also available in stsci_python)

```
>>> import imagestats
>>> import pyfits
>>> import ndimage as nd
>>> chip = pyfits.getdata('acs.fits','sci',1)
>>> # Perform morphological closing and opening to filter image of any
>>> # source smaller than (5,5).
>>> # A size of (3,3) still left some residuals for ACS data
>>> closechip = nd.grey_closing(chip,size=(5,5))
>>> occhip = nd.grey_opening(closechip,size=(5,5))
>>> # compute sigma of background
>>> sigma = imagestats.ImageStats(occhip,nclip=3).stddev
>>> # create mask using difference between original input and filtered image.
>>> mask = (chip - occhip) > sigma
```

### 3.7.9 Source extraction

Extract magnitudes and positions of sources in image (similar to `daofind`)

```
>>> import pyfits
>>> import imagestats
>>> import ndimage as nd
>>> sci, hdr = pyfits.getdata('acs2.fits','sci',1,header=True)
>>>
>>> # compute background value, clipping out bright sources
>>> scistats = imagestats.ImageStats(sci,nclip=3)
>>>
>>> # create a binary image flagging all sources in image
>>> # with values greater than the mean of the background
>>> # For crowded fields, extra care/work will need to be
>>> # done to separate blended sources.
>>> sci_clip = sci >= scistats.mean
>>>
>>> label each source with its own ID index
>>> sci_labels,sci_num = nd.label(sci_clip)
>>>
>>> # Compute a sum for each object labeled and return as a list
>>> counts = nd.sum(sci,sci_labels,range(sci_num))
>>>
```

```
>>> # Get position of object using its center of mass
>>> pos = nd.center_of_mass(sci,sci_labels,range(sci_num))
>>>
>>> # Retrieve photometric keywords from image header
>>> photflam = hdr['photflam']
>>> photzpt = hdr['photzpt']
>>> # Convert counts to magnitudes for each object
>>> mag = photzpt - 2.5*log10(array(counts)*photflam)
```

### 3.7.10 Other issues regarding efficiency and performance

Even if a problem can be cast into a purely array manipulation form, one may encounter other barriers to performance. The most likely is that you will run into memory limitations. If the algorithm involves computations on large arrays, and many temporary or ancillary arrays are needed as part of the computation, then one can easily run out of available memory, or if not virtual memory, real memory, leading to unacceptable system paging. If the algorithm essentially is "ufunc"-like, that is computations are performed independently on pixels, then the array can be segmented and iterated over the segments. For two dimensional arrays in IDL this typically meant iterating over rows in images. That can be done in numarray as well, but there are other approaches that can be used. Even when algorithms are not strictly independent of neighboring pixels, so long as the algorithm is reasonably local, then one can iterate over segments that overlap to the necessary degree. Many problems fall in this category. A solution of this sort will be illustrated in tutorial 4.

Some algorithms result in many array creations and destructions. Even though in theory no memory is being consumed over the long run, it is possible to eventually fragment the available memory as to prevent allocating arrays of sufficient size (this is a problem with IDL and many other systems as well). In such cases it makes sense to reuse existing arrays (if sizes don't change) in iterations. This can be done by assigning to an existing array through slice assignment. For example:

```
>>> im = 2*im # replaces the array im used to refer to
              # with a new array
>>> im[:,:] = 2*im # writes back into the array im
>>> im *= 2 # also reuses im array
            # (but be careful of type downcasts!)
>>> multiply(im, 1, im) # use of optional output array
```

### 3.7.11 Customizing numeric error handling

By default, numarray notices if any numerical errors have occurred and warns you. It is possible to change that behavior for each kind of error individually for for all (divide-by-zero, invalid result, overflow, and underflow). There are three choices: ignore (no warnings), warn (print a warning), or raise (raise an exception). This works for integers as well as floats and complex numbers. See the numpy book for details on how to change the default behavior (section 9.1.4, 9.55)

## Exercises

1. Read each of the image extensions in the FITS file `tut3f1.fits` using the object-oriented interface, assemble an image cube from the 2-d images in each of the extensions (they are all the same size), and without loops, generate a 2-d result that contains the maximum value at that pixel for the whole stack of images. Display the result. The answer will be obvious if you did it correctly.

2. Add the keyword/value pair `IMNUM=` <extension number> to each of the headers `tut3f1.fits` right after the TARGET keyword. While you are at it, add a history keyword. Verify the headers have been updated with your favorite FITS header viewing tool (i..e, not PyFITS)

3. Using the random number module, generate a million random points with $x$,$y$ coordinates between 0,1. What fraction of these points lie within a radius of 1 from the origin? How close is this to the expected result?

4. The irregularly sampled Discrete Fourier Transform (DFT) is given by

$$F(\omega) = \sum\nolimits_{n=0}^{N-1} f_n e^{-i\omega n \Delta t}$$

   Given an array of time samples $f_n$, desired frequencies to sample $\omega_m$(not necessarily uniformly spaced), and$\Delta t = 1$ compute the DFT at those frequencies without using any loops.

# 4 Programming in Python

## 4.1 Introduction

This tutorial will focus on writing Python programs and scripts that can be used to aid or augment interactive analysis. If you find yourself repeating the same pattern of commands more than a few times, or need to write an algorithm that involves more than a few lines of Python, it would be silly not to write a script or function to do the same.

### 4.1.1 Namespaces

First, let's have a quick look under the hood. When you start up Python, there are a few environmental objects set up that you can interrogate with the `dir()` function.

```
>>> dir()
['__builtins__', '__doc__', '__name__']
```

As you can see, the `dir()` function returns a list of 3 items. The contents of the strings are:

```
__builtins__    is a module
__doc__         is of type NoneType
__name__        is a string
```

The`__name__` object is just a character string, which we can print out:

```
>>> print __name__
__main__
```

So when we're running the Python interpreter, `__name__ = '__main__'`. Remember this.
Since`__builtins__` is a module, we can find out its attributes by using the `dir()` function:

```
>>> dir(__builtins__)
['ArithmeticError', 'AssertionError', 'AttributeError',
'DeprecationWarning', 'EOFError', 'Ellipsis', 'EnvironmentError',
'Exception', 'False', 'FloatingPointError', 'FutureWarning',
'IOError', 'ImportError', 'IndentationError', 'IndexError',
'KeyError', 'KeyboardInterrupt', 'LookupError', 'MemoryError',
'NameError', 'None', 'NotImplemented', 'NotImplementedError',
'OSError', 'OverflowError', 'OverflowWarning',
'PendingDeprecationWarning', 'ReferenceError', 'RuntimeError',
'RuntimeWarning', 'StandardError', 'StopIteration', 'SyntaxError',
'SyntaxWarning', 'SystemError', 'SystemExit', 'TabError', 'True',
'TypeError', 'UnboundLocalError', 'UnicodeDecodeError',
'UnicodeEncodeError', 'UnicodeError', 'UnicodeTranslateError',
'UserWarning', 'ValueError', 'Warning', 'ZeroDivisionError', '_',
'__debug__', '__doc__', '__import__', '__name__', 'abs', 'apply',
'basestring', 'bool', 'buffer', 'callable', 'chr', 'classmethod',
'cmp', 'coerce', 'compile', 'complex', 'copyright', 'credits',
'delattr', 'dict', 'dir', 'divmod', 'enumerate', 'eval', 'execfile',
'exit', 'file', 'filter', 'float', 'frozenset', 'getattr', 'globals',
'hasattr', 'hash', 'help', 'hex', 'id', 'input', 'int', 'intern',
'isinstance', 'issubclass', 'iter', 'len', 'license', 'list',
'locals', 'long', 'map', 'max', 'min', 'object', 'oct', 'open',
'ord', 'pow', 'property', 'quit', 'range', 'raw_input', 'reduce',
'reload', 'repr', 'reversed', 'round', 'set', 'setattr', 'slice',
'sorted', 'staticmethod', 'str', 'sum', 'super', 'tuple', 'type',
'unichr', 'unicode', 'vars', 'xrange', 'zip']
```

This exciting-looking list has all the types, objects and functions that are part of the 'built-in' objects. Although they don't show up when you use `dir()`, they are normally part of every namespace.

There are disadvantages of trying to import too many things into your namespace. The biggest problem occurs when one of the modules has a function that is the same as a built-in function. That's usually not good practice, and most modules avoid that, but it does happen. More likely is when you have two modules that use the same name for a function or object. To illustrate:

```
>>> from numpy import *
```

The namespace now contains a very large number of items:

```
>>> dir()
['ALLOW_THREADS, 'BUFSIZE', 'CLIP', 'ERR_CALL', ERR_DEFAULT',
...
'where', 'who', 'zeros', 'zeros_like']
```

Over four hundred if you are counting. Now let's do something simple:

```
>>> x = arange(2.)
>>> sin(x)
array([ 0.      , 0.84147098])
# Now lets import the math module and retry the last command
>>> from math import *
>>> sin(x)
Traceback (most recent call last):
   File "<stdin>", line 1, in ?
[...]
TypeError: Only length-1 arrays can be converted to Python scalars
```

What happened? Turns out the `math` module also defines `sin()`. When we did `from math import *` we overwrote the numpy version. The strange error message occurs since the math module asks the argument if it can turn itself into a floating point number if isn't one already. Numpy can in one instance (for rank-0 or 1 element-1-d arrays) but raises an exception in all other cases.

When you do overwrite functions or objects, the results can be very confusing. That's why it is recommended that you avoid the `from zzz import *` style within modules and scripts. If the module name is very long and inconvenient to type, it is very acceptable to import as a different name, e.g.,

```
>>> import numarray as np
>>> np.sin(arange(2.))
```

When using something like numpy or pylab interactively it is fine to use the `from zzz import` style since each of these packages essentially form the bulk of your working environment (but do note that there are some collisions between pylab and numpy that aren't compatible; these will be discussed later). But when working interactively, be careful about using that style with many other modules unless you are confident that there are no name collisions.

If you must overload (i.e., replace) the name of a builtin object or function it is still possible to use it. Suppose you want to define an open function within your module. PyFITS does this; however, PyFITS does not allow its `open` function to come into the importing namespace as `open`. Instead it is aliased to `fitsopen` to prevent name collisions with the builtin `open`. Look up the `__all__` attribute for modules to see how that is accomplished). By overloading open doing so you can't use `open` to open a file using the builtin. But this does accomplish the same thing:

```
>>> f = __builtins__.open('junk.txt','w')
```

When you import a module as follows

```
>>> import pyfits
```

then only pyfits appears in your namespace, and the pyfits module object has its own, local namespace for all it contains.

```
>>> dir()
['__builtins__', '__doc__', '__name__', 'pyfits']
```

So your PyFITS functionality is restricted to its own namespace:

```
>>> dir(pyfits)
['ASCIITNULL', 'AllHDU', 'BinTableHDU', 'Boolean', 'Card',
'CardList', 'ColDefs', 'Column', 'CorruptedHDU', 'DELAYED',
'ExtensionHDU', 'FALSE', 'FITS_FatalError', 'FITS_SevereError',
'FITS_Warning', 'FITS_rec', 'GroupData', 'GroupsHDU', 'HDUList',
'Header', 'ImageBaseHDU', 'ImageHDU', 'Memmap', 'PrimaryHDU',
'Section', 'TAB', 'TRUE', 'TableBaseHDU', 'TableHDU',
'UNDEFINED', 'Undefined', 'UserList', 'ValidHDU', 'VerifyError',
'_Card_with_continue', '_ErrList', '_File', '_FormatP',
'_FormatX', '_Group', '_KeyType', '_LineSlice', '_OnePointAxis',
'_SinglePoint', '_SteppedSlice', '_TempHDU', '_VLF', '_Verify',
'_WholeLine', '__builtin__', '__builtins__', '__credits__',
'__doc__', '__file__', '__name__', '__version__', '_eval',
'_floatFormat', '_get_tbdata', '_iswholeline', '_makep',
'_normalize_slice', '_pad', '_tmpName', '_unwrapx', '_wrapx',
'blockLen', 'chararray', 'commonNames', 'convert_ASCII_format',
'convert_format', 'exceptions', 'fits2rec', 'fix_table',
'get_index', 'isInt', 'key', 'keyNames', 'maketrans',
'memmap_mode', 'ndarray', 'new_table', 'num', 'objects', 'open',
'operator', 'os', 'padLength', 'parse_tformat', 'python_mode',
're', 'rec', 'rec2fits', 'sys', 'tdef_re', 'tempfile',
'tformat_re', 'types']
```

Now we have access to all of PyFITS's functionality, and there's no confusion with built-in functions. The only down side is that you have to prepend each function or attribute with `pyfits.` to access it. But it does make for clearer code; there's no ambiguity as to where the attribute or function you're using comes from.

You should be aware that the names that appear in the local names space when you do from pyfits import * do not contain all the names present in the module namespace for two possible reasons. First, Python automatically excludes all names beginning with `_`. Secondly, the module can define `__all__` with a list of names that it does not wish to be imported into the local namespace when the `from zzz import *` form is used (this is how pyfits excludes open)

## 4.2 Functions

### 4.2.1 The basics

As in many programming languages, functions are a way to do the same thing repeatedly but with different values (or arguments). They save typing the same code over again. Basic function declarations in Python are very simple as illustrated by the following example:

```
def cube(x):
    '''take the cube of x'''
    return x*x*x
```

This illustrates that functions are defined with a `def` statement, followed by the name of the function, and then a comma-delimited list of arguments enclosed in parentheses. The argument list is optional, but the parentheses aren't. After the argument tuple, there is a colon to indicate that Python expects the body of the function either on the same line or in an indented block in the following lines. Functions take an optional docstring. If you provide the docstring, many tools can be used at runtime (as previously shown) to display it. Functions use a `return` statement to return a value (but return statements are optional; if the end of the function is reached with no `return`, the function automatically returns a `None` value). Finally, functions can be passed as arguments or assigned to other variables:

```
>>> cube(3)
27
>>> cube(2.2)
10.648000000000003
>>> cube()
Traceback (most recent call last):
   File "<stdin>", line 1, in ?
TypeError: cube() takes exactly 1 argument (0 given)
>>> cube('2')
Traceback (most recent call last):
   File "<stdin>", line 1, in ?
   File "<stdin>", line 3, in cube
TypeError: can't multiply sequence by non-int
>>> cube.__doc__
'take the cube of x'
>>> calias = cube # calias points to the same function 'object'
>>> calias(3)
27
>>> def integrate(function, start, stop):
...      '''very crude integration function'''
...      total = 0
...      for value in range(start,stop):
...          total += function(value)
...      return total
...
>>> integrate(cube,1,10)
2025
```

The argument of the `cube` function can be anything that supports the `*` operator. (Technically, it must implement a `__mul__` method; see the next tutorial to find out more about this). So, for example, we can use it with numpy arrays

```
>>> data = arange(10)
>>> data
array([ 0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> data3 = cube(data)
>>> data3
array([   0,   1,   8,  27,  64, 125, 216, 343, 512, 729])
```

### 4.2.2 Function argument handling

*Is this a five minute argument or the full half hour?*
(www.mindspring.com/~mfpatton/sketch.htm)

Python provides many conveniences to make argument handling flexible. There are two kinds of arguments possible; "positional" and "keyword". The distinction can be a bit confusing depending on whether you are defining arguments or using them. This is illustrated by the `cube` example. The parameter `x` is a positional parameter since it can be specified simply by putting a value in the order expected (with only one argument, order isn't really an issue in this case). But one can also use keyword syntax for positional arguments:

```
>>> cube(x=3)
```

But that doesn't change the fact that it is a positional argument.

Arguments may have default values specified for them. E.g.,

```
def integrate(function, start=0, stop=10):
```

All the arguments of integrate are positional arguments, but the last two have default values, thus

```
>>> integrate(cube)
```

will use 0 for start and 10 for stop since they were not specified for this call. All the following variants are acceptable given the definition of integrate:

```
>>> integrate(stop=5, start=1, function=cube)
>>> integrate(cube, 3) # stop will be 10
```

But this is not legal:

```
>>> integrate(cube, start=2,7)
```

because it is not permitted to use a positional argument form after a keyword form specification (Python no longer is sure that you are adhering to positional order once you start using the keyword form). When you use the keyword form to refer to positional arguments, order no longer matters for that value and following keyword-like arguments. You also cannot follow arguments definitions that have a default specified with arguments definitions that have no defaults (think about why that cannot be permitted).

Variable numbers of arguments are easy to handle as well as arbitrary keywords. Here is an example of the first:

```
def average(*args):
     total = 0.
     for arg in args:
         total += arg
     return total/len(args)
```

The syntax for `args` indicates that a variable number of positional parameters are expected. These will be stuffed into a variable named `args` (you can choose any legal name you wish) as a list. Likewise, one can do something similar for keywords:

```
def makedict(**keywords):
     '''Make a dictionary from a function keyword=value args list'''
     newdict = {}
     for keyword in keywords.keys():
         newdict[keyword] = keywords[keyword]
     return newdict    # note that we could have simply returned keywords!
```

This syntax indicates that all keyword argument specifications will be stored in a dictionary as keyword:value pairs with the dictionary referred to by the variable name keywords (name is up to you).

All three forms may be combined:

```
def wild_and_crazy_function(mode, *filenames, **options):
```

This function expects one mandatory positional keyword, an optional list of filenames, and keyword form for `options` (whether the values in the list of filenames are acceptable or the keywords used are permitted must be handled in the function code).

## 4.3 Python scripts

First, a little clarifying terminology. A script is typically invoked from the operating system command line, though if no arguments need to be passed, then scripts are easily run from the various Python interpreters. Functions are just that, they take arguments and return values, and can be used in expressions. Modules are Python files that can contain script-like code. It is possible to write modules that are both useful in a scripting context and for importing functions, classes, and objects. Python also has a higher level organization of code called packages. All these elements will be described in this tutorial. While it is possible to define functions and classes interactively, it is normally easier to define them in a module with an editor (see Appendix E for a link to Python-friendly editors). Python scripts, at their simplest level, just consist of code that one might have typed at the command line. It is a way of creating a batch file of commands that can be executed every time it is run. On Unix systems, if the first line of the file contains `#!/usr/bin/env python` or acceptable variants, and the file is marked as executable, then the command can be invoked by just typing the name of the file. (The `#!` combination is sometimes called 'shebang'; see http://catb.org/~esr/jargon/html/S/shebang.html), a good way to remember the syntax.)

For example, if one creates a file called `test` containing:

```
#!/usr/bin/env python
print 'script starting up'
for item in [1,4,9]:
     print item
```

followed by changing the mode of the file (on Unix) to be executable:

```
% chmod a+x test
```

Then the script can be executed by typing`./test` (or just `test` if its directory is in the standard path). Where the `#!` functionality is not supported, one executes scripts instead by typing

```
% python test
script starting up
1
4
9
```

Scripts with no command line options can be invoked from any of the Python interpreters by using the `execfile()` function. E.g.,

```
>>> execfile('test')
script starting up
1
4
9
```

IPython provides the convenient run command to do the same:

```
In[1]: run test
script starting up
1
4
9
```

Later we will revisit scripts that expect command line arguments. Scripts can contain loops and conditional code (and even function and class definitions for their own internal use).

## 4.4 Modules

Let's get back to our `cube` example. Instead of having to type out all that code, we can put it in a module. Modules correspond to Python files. They are either simple Python source files (and in that case must have a `.py`, filename extension) or they are shareable object file (.so files for Unix and .dll files for MS Windows).

Modules can contain all sorts of things: any number of function definitions, class definitions, and variable definitions. Modules can also contain any amount of code that is executed when the module is imported (initialization, etc.). Modules can import other modules.

Module importing is only done once within a Python session. If another module has imported a given module, Python notes that internally; any subsequent import of that module checks to see if the import has already been done and if so, just refers to the module already imported. When debugging a module you have written it is necessary to use the `reload()` function in order to force the module to be imported again if changes are made to it:

```
>>> import mymodule
[test fails]
[edit mymodule.py]
>>> reload(mymodule)
[retest module]
[and so on]
```

Reloading is simple when you are only dealing with one module. If you have a larger software system that involves multiple modules you have written that depend on each other, it is also important to reload all other modules that depend on the module you've changed and reloaded. The reloading of the modules must be done in the order that the modules are imported. Generally, when there are many such dependencies, it is easier to just start with a fresh Python session. Reloading does not work with modules that are not written in Python (`.so` and `.dll` modules).

Make a module called `cube.py` with the following lines:

```
def cube(x):
   '''Take the cube of x'''
   return x*x*x
```

As previously noted there are several ways to import modules:

```
>>> import cube
>>> import cube as mm # use mm as name for cube
>>> from cube import * # import all exposed names into local namespace
>>> from cube import cube # only import specified items into local >>> namespace
```

When debugging a module, it is most useful to use one of the first two forms since reloading does not update the objects in the local namespace with the new definitions. Pay special heed to this or you will wonder why your edits to your module do not appear to have any effect on the problems you are seeing!

Now we can use our cube function; assume we did

```
>>> import cube
```

Here's what happens when we try to use it:

```
>>> cube(3)
Traceback (most recent call last):
   File "<stdin>", line 1, in ?
TypeError: 'module' object is not callable
```

The reason is that the import statement imported the `cube` **module** into the local namespace, but the `cube` **function** lives in the cube namespace. So if we want to use the `cube` function, we have to do:

```
>>> cube.cube(3)
27
```

Let's put another line in to see what the value of the __name__ attribute is from inside cube:

```
def cube(x):
   '''Take the cube of x'''
   print __name__
   return x*x*x
```

Save, and then do

```
>>> reload(cube)
<module 'cube' from 'cube.py'>
>>> cube.cube(3)
cube
27
```

Now`__name__` is equal to the enclosing namespace, which in this case is the function `cube`. This gives us a mechanism for using modules both as shell commands and as Python modules to be `import`ed. Let's add some lines to `cube.py`:

```
#!/usr/bin/env python
import sys
def cube(x):
   '''Take the cube of x'''
   print __name__
   return x*x*x
if __name__ == '__main__':
   _nargs = len(sys.argv)
   if _nargs != 2:
     print 'Usage: cube x'
   else:
     print cube(float(sys.argv[1]))
```

When you use a module from the shell, the `__name__` object is equal to `'__main__'`, so the code in the conditional block is executed. To pass arguments to the cube function when used as a standalone module, we use the `sys.argv` attribute; this is a Python list whose first element is a string containing the name of the module, while subsequent list elements are the following whitespace-delimited elements turned into strings. Since `cube()` doesn't like strings, we have to turn the argument into a float before evaluating the cube.

Now we can exit Python and do:

```
machine> python cube 5
__main__
125.0
```

which demonstrates that we can use our `cube.py` module from the command line, and from inside Python we can do

```
>>> import cube
>>> cube.cube(3)
cube
27
```

## 4.5 Exception handling

Python has some nice support for exception handling, but it takes a bit of getting used to if you're not familiar with this kind of approach. Languages that don't have exception handling built in (e.g. FORTRAN, C) tend to have code that is sprinkled with code like this:

```
ratio = 0.0;
if (x == 0) {
     printf("Divisor = 0\n");
} else {
     ratio = y/x;
}
```

You trap the condition that would lead to an error, and then go on and execute the code knowing that the error won't occur. In Python (and C++, Java and other more modern languages), an error will "throw an exception", which you can then handle. So the equivalent code in Python would look like this:

```
ratio = 0.0
try:
   ratio = y/x
except ZeroDivisionError:
   print 'Divisor = 0'
```

The `try/except` syntax has the advantage that what you want to do appears first, and the exception handling appears later so you don't have to read past a lot of error trapping code to find out what a particular block of code is doing.

When an exception occurs, the program stops and Python looks for a handler to deal with the exception. If the exception occurs during the execution of a function call and there is to handler in the function, the function immediately returns and passes control and the exception to its calling block. If there is an appropriate handler there, it can catch the exception and deal with it, otherwise it stops execution and passes control and the exception back up to its calling block, and so on, until a suitable exception handler is found. If no handler is found to deal with the exception, Python prints an error message and returns to the interpreter prompt (or if the error occurred in a script called from the shell, the script halts, an error message is printed and control passes back to the shell).

The `except` block "catches" the exception so that no other exception handlers (including the one built into the Python interpreter) will see it. If you want to catch an exception, do some processing (for example, print something informative), and then propagate the exception further up the chain, your code can throw the exception for something else to catch by using the `raise` statement:

```
try:
   [do some processing]
except SomeError:
   [respond to this particular error condition]
   raise SomeError        # now let something else handle the error
```

It is also possible to set up a clean-up handler to make sure that a certain block of code is executed whether an exception occurs or not by using the `try/finally` syntax. For example:

```
f = open('thisfile.txt','r')
try:
   [do something with the file]
finally:
   f.close()
```

The `finally` block is executed even if the `try` block throws an exception that would cause Python to terminate processing.

Python provides a large number of exception types so that your code can respond to the specific exception thrown. It is usually not a good idea to catch every kind of exception, for example, by using something like

```
try:
   [do stuff]
except:
   [respond to every type of exception]
```

because it makes it difficult to debug exactly what happened; have your code respond to specific exceptions if you need it to, and let Python print an error message so that you get some feedback as to the type of exception thrown, and where it occurred.

Finally, you can end your Python session by raising a `SystemExit` exception.

## 4.6 Garbage (cleaning up after yourself)

Something we have glossed over throughout is how the memory used by Python objects is handled. Users of C or similar languages are used to having to explicitly allocate and free memory for new objects. That generally isn't necessary for Python (nor IDL or Java). So what does happen to that large array you created? Does it stay around forever until you end your Python session? Well, it depends. The simple answer is that it stays around as long as something is using it, and as soon as nothing is using it, Python frees the memory it uses. That sounds simple, but what does it mean exactly? If you recall, it was mentioned that variables are not the objects themselves, but only contain references to objects. Python keeps track of all things that refer to an object. Once it notices that nothing refers to the object, it deletes the object and it frees the memory it uses.

In a generic sense, this sort of automatic memory management is often called"garbage collection". The system Python uses is called reference counting and it is considered a fairly primitive form of garbage collection (compared to what Java uses, for instance). Even so, it has some significant advantages, generally works reasonably well, and it is comparatively easy to understand.

When one deals with large memory objects (such as astronomical images), it pays to have some understanding of what is going on with regard to memory management, otherwise you are bound to run into situations when you run out of memory, and you don't understand why you ran out of memory. The primary rule to understand is that if you want to remove an image from memory, make sure nothing refers to it. This can sometimes be more subtle than one realizes. Let's start with simpler cases and move to more subtle cases.

Assume all cases start with creating an image array as follows:

```
>>> im = pyfits.getdata('pix.fits') # now an image sits in memory
```

Case 1:

```
>>> im = 0 # now im points to a memory location with a zero in it
```

Case 2:

```
>>> del im # same effect as Case 1, since there is not even a variable im  anymore
```

Note that by reassigning the variable `im` to point to the scalar 0, nothing refers to the image. As soon as the reassignment is done, Python decreases the reference count for the image array, notices that it is now 0, and deletes it immediately (one advantage of this approach is that the memory is freed immediately, unlike more sophisticated garbage collectors).

Case 3:

```
>>> sim = im
>>> im = 0 # image is not deleted, sim still refers to it
>>> sim = 0 # now it is freed
```

Case 4:

```
>>> sim = im[:1,:1]
>>> im = 0 # image data buffer not deleted, as slice has a reference to  the data buffer
>>> sim = 0 # now it is deleted
```

In this case, even if the slice is a minuscule part of the array (1x1 array), the whole array buffer still has a reference to it, and is not deleted until the slice is deleted.

The fact that numpy allows many views into the same object means that the object will not be deleted until all the views are removed.

Case 5:

```
>>> mylist = [1, 'hello', im]
>>> im = 0 # image not deleted, list still contains a reference
>>> mylist[2] = 0 # now it is deleted
```

In other words, if you save references to the image in any data structure (lists, tuples, dictionaries, object attributes, etc), the array will not be deleted until those references are removed.

Case 6:

```
>>> imshow(im)
>>> im = 0 # image is not deleted!
>>> cla() # now it is!
```

This illustrates a more subtle case. What may not be apparent is that when `matplotlib` displays an image, it saves a reference to it (how do you think it manages to be able to resample the image when you resize the window?) You must force `matplotlib` to remove that reference (`cla()`, which clears the plot, happens to do that). This points to a potential problem, that is, use of modules that somehow retain references to objects you pass to functions or objects, and where it may not be obvious that is happening.

Case 7:

```
>>> list1 = [1, im]
>>> list2 = [list1]
>>> list1[0] = list2
>>> im = list1 = list2 = 0 # what happens to this case?
```

Here we have set up a cyclic reference. The list created for `list1` refers to the image, and also has a reference to `list2` after we define `list2`. The list defined for `list2` refers to the first list. We can remove the references by `im` to the image, and `list1` and `list2` to the lists that were created. However these two lists still have references to each other even if the variables no longer do, so these lists won't be deleted as a result, right? (and thus, the image they contain won't either). Well it depends. In much older versions of Python, they wouldn't be, but version 2.2 and later detect when there are cyclic references with no connection to any variable, and it does delete these.

When you are dealing with large memory objects, or when you create large numbers of objects within loops, it pays to understand when they are being deleted and when they aren't.

## 4.7 Miscellany:

Here are a few topics that don't fit into any of the previous sections, but are of general interest.

### 4.7.1 Interactive programs

Say you have a Python program where you want to prompt the user for a value to be used in processing. This can be handled by the `raw_input()` function. Going back to our cube example, we could handle the case of no argument being provided to the script (signalled by the fact that `sys.argv` has length 1) by prompting the user for a value:

```
#!/usr/bin/env python
import sys
def cube(x):
   '''Take the cube of x'''
   return x*x*x
if __name__ == '__main__':
   _nargs = len(sys.argv)
   if _nargs  == 1:
     x = raw_input("Enter number to be cubed:  ")
   else:
     x = sys.argv[1]
   print cube(float(x))
```

`raw_input` always returns a string, so you have to do the conversion from a string to a number of you're expecting a numeric input.

### 4.7.2 Text Handling

A lot of people use Perl for text handling, but Python has its own strengths in this area. For example, you can read a text file into a list object, one line per element using the `readlines()` function:

```
>>> f = open('login.cl','r')
>>> flist = f.readlines()
>>> flist[0]
'# LOGIN.CL -- User login file for the IRAF command language.\n'
```

We can turn strings into individual words by using the split method of strings:

```
>>> words = flist[0].split(' ')
>>> words
['#', 'LOGIN.CL', '--', 'User', 'login', 'file', 'for', 'the', 'IRAF',
'command', 'language.\n']
```

Now we could reverse the order of the words:

```
>>> words.reverse()
>>> words
['language.\n', 'command', 'IRAF', 'the', 'for', 'file', 'login', 'User', '--',
  'LOGIN.CL', '#']
```

And we can join them back up again:

```
>>> flist[0] = ' '.join(words)
>>> flist[0]
'language.\n command IRAF the for file login User -- LOGIN.CL #'
```

Why you would want to do this is questionable, but it does illustrate the power of Python's text handling capabilities. To quickly review what methods strings have, just type:

```
>>> dir('')
```

### 4.7.3 String formatting

So how does one customize the printing out of numbers, particularly floating point numbers? In Python you can define a format string that is very similar to format descriptions in C. The format string is applied through use of the `%` operator. A few examples will explain best:

```
>>> x = 1100003
>>> 'maximum value = %f' % x
'maximum value = 1100003.000000'
>>> 'maximum value = %g' % x
'maximum value = 1.1e+06'
>>> 'min = %d, max = %d' % (3, 7.2)
'min = 3, max = 7'
```

The % operator when used with a string as the first argument expects either a single value or a tuple of appropriate values as the second argument (with the length matching the number of format elements in the format string). The following table summarize the different formatting codes.

| Conversion Code | Meaning |
|---|---|
| `d, i` | Signed decimal integer |
| `o` | Unsigned octal (alternate form uses leading zeros) |
| `u` | Unsigned decimal |
| `x, X` | Unsigned hexadecimal (lower/upper case) (alternate form: leading 0x/0X) |
| `e, E` | Floating point exponential (lower/upper case) |
| `f, F` | Floating point decimal |
| `g, G` | Same as `e,E` if exponent > -4 or less than precision, '`f,F`' otherwise |
| `c` | Single character |
| `r` | String (implicitly converts any Python object using `repr()` |
| `s` | String (implicitly converts any Python object using `str()` |
| `%` | Results in literal `%` |

The code characters that differ only by case affect the case of the output result. The codes d and i are equivalent.

Conversion codes can be prefixed with the following optional items (in the order noted)

1. A mapping key as a parenthesized string of characters that is a key in the dictionary used (see example below)
2. One or more conversion flags (see table below)
3. Minimum field width (see documentation for use of *)
4. Precision given as a '.' followed by the precision (see documentation for use of *)

| Flag | Meaning |
|---|---|
| `#` | Use alternate form (where applicable) |
| `0` | Pad numeric values with 0 |
|  | (a space) insert space before positive numbers or empty strings |
| - | Left adjust converted value (overrides 0 if also specified) |
| + | Always use a sign character (+/-) |

The following example illustrates a few of the more advanced formatting features. Note the use of the dictionary to populate named elements in the format string. This is quite handy for complex strings, particularly where the contents may change the number or order of formatted items in later versions of the program.

```
>>> '%(employee)s: ID = %(ident)08d, salary = %(salary)10.2f' % \
{'salary':33333.3, 'employee':'John Doe', 'ident':13}
'John Doe: ID = 00000013, salary =   33333.30'
```

### 4.7.4 More about `print`

If you place a trailing comma on the print statement line, that will suppress the newline normally appended to the printed string. E.g.,

```
>>> print 'hello' ; print 'there'
hello
there
>>> print 'hello', ; print 'there
hello there
```

You can also redirect the printed output to any 'file-like' object as follows:

```
>>> f = open('mylogfile.txt','w') # open file for writing
>>> print >> f, 'test line for file' # write to file
```

### 4.7.5 Line continuations

Python has no specific limit on the length of a line of code. Generally it is a good idea to limit line lengths to less than 80 characters or less (some prefer 72). Lines are continued in two basic ways:

- By ending the line with a backslash `'\'` (before any comment).
- By use of an unclosed parenthesis, bracket or braces.

The latter is illustrated by some examples:

```
x = (1 +
     2)
y = {2:4,
     'Ted':5,
     (2,3):7}
z = 'hello there'[
        2:5]
```

### 4.7.6 Variable name conventions

Apart from not being allowed to use variables with reserved names like `try` or `import`, there aren't many restrictions on the names of variables that you can use in Python other than the names must only contain alphanumeric characters, `'_'`, and not start with a digit. There is a convention that variable, attribute, method, or class names names that begin with a single `'_'` are considered private and not part of the public interface of the module or class. So while there's nothing preventing you from accessing these variables or functions, it usually isn't wise since such private elements may change in future versions by changing their meaning (and classes and methods changing their interface) or even disappearing. Names that begin underscores will not normally appear in the local namespace when using the `from mymodule import *` form of importing.

### 4.7.7 Division

Normally, if you divide an integer by an integer in Python, the result is truncated. So `2/4` results in zero, while `2.0/4.0` results in `0.5`. However, this will change with Python v3.0 when division of integers will result in floating point values. Buy using this special import statement, you can cause Python to use its future division behavior now (and avoid having to check or change your scripts and modules when that happens!):

```
>>> 2/4
0
>>> from __future__ import division
>>> 2/4
0.5
```

Note that by using this special import, numpy will also change the behavior of division. Also realize that this import only affects the module that uses it. Those that don't will continue with the current default behavior. Python has defined the operator // to implement integer (truncating) division so that capability remains available.

### 4.7.8 Implicit tuples and tuple assignment

Whenever you type a comma-separated list of variables, Python interprets it as a tuple. So if you type:

```
>>> x = 1,2,3,4,5
>>> type(x)
<type 'tuple'>
```

Python also applies the same rule on the left side of assignment statements meaning that one can assign to elements of tuples by assigning a identically sized tuple on the right hand size:

```
>>> x,y,z = 2,5,6
```

and `x` will be set to 2, `y` to 5 and `z` to 6.

### 4.7.9 What if your function needs to return more than one value?

The standard idiom in Python is to return a tuple of the multiple values. For example:

```
>>> def powers(x):
....   square = x*x
....   cube = x*x*x
....   fourth = x*x*x*x
....   return square, cube, fourth

>>> powers(3)
(9, 27, 81)
```

Combined with tuple assignment, this makes for a convenient way of handling the multiple values:

```
>>> square, cube, fourth = powers(3)
```

In C, if you want to return more than one value, you have to create a struct, or change what one of the arguments points to. In IDL you would either return a structure or provide the extra return values as extra arguments.

Implicit tuples also make it easy to swap values without using a temporary value:

```
>>> x, y = 10,6
>>> x,y = y,x
>>> x,y
(6, 10)
```

### 4.7.10 Equality versus identity

Items that satisfy the equality test (==) are not necessarily identically the same object. If you wish to test whether two variables or reference refer to the exact same object, use the `is` operator:

```
>>> x is y
False
```

## 4.8 Python module overview

Standard Python comes with a large number of modules. Here's just a sample of some of them:

| Module(s) | Use |
|---|---|
| sys | Information about Python itself (path, etc.) |
| os | Operating system functions |
| os.path | Portable pathname tools |
| shutil | Utilities for copying files and directory trees |
| filecmp | Utilities for comparing files and directories |
| glob | Finds files matching wildcard pattern |
| fnmatch | Tests filename against wildcard pattern |
| re | Regular expression string matching |
| time | Time and date handling |
| datetime | Fast implementation of date and time handling |
| doctest, unittest | Modules that facilitate unit tests |
| pdb | Debugger |
| profile | Code profiling (to find bottlenecks in performance) |
| pickle, cpickle, marshal, shelve | Used to save objects and code to files |
| getopt, optparse | Utilities to handle shell-level argument parsing |
| math, cmath | Math functions (real and complex). Numarray has all these, but these are faster for scalars |
| random | Random generators (likewise) |
| gzip | read and write gzipped files |
| struct | Functions to pack and unpack binary data structures |
| StringIO, cStringIO | String-like objects that can be read and written as files (e.g., in-memory files) |
| types | Names for all the standard Python types |

There are many other modules dealing with process control, language parsing, low-level Unix interfaces, and particularly many network, web, and XML libraries that are beyond the scope of this tutorial. There are many GUI frameworks available. The one bundled with Python is Tkinter (based on Tk).

## 4.9 Debugging

Believe it or not, many Python programmers simply rely on using traceback information along with appropriately placed print statements. Nevertheless, Python has a debugger, which is in the `pdb` module. The Python library documentation gives the full details on using the debugger. While the debugger does support a number of powerful features, it is a command-line debugger, which means that it is clumsier to use than a GUI-based one (GUI-based Python debuggers do exist; these are briefly mentioned in the appendix on editors and IDEs). This part will only highlight the most common commands. There are two common ways of invoking the debugger. One can run the function from the debugger or one can start the debugger in a 'post-mortem' mode after an uncaught exception has been raised. We'll illustrate both with a contrived example. In a file `fact.py`:

```
def factorial(n):
    if n<1 or type(n) not in [type(1), type(1L)]:
        print 'argument must be positive integer'
        raise ValueError
    if n == 1:
        return 1
    else:  # intentional exception raised when n=5
        if n == 5: 0/0
        return n*factorial(n-1)
```

Note that this is a recursive function, i.e., it calls itself. It has been written to intentionally raise a divide-by-zero exception when the argument is 5 (given the way it is written, that will always happen for values >= 5) . First we show it working:

```
>>> import fact
>>> fact.factorial(4)
24
```

Now let's try a case that fails, then invoke the postmortem feature:

```
>>> fact.factorial(7)
[...]
ZeroDivisionError: integer division or modulo by zero
>>> import pdb # the debugging module
>>> pdb.pm()   # start postmortem debugging
> [...]/fact.py(8)factorial()
-> if n == 5: 0/0
(Pdb)
```

The debugger now is at the level that started the exception. While in that level you may inspect the contents of all the variables, move to other levels of the stack, etc. While it is possible to single step and restart execution, the exception cases generally make those options less useful. Post-mortem mode is mainly for looking at the state that it failed in rather than executing. The following shows some examples.

```
(Pdb) p n # print the value of n
5
(Pdb) w   # where in the call stack are we?
  <stdin>(1)()
  [...]/fact.py(9)factorial()
-> return n*factorial(n-1)
  [...]/fact.py(9)factorial()
-> return n*factorial(n-1)
  [...]/fact.py(8)factorial()
-> if n == 5: 0/0
(Pdb) u # move up one level in the stack
> [...]/fact.py(9)factorial()
-> return n*factorial(n-1)
(Pdb) p n # print the value of n
6
```

The prompt for the debugger is `(Pdb)`. Many of the debugger commands show where it currently is in the calling stack by printing the name of source file that contains the code (the path is shown as `[...]` since that will be dependent on the location of your code and the function or method that is being executed followed by the source line. Many commands can be invoked with a one or two character abbreviation (the example makes use of these abbreviations).

Since this is a recursive function, when it is called with the argument 7, it then calls it self with an argument of 6, then again with 5 and stops there because an exception is raised. That's why you see the repeated `fact.py(x)factorial()` references. Three different levels are in the very same function. The top two at line 9 and the last at line 8. As we would expect, printing out the value of `n` where the exception occurs shows it to be 5. The `up` command (`u`) moves to the previous call level; the value of `n` at that level is 6, as expected. Here are the commands most useful for postmortem examination (parentheses are used to show the alternate forms of the command, e.g., `h` or `help`):

**h(elp)** [command] list commands, or given specific command, give details of that command

**w(here)** show stack trace and location of current location

**d(own)** move down in the stack of calls

**u(p)** move up in the stack of calls

**l(ist)** [start[, end]] list code. Defaults to 11 lines centered at current location.

**p** expression print value of expression in the current context

**pp** expression pretty print value of expression

**a(rg)** print the current function's argument list

**q(uit)** quit the debugger mode

If you are using IPython, you can set it so that it automatically goes into post-mortem mode by starting IPython with the -pdb option, or by typing pdb at the IPython prompt. When it is in this mode it is similar to how IDL behaves when errors occur.

The simplest way of inserting effective breakpoints in the postmortem mode is to place `0/0` where you wish it to stop in your code (presuming nothing will trap that error!).

The function can be run from the start with the debugger. In that mode it is possible to set breakpoints (with options to ignore the breakpoint some specified number of times–useful for stopping after so many iterations), clear breakpoints, etc. One can also single step through the program, jump to other locations, define aliases, and a standard configuration file. See the Python documentation for a listing of the commands. The following shows a brief example of stepping through the code.

```
>>> pdb.run('fact.factorial(7)')
> <string>(1)?()
(Pdb) s # start stepping
--Call--
> [...]/fact.py(1)factorial()
-> def factorial(n):
(Pdb) # typing <Return> (blank line) executes last command, i.e., s
> [...]/fact.py(2)factorial()
-> if n < 1 or type(n) not in [type(1), type(1L)]:
(Pdb) b factorial # set breakpoint to first statement in function
Breakpoint 1 at [...]/fact.py:2
(Pdb) c # continue execution until end or next breakpoint
> [...]/fact.py(2)factorial()
-> if n < 1 or type(n) not in [type(2), type(1L)]:
(Pdb) p n
6
```

## 4.10 PyRAF

[This section can be skipped by non-astronomers]

### 4.10.1 Basic features

PyRAF was written here at STScI to replace the IRAF CL, with the goal of allowing the running of IRAF tasks and scripts from a Python environment. IRAF has an extremely rich set of tasks, but using the CL isn't everyone's cup of tea. With PyRAF, it is possible to use Python syntax as well as CL syntax, and this alone greatly enhances the power available to PyRAF users.

The PyRAF tutorial gives a good introduction to using PyRAF, highlighting some of its most important features:

- Almost all of the CL functionality is available
- CL scripts will run under PyRAF

- Easier debugging of CL scripts
- Command-line recall!
- Tab-completion!
- GUI parameter editor
- Powerful graphics system

It is possible to write Python functions that will run under PyRAF using the same parameter passing mechanism as IRAF and the same `epar` interface.

### 4.10.2 Using PyRAF

Using Python in PyRAF makes is relatively easy to do complex tasks. For example, MultiDrizzle is written almost entirely in Python (there are some parts that were written in C to improve the execution speed). To give a useful example, one of the most frustrating aspects of IRAF is that it is very difficult to operate on a set of FITS extensions. Doing

```
---> imstat *.fits[sci,*]
```

doesn't work, and nor does making a file list using files:

```
---> files *.fits[sci,*] > filelist
```

But it is relatively easy to make a simple function to do extension processing, returning a list of files with extensions that match a specification. Here's the code

```
import pyfits
from pyraf import pyraf
def extensions(filespec, ext=None):
   '''A module to return a list of files that meet the specification'''
   filelist = iraf.files(filespec, Stdout=1)
   outlist = []
   for exposure in filelist:
     thisfile = pyfits.open(exposure)
     _nextensions = len(thisfile)
     for i in range(_nextensions)[1:]
       if(thisfile[i].header['extname'] == ext.upper():
         extver = thisfile[i].header['extver']
         outlist.append(exposure + '[' + ext + ',' + str(extver) + ']')
     thisfile.close()
   return outlist
```

Since the IRAF `files` task does wildcard filename processing, it seems a waste not to use it. Note the syntax of using `Stdout=1`; this puts the output from the `files` task into a list which the `filelist` variable is set to. We use the `extensions` function by doing:

```
---> from extensions import *
---> extensions('j*flt.fits','SCI')
['j6me13q9q_flt.fits[SCI,1]', 'j6me13q9q_flt.fits[SCI,2]',
'j6me13qaq_flt.fits[SCI,1]', 'j6me13qaq_flt.fits[SCI,2]',
'j95t20hmq_flt.fits[SCI,1]', 'j95t20hmq_flt.fits[SCI,2]',
'j95t20hoq_flt.fits[SCI,1]', 'j95t20hoq_flt.fits[SCI,2]',
'j95t20hrq_flt.fits[SCI,1]', 'j95t20hrq_flt.fits[SCI,2]',
'j95t20huq_flt.fits[SCI,1]', 'j95t20huq_flt.fits[SCI,2]',
'j95t20hyq_flt.fits[SCI,1]', 'j95t20hyq_flt.fits[SCI,2]',
'j95t20i1q_flt.fits[SCI,1]', 'j95t20i1q_flt.fits[SCI,2]',
'j95t20i4q_flt.fits[SCI,1]', 'j95t20i4q_flt.fits[SCI,2]',
'j95t20i7q_flt.fits[SCI,1]', 'j95t20i7q_flt.fits[SCI,2]']
---> for extension in extensions('j*','SCI'):
...  iraf.imstat(extension)
[lots of imstat output]
```

### 4.10.3 Giving Python functions an IRAF personality

One of the powerful aspects of PyRAF is that it allows you to write Python functions and then wrap them in such a way that they can be run as though they were IRAF tasks with the same CL syntax that IRAF tasks can be invoked with. The following is an example that uses many of the capabilities that PyRAF provides. In this case, write a short Python function to find the maximum value of an image or images in a fits file after smoothing by a boxcar. It needs 3 arguments: the name of the input file, the extension number, and the size of the boxcar filter.

In a file smax.py:

```
from convolve import boxcar
import pyfits
def smax(input, next, bsize=5):
    if next:
        im = pyfits.getdata(input, next)
    else:
        im = pyfits.getdata(input)
    return boxcar(im, (bsize,bsize)).max()
```

In a separate file smax_iraf.py (though it isn't necessary; it's just to keep the IRAF aspects isolated from the pure Python functionality.

```
from pyraf import iraf
import smax
def _smax(image, bsize, max, verbose):
    '''Use Python function smax to determine maximum smoothed value'''
    pos = image.find('[') # name contain extension spec?
    if pos>0:
        filename = image[:pos]
        nextstr = image[pos+1:-1]
        try:   # integer ext or name?
            next = int(nextstr)
        except TypeError:
            next = nextstr
    else:
        filename = image
        next = None
    max = smax.smax(filename, next, bsize)
    if verbose:
        print 'smoothed maximum =', max
    iraf.smax.max = max

parfile = iraf.osfn('home$scripts/smax.par')
t = iraf.IrafTaskFactory(taskname='smax', value=parfile, function=_smax)
```

Finally, create a file named smax.par (in home$scripts, though it can be anywhere you'd like so long as the reference to that directory in smax_iraf.py is consistent) that contains:

```
input,s,a,"",,,"input file (including extension)"
bsize,i,a,5,,,"size of boxcar to smooth with"
max,f,h,0.,,,"maximum found"
verbose,b,h,yes,,,"Print value?"
mode,s,h,"al"
```

Either in PyRAF at the command line or in a CL package script (see *PyRAF Programmer's Guide* for details)

```
--> pyexecute('home$scripts/smax_iraf.py')
```

At this point is is possible to use the task like any other IRAF task. You can then:

```
--> epar smax
[...]
--> lpar smax
        input = pix.fits          input file (including extension)
        bsize = 5                 size of boxcar to smooth with
         (max = 0.)               maximum found
     (verbose = yes)              Print value?
        (mode = al)
--> smax pix.fits[0] 11 verbose+
```

The wrapper function `_smax` is essentially taking the inputs from the IRAF interface and adapting them to the Python function. It is separating the filename into the two components (if there is an extension specification). The rest of the `smax_iraf.py` file is creating an IRAF task object for PyRAF to use by pointing to the parameter file and giving the appropriate name for the task.

If you are particularly fond of working with CL command-style syntax, this a way of accessing Python programs within that environment (or allowing colleagues to do so).

## 4.11 Final thoughts

We like Python because it's possible to be productive very quickly. You can write some ugly quick and dirty code to get what you want done. And then you can throw that code away. If you need to write production code, you can do that too; Python is very robust and full-featured, and chances are there's a module somewhere that will help you out.

## Exercises

1. Write a function to do a regular expression match on FITS header keywords and print all that match given a filename and regular expression string (see the `re` module documentation for usage).

2. Wrap the previous function as a PyRAF task.

# 5 What is this object-oriented stuff anyway?

The object-oriented features of Python provide capabilities that are hard to obtain by any other means. This tutorial won't make you a wizard at object-oriented design, nor will it come close to even giving you a solid grounding, but it will give you a flavor of the advantages that the object-oriented features of Python provide. The focus will be much more pragmatic than you will normally find in introductions to object-oriented programming.

## 5.1 Class basics

### 5.1.1 Class definitions

A class defines its attributes and methods as follows

```
class Clown:
    '''Educational Class''' # docstring
    def __init__(self, noise='Honk Honk'):
        self.noise=noise
    def makenoise(self):
        print self.noise
```

This creates class called `Clown` that has one attribute (`noise`) and one method (`makenoise`). There are a couple things about this class definition that are not what they seem. First of all, all methods assume that the first parameter will be a reference to the object itself. By convention, virtually everyone uses the name self for that parameter, though Python does not require you to use that name. If you know what's good for you, you'll also use that convention.

So, fair enough, the first argument is a reference to the object. But note that the first argument is not used when calling the method for a given object, Python puts it in for you. This aspect is bound to confuse you at least a couple times. The example of usage later will illustrate this point.

The second aspect of this class definition that isn't obvious is the `__init__` method. As previously mentioned, methods with names of the form `__zzz__` indicate some sort of indirect effect. The `__init__` methods is the initialization method. It is what is called when you create an instance of the class. But normally you don't call it directly. For example (in a file `clown.py`)

```
>>> import clown
>>> bozo = clown.Clown() # create first clown object
>>> weepy = clown.Clown('Boo Hoo') # create second clown object
>>> bozo.makenoise()
Honk Honk
>>> weepy.makenoise()
Boo Hoo
```

Calling the class as a function in effect calls the `__init__` method on a new instance of that class. It is the `__init__` method that typically sets up the attributes of the object. Generally the values of the attributes are passed as parameters (but can also be set indirectly or from the general environment; e.g., the current time). Since the noise defaulted to `'Honk Honk'`, not supplying an argument resulted in the noise attribute set to that value. Also note that Python takes the method call and effectively transforms it into the form of the last line of the example; that's where the value of `self` gets set. You have to get used to the idea that the definition of the method has an extra parameter than the way it will be used.

One point about OO terminology needs to be hammered home. Classes and objects are not the same thing. A class defines things about the object, but it should not be confused with those objects. In the previous example, `Clown` is the class. The variables `bozo` and `weepy` refer to objects created from that class. There is only one class, but many potential objects that can be created from it. The relationship is similar to that between types of variables and specific variables. In fact, you can think of classes as user-defined types that have associated programs (methods) that come along with those types. A common beginner mistake is to be sloppy about the distinction between the two concepts.

Frequently objects are referred to as 'instances of' of classes, or objects being 'instantiated' from a class, or the act of creating a class instance as 'instanciation'.

### 5.1.2 Python isn't like other object oriented languages

Python allows some things that most other object oriented languages don't permit. That it does fills some purists with shock and horror. Like freedom in general it can be abused, but generally it is not a problem and sometimes a very useful capability.

Python permits new attributes to be added to classes after their creation. And methods. You can add whatever attributes or methods you desire at any time you want. Continuing the previous example:

```
>>> bozo.realname = 'Clark Kent'
>>> def yell(cstr=''): print cstr.upper()
>>> bozo.yell = yell # adding a new method just for this object
>>> print bozo.realname
Clark Kent
>>> bozo.yell('hey you')
HEY YOU
```

The case of adding a method is a bit of a cheat in that you may notice that the function has no reference to self and methods added that way can't get at the attributes or methods of that instance. To do that requires a little more trickery:

```
>>> def yellname(self): print self.realname.upper()
>>> bozo.__class__.yellname = yellname
>>> bozo.yellname()
CLARK KENT
```

In effect we have dynamically added a method to the class rather than the instance which does allow it to reference self.

As far as unrestricted freedom to add to objects, this isn't entirely true. Python does provide mechanisms to prevent arbitrary additions of attributes and methods. But it is true that by default nothing keeps one from doing so.

Another thing that Python does differently is that it doesn't provide an means of protecting or hiding methods and attributes from external clients of the objects as is common with most OO languages. Python takes a decidedly different philosophy on this issue. Rather than devising mechanisms to prevent programmers and users from getting at internals, it expect them to use conventions indicating that some items are private and shouldn't normally be messed with (e.g., any attribute or method name that begins with an underscore). It expects you to be sensible, but won't prevent you from violating the convention (and wouldn't you know it, sometimes it's necessary to violate the convention if there is no other way of getting the job done). If you do so and suffer as a result, it's your fault, not the language's. Python's point of view regarding this is "We are all adults here".

### 5.1.3 Classes as a generalized data structure

This leads us to our first (if somewhat trivial) practical use of classes. Some may have noticed that Python has no structure mechanism similar to that available in C or Java. Often, it's possible to just use lists, tuples or dictionaries (particularly the latter if it is important to refer to the structure member by name) instead. But there are times where it's just nice to be able to use the `var.member` syntax that structure provide. Classes allow that. One can define special purpose classes as structures, where there are no methods (aside from the `__init__` method, and if one intends to add the attributes after the structure creation, even that isn't needed). One can either define an `__init__` that expects all the structure elements, or create a very bare class from which one will add attributes later. For example:

```
class Point:
    '''structure to hold coordinates of a point'''
    def __init__(self, x, y):
        self.x = x
        self.y = y
>>> import point
>>> p1 = point.Point(0.,0.)
>>> p2 = point.Point(10.3, -22)
>>> p2.x
10.3
>>> p1.y = 100
```

### 5.1.4 Those 'magic' methods

So far we've ignored all those strange methods that are of the form `__zzz__`. What the heck are they for? They are all generally hooks that allow your classes to take advantage of special Python syntax or behaviors. If you'd like to write a class whose objects can be indexed like lists, tuples or dictionaries you can do that by defining the `__getitem__` method for your class. If you define that method suitably, then you take full advantage of indexing syntax. The following example will illustrate by defining a class that can collect items in a list, but effectively keep them sorted when retrieved by index. It's not very useful, but it shows how it works. In file `sortedlist.py`

```
class SortedList:
    def __init__(self):
        self.values = []
    def append(self, value):
        self.values.append(value)

    def __getitem__(self, index):
        self.values.sort()
        return values[index]
    def __len__(self):
        return len(self.values)

>>> import sortedlist as sl
>>> x = sl.SortedList()
>>> x.append("apple")
>>> x.append(3)
>>> x.append("pear")
>>> x.append(7)
>>> x.append("mango")
>>> x.append(11)
>>> x.append("orange")
>>> for v in x:   print v
3
7
11
apple
mango
orange
pear
```

Nothing requires a class that uses `__getitem__` to be finite in the keys that are possible.

The magic methods allow one to take advantage of many of Python's conveniences. The following lists all the magic methods and the behavior they affect. Note that a number are associated with built-in Python functions. The first shown (`__len__`) means that if you define it for your class, than an instance of that class will work with `len()` (even though the built-in function has no idea of what your class is). These are hooks to allow your class to give the necessary information to many of the standard built-in functions.

**Container methods:**

`__len__(self)`: What the built-in function `len()` uses to determine how many elements a class contains. If it isn't present, `len()` doesn't work for that class

`__getitem__(self, key)`: Used when an object is indexed with key (returns `self[key]`).

`__setitem__(self, key, value)`: Used for assigning to indexed objects (`self[key]=value`)

`__delitem__(self, key)`: Used to delete `self[key]`.

`__iter__(self)`: Used when next element of an iterator is asked for.

`__contains__(self, item)`: Used for the expression `item in self`.

**Sequence methods:**

`__getslice__(self, i, j)`: Returns `self[i:j]`. In many respects, this method is no longer needed since `__getitem__` can handle all slicing (and is necessary if strides are used).

`__setslice__(self i, j, sequence)`: Used for `self[i:j]=`*sequence*. Like `__getslice__`, this method isn't really necessary since `__setitem__` can handle all slicing cases (including strides).

`__delslice__(self, i, j)`: Used to delete slices.

**General methods**

`__new__(cls...), __metaclass__`: for experts only.

`__init__(self, ...)`: You've met this one already

`__del__(self)`: called when reference count goes to 0. Usually used when some sort of cleanup is needed that can't be expected to be handled by simply deleting all references within the object. Some subtleties in when this is guaranteed to be called. See documentation.

`__repr__(self)`: called by the built in `repr()` (also used at interactive prompt) to print info about object

`__str__(self)`: called by the built-in `str()` to print string representation for object (e.g., `print obj`)

`__lt__,__le__,__eq__,__ne__,__gt__,__ge__`: called for `<, <=, ==, !=, >, >=` operators respectively with `(self, other)` as arguments.

`__cmp__(self, other)`: called by comparison operators if appropriate specific operator magic method not defined. Should return negative integer if `self<other`, 0 if `self==other`, positive integer if `self>other`.

`__hash__(self)`: Used to convert key for dictionary into 32-bit integer. If you don't know what this means, ignore it for now.

`__nonzero__(self)`: Called when object is used as a truth value. Normally returns `False` or `True`.

`__unicode__(self)`: used by built-in `unicode()`

`__call__(self, args...)`: Called when object is "called" as though it were a function (e.g., IRAF tasks objects use this trick)

**Attribute methods:**

`__getattr__(self, name)`: Called when an attribute of the specified name is not found `__setattr__(self, name, value)`: Called when trying to set the value of an attribute. Always called regardless of whether such an attribute exists (thus a bit tricky to use; see documentation for examples)

`__delattr__(self, name)`: Called when attribute is deleted (e.g., `del self.name`)

`__getattribute__`, `__get__`, `__set__`, `__delete__`, `__slots__`: are powerful and very useful, but are beyond the scope of this introduction. In particular these allow one to restrict what attributes are allowed for an object, as well as associate functions to be called when getting or setting the value of the given attributes. See the documentation for details.

**Numeric methods** (used to overload numeric operations). The following table shows the magic methods that are called when numeric operators or standard functions are called. They all have the same function arguments: `(self, other)`. There are three different magic methods for each operator. To illustrate we'll use the addition operator as an example. Given your object obj, when Python encounters the expression `obj+3` it sees if you have defined `__add__`, if so it will call `obj.__add__(3)`. You use that method to define what should happen when you try to add something to it. You may only accept numbers as the "other" argument. Or you may only accept other instances of the same class. It's up to you. When Python encounters `3+obj`, it will find that '3' doesn't know what to do with `obj`, it then sees if `obj` knows what to do, then it calls `obj.__radd__(3)`. The second column refers to when the object is the rightmost part of a binary operator. The last is when you find "augmented" assignment statements. For example: `obj += 3` will result in `obj.__iadd__(3)` being called.

| `self op. other` | `other op. self` | `self op= other` | `Operator` |
|---|---|---|---|
| `__add__` | `__radd__` | `__iadd__` | `+` |
| `__sub__` | `__rsub__` | `__isub__` | `-` |
| `__mul__` | `__rmul__` | `__imul__` | `*` |
| `__floordiv__` | `__rfloordiv__` | `__ifloordiv__` | `/ or //` |
| `__mod__` | `__rmod__` | `__imod__` | `%` |
| `__divmod__` | `__rdivmod__` | `__idivmod__` | `divmod()` |
| `__pow__` | `__rpow__` | `__ipow__` | `**` |
| `__lshift__` | `__rlshift__` | `__ilshift__` | `<<` |
| `__rshift__` | `__rrshift__` | `__irshift__` | `>>` |
| `__and__` | `__rand__` | `__iand__` | `&` |
| `__xor__` | `__rxor__` | `__ixor__` | `^` |
| `__or__` | `__ror__` | `__ior__` | `\|` |
| `__truediv__` | `__rtruediv__` | `__itruediv__` | `/` |

`__coerce__(self, other)`: Called by numeric operations. Should return a tuple of (self, other) where one or both have been converted to a common numeric type (see below).

**Unary operators:**

`__neg__(self)`: `-self`

`__pos__(self)`: `+self`

`__abs__(self)`: `abs(self)` [built-in `abs()`]

`__invert__(self)`: `~self` (bit inversion)

`__complex__(self)`: `complex(self)` [should return complex value]

`__int__(self)`: `int(self)` [should return integer value]

`__long__(self)`: `long(self)` [should return long integer value]

`__float__(self)`: `float(self)` [should return float]

`__oct__(self)`: `oct(self)` [should return string]

`__hex__(self)`: `hex(self)` [should return string]

### 5.1.5 How classes get rich

They inherit, that's how. Before discussing what they inherit we'll note that usually by now there is some explanation of why classes are so wonderful with regard to the theory of object oriented programming. You'd see terms like abstraction, encapsulation, and polymorphism. These are very nice terms, but we are going to avoid them for a while. Instead we will take a different track in demonstrating why classes can be useful. One of the other common OO terms is inheritance. What it essentially means is that classes can steal work that has been done for other classes, particularly if that other class already does an awful lot of what you need to do, but not exactly. Generally speaking, when you inherit from another class, it is expected that you will be able to do all that class can do, and perhaps more. You may not do it the same way, but you will have all the same public methods and attributes (those that convention has not indicated are to be kept private; see 4.7.6). Nothing enforces this though. If you want to be antisocial, you are free to be antisocial.

As usual, examples are the best way of showing what this is all about. Suppose you love dictionaries and want to use them in your program. But for some reason, you only will accept strings as keys, and want keys to be case-insensitive. Does this mean you have to rewrite all the machinery for dictionaries? Hardly. Here's how it can be done with very little code

```
class SDict(dict):
    '''Dictionary that only accepts case-insensitive string keys'''
    def __init__(self, idict = {}):
        '''If intializing dict is non-null, examine keys'''
        keys = idict.keys()
        values = idict.values()
        for i in range(len(keys)):
            if type(keys[i]) != type(''):
                raise TypeError
            keys[i] = keys[i].lower()
        dict.__init__(self)
        for key, value in zip(keys, values):
            self[key] = value
    def __getitem__(self, key):
        if type(key) != type(''):
            raise TypeError
        return dict.__getitem__(self, key.lower())
    def __setitem__(self, key, value):
        if type(key) != type(''):
            raise TypeError
        dict.__setitem__(self, key.lower(), value)
>>> import sdict
>>> sd = sdict.SDict({'Bob':'555-1234','Hubble':'338-4700'})
>>> sd
{'bob': '555-1234', 'hubble': '338-4700'}
>>> sd[3]=4
[...]
TypeError:
>>> sd['BOB']
'555-1234'
```

Note now that the class name has an argument `dict`. This is the mechanism to indicate that this class is inheriting from `dict`, which happens to be the class name associated with standard Python dictionaries.

To really do this right, a few other dict methods should be overridden to handle keys properly. These include `has_key()`, `update()`, `get()`, and `setdefault()`. So with about a page of code, you have completely customized a powerful data structure for a more specialized use.

One final remark about inheritance. The built-in function `isinstance()` will return `True` if the class the object is being compared to is anywhere in its inheritance hierarchy. For example:

```
>>> isinstance(sd, dict)
True
```

So even though `sd` is an instance of `SDict`, it is also considered an instance of every class it inherits from (`dict` here). This can be used to ensure that any object inherits from a given class (but see the discussion about duck typing [yes, that's duck] later, before using this too heavily)

## 5.2 A more complex example: Representing Source Spectra

### 5.2.1 Goals

This section explores a more realistic problem in more depth. We'll start with a simpler version of the general problem, and do a comparatively simple implementation. Then we'll discuss how new features can be added, without necessarily doing all the actual work, to illustrate the advantages of the object-oriented approach over a more traditional procedural approach. The example chosen is far from an academic exercise.

The problem to solve is modeling source spectra. Ultimately, we'd like a very general approach that provides many features; but we'll start with more modest goals: we want to be able to build up a source spectrum from an unlimited number of analytic source components and be able to sample the net spectrum at whatever wavelengths we choose without using resampling. We'll address flux integration and tabulated source models later. To keep the example short, we'll only implement two analytic models: Gaussian lines and black bodies (adding others is straightforward). We'll also assume that wavelengths are always in angstroms and the source spectra are in units of $F_\lambda$.

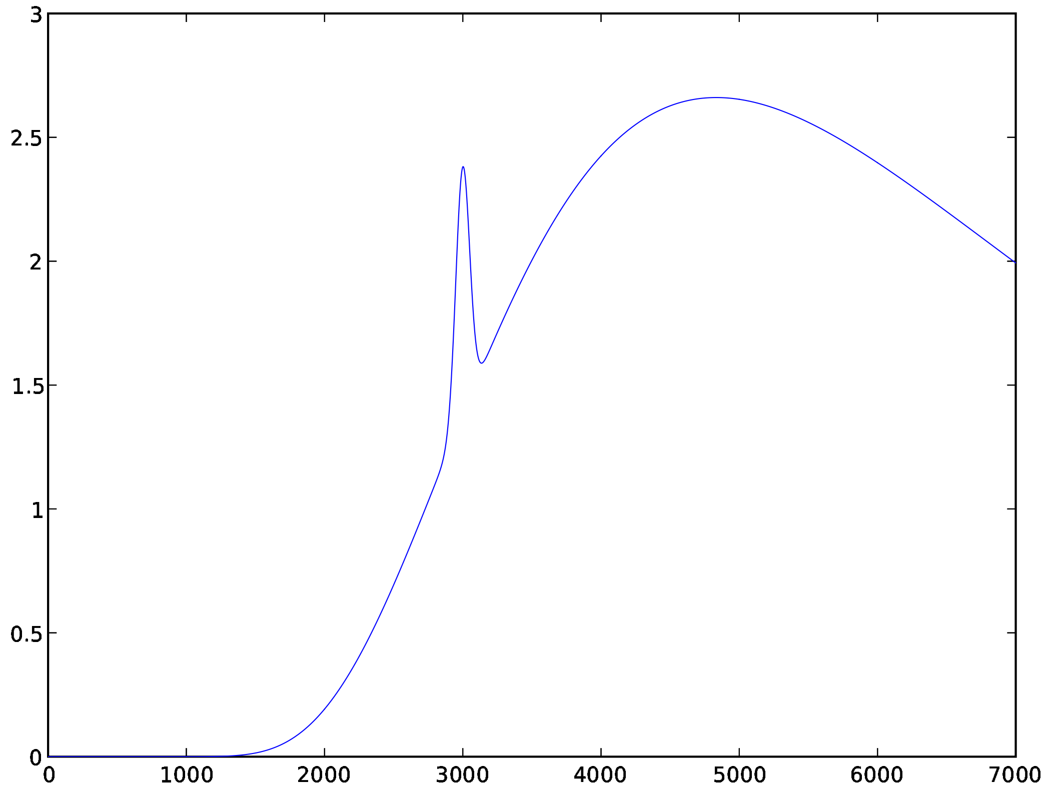
### 5.2.2 Initial Implementation

The approach taken for the models may strike many as unusual, but it allows great flexibility. We'll show the source code for the basic implementation, and then go into a lot of detail explaining how it works. It probably will appear unintelligible at first glance even though it is relatively short. Have patience. This example makes use of inheritance and abstract classes. The latter is an important and often used technique. Abstract classes are generally incomplete implementations that are never expected to have an instance created of it directly. They are intended to be inherited by other classes that will fill out the functionality. Classes that will have instances created are sometimes called concrete classes in contrast to abstract.

```
import numpy as n

class SourceFunction:
    '''Abstract Class representing a source as a function of wavelength

Units are assumed to be Flambda
'''
    def __add__(self, other):
        return CompositeSourceFunction(self, other, 'add')
        # __radd__ not needed

class CompositeSourceFunction(SourceFunction):
    '''Source function that is a binary composition of two other functions
'''
    def __init__(self, source1, source2, operation):
        self.comp1 = source1
        self.comp2 = source2
        self.operation = operation
    def  __call__(self, wave):
        if self.operation == 'add':
            return self.comp1(wave) + self.comp2(wave)
    class BlackBody(SourceFunction):
        def __init__(self, temperature):
            self.temperature=temperature
        def __call__(self, wave):
            BBCONST =6.625e-34 * 3e8/(1.38e-23 * 1.e-10)
            exparg = BBCONST/(n.array(wave)*self.temperature)
            exparg[exparg>600] = 600. # to prevent overflows
            return 1.e21/(wave**5 * (n.exp(exparg)-1.))

    class Gaussian(SourceFunction):
        def __init__(self, center, width):
            self.width=width
            self.center=center
        def __call__(self, wave):
            return n.exp(-(wave-self.center)**2/(2*self.width**2))
```

Before explaining how it works, we'll give some context by showing how it is used.

```
>>> import spec as s
>>> from pylab import *
>>> spectrum = s.BlackBody(6000) + s.Gaussian(3000, 50)
>>> wavelengths = arange(7000) + 1.
>>> plot(spectrum(wavelengths))
```



A composite spectrum is built simply by adding basic elements together as an expression (one could add more Gaussian components at different wavelengths and widths just by adding more terms in the expression).

Although spectrum is an object, it can be called as though it were a function. When called with an array of wavelengths, it returns an array of fluxes that is then plotted.

While the use is deceptively simple, and the code is relatively short, more is happening than immediately meets the eye. This example uses a number of Python's object-oriented capabilities. We will introduce these not in the order that they appear in the source file, but in the order they are used in the example.

### 5.2.3 Basic object creation

The first things that happen are two basic spectrum objects are created. One is a an instance of a `BlackBody` class. Looking at the source code, notice that the `__init__` method (what gets called as `s.BlackBody.__init__(self, 6000)` when `s.BlackBody(6000)` is executed) is very simple. All it does is save the temperature as an attribute. Nothing else at all is done. Likewise, when `s.Gaussian(3000,50)` is executed, its `__init__` method simply saves the parameters of the specified Gaussian. So far, not a whole lot has happened. Two new objects exist, but they haven't really done anything.

### 5.2.4 Spectrum addition

When these two objects are added is when things get interesting. As we mentioned in an earlier section, Python lets you define what should happen when various operators are encountered. We didn't give much detail about how that happened. When Python finds two objects combined with one of its standard operators (addition in this case) it looks at the first object and sees if it has a `__add__` method defined. If it does, it calls it, giving it the other object as an argument. Fine you say, but what about the case when this method isn't present, which at first glance, it doesn't appear to be for either of these classes. But there is. Notice that both of these classes inherit from `SourceFunction`. And in particular they inherit its methods. There is only one method defined for SourceFunction, and wouldn't you know it, it's `__add__`. Any class that inherits `SourceFunction` automatically gets the `__add__` method for free. It is written in such a way that it has no dependence on the details of the class that inherits it.

So `s.SourceFunction.__add__` will be called with the `BlackBody` object as `self`, and the `Gaussian` as `other`. This method is quite simple, but you will quickly notice that it returns an instance of a 3rd class: `CompositeSourceFunction`. This 3rd class also inherits from `SourceFunction`, and like `BlackBody` and `Gaussian`, it also defines an `__init__` and `__call__` method. Instead of saving the attributes of a specific spectrum model (like temperature or central wavelength), it saves references to the two objects that are supposed to be added. And that's all! Nothing seems to really be added. At this point it is easy to think that this object stuff is all smoke and mirrors. Where's the real action?

That comes later. To briefly review what has happened in the creation of spectrum, Two basic source function objects are created, and when added together, generate a `CompositeSourceFunction` object that contains a reference to each of the two basic objects, but otherwise hasn't really done any real computation.

### 5.2.5 Evaluation of the spectrum at given wavelengths

Now we encounter `spectrum(wavelengths)`. As previously mentioned, when an object is called as a function, Python sees if the object has defined a `__call__` method. If it has, it is called with the arguments given (and if not, an exception is raised). As you can see from the source, all the concrete (i.e., non-abstract) classes have defined `__call__`. For the case of the `CompositeSourceFunction`, its `__call__` method is called with `wavelength` as the argument. What it does is call each of the two source function objects it refers to with the same `wavelength` argument. So the respective `__call__` methods of the `BlackBody` and `Gaussian` are, in turn, called with the same wavelength array. You will see that the `__call__` methods are where the real action takes place. This is where the spectrum model computation resides. As a result, each call results in an array of fluxes that is returned to the `CompositeSourceSpectrum` object `__call__` method, and then these are added, and the resulting array is returned.

### 5.2.6 Why this is better than the traditional approach

Answering this first requires understanding what the traditional approach would be. And that's not so obvious. How would you do it? There are two variants of 'traditional' that can be considered: writing this in a language like C or Fortran, or writing it in IDL using arrays. Let's take these in turn. With the example above, we can construct a composite spectrum from any number of basic elements by adding them together. So the traditional C/Fortran approach must be able to deal with an unlimited number of components of many types. That may not seem so hard, just provide a list somehow. Yes, that works for this basic version. But the example above hasn't yet addressed multiplicative factors, which are easy to address in this framework (and a later version will show that). Thus the software will have to deal with arbitrarily complex expressions of spectral components. It is hard to escape the fact that one needs to write an expression parser (as synphot does). That is no simple matter at all. For the Python object-oriented approach, it is completely unnecessary since Python is doing the parsing for you. This alone is a huge advantage.

Is this an advantage over IDL as well? That depends on how you approach the problem. If the approach is to take advantage of the array capabilities, one might consider generating an array for each component at a specified set of wavelengths. If one can do this for all components using the same set of wavelengths, then IDL can handle combinations of spectra using its array expression facilities. Parsing expressions would not be necessary. But this approach is fraught with difficulties. What wavelengths to choose? If you don't choose a set that is fine enough, you risk missing important features in the components. What if someone chooses a Gaussian line width of 0.01 angstroms and you only sample every angstrom? No matter what your default choice, eventually someone will find it a problem. What range of wavelengths should you cover? That involves choices as well. Arbitrary restrictions will come back to bite you eventually. When someone asks for fluxes for a specific wavelength set, how do you get these from the sampled wavelengths? Interpolation? What kind of interpolation? Choices there can often backfire (suppose it generates negative values when the spectrum component model was always positive). When the spectrum model can use tabular spectra in addition to analytic spectra, will the resampling of the tabular spectra onto a standard wavelength set introduce unacceptable errors, particularly in view of the fact that there may be subsequent resamplings?

In fact, the use of arrays to represent all components is a possible choice for C or Fortran implementations as well, and the same issues arise there also. Indeed, that's how synphot was implemented. And every one of the concerns listed have been manifested as actual problems in practical usage of synphot at one time or another. There has never been a truly satisfactory solution to them using standard wavelength sets.

We'll detail other advantages of object-oriented approach after adding some more features and capabilities.

### 5.2.7 Take 2: handling multiplicative effects

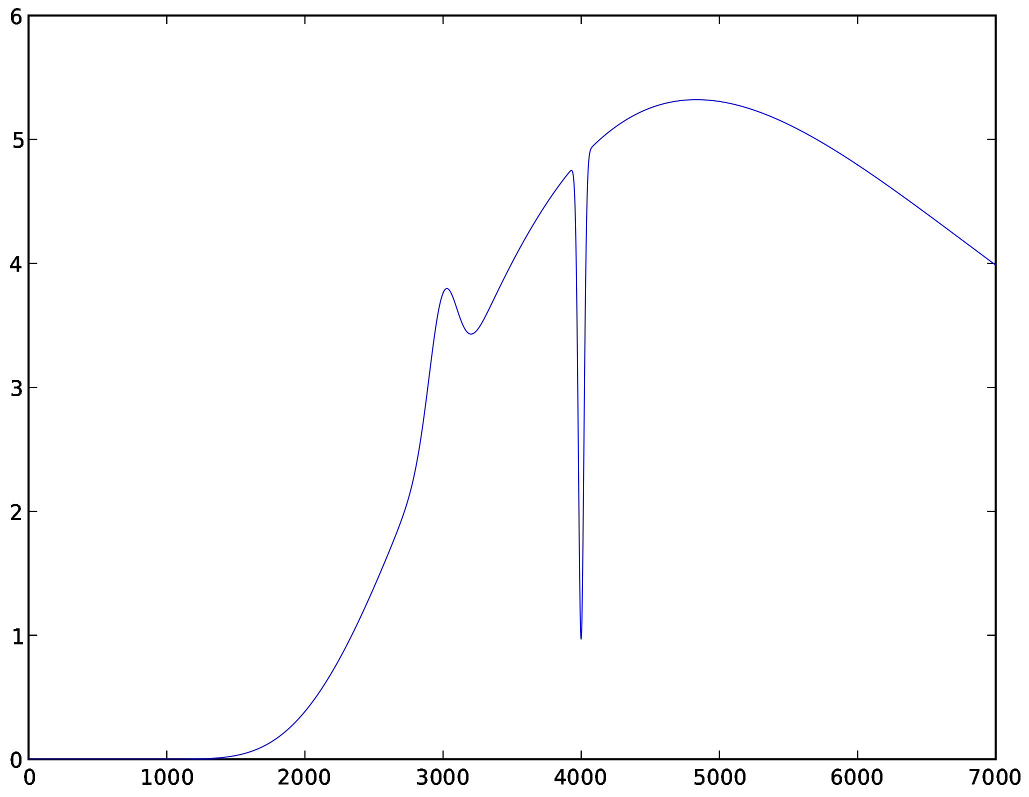
Simply adding fixed components together isn't very useful. There must be a way of handling scaling each component as well as handing effects that are multiplicative such as absorption lines or reddening. This next version adds these capabilities (new or modified code is shown prefaced with |).

```
  import numpy as n

| class TransmissionFunction:
|     '''Abstract Class representing a transmission function of wavelength
|
| Unitless'''
|     def __mul__(self, other):
|         if isinstance(other, TransmissionFunction):
|             return CompositeTransmissionFunction(self, other)
|         if isinstance(other, SourceFunction):
|             return CompositeSourceFunction(self, other, 'multiply')
|         if type(other) in [type(1), type(1.)]:
|             return CompositeTransmissionFunction(
|                 self, ConstTransmission(other))
|         else:
|             print "must be product of TransmissionFunction, SourceFunction or constant"
|     def __rmul__(self, other):
|         return self.__mul__(other)
|
| class CompositeTransmissionFunction(TransmissionFunction):
```

```
|     '''Transmission function that is a product of two other transmission functions'''
|     def __init__(self, tran1, tran2):
|         if (not isinstance(tran1, TransmissionFunction) or
|             not isinstance(tran2, TransmissionFunction)):
|             print "Arguments must be TransmissionFunctions"
|             raise TypeError
|         self.tran1 = tran1
|         self.tran2 = tran2
|     def __call__(self, wave):
|         return self.tran1(wave) * self.tran2(wave)
|
| class ConstTransmission(TransmissionFunction):
|     def __init__(self, value):
|         self.value = value
|     def __call__(self, wave):
|         return 0.*wave + self.value
|
| class GaussianAbsorption(TransmissionFunction):
|     def __init__(self, center, width, depth):
|         self.center = center
|         self.width = width
|         self.depth = depth
|     def __call__(self, wave):
|         return 1. - self.depth*n.exp(-(wave-self.center)**2/(2*self.width**2))

  class SourceFunction:
      '''Abstract Class representing a source as a function of wavelength

  Units are assumed to be Flambda
  '''
      def __add__(self, other):
|         if not isinstance(other, SourceFunction):
|             print "Can only add SourceFunctions"
|             raise TypeError
        return CompositeSourceFunction(self, other, 'add')
        # __radd__ not needed
|     def __mul__(self, other):
|         if type(other) in [type(1), type(1.)]:
|             other = ConstTransmission(other)
|         if not isinstance(other, TransmissionFunction):
|             print 'Source functions can only be '+ \
|              'multiplied by Transmission Functions or constants'
|             raise TypeError
|         return CompositeSourceFunction(self, other, 'multiply')
|     def __rmul__(self, other):
|         return self.__mul__(other)
  class CompositeSourceFunction(SourceFunction):
      '''Source function that is a binary composition of two other functions
  '''
      def __init__(self, source1, source2, operation):
          self.comp1 = source1
          self.comp2 = source2
          self.operation = operation
      def  __call__(self, wave):
            if self.operation == 'add':
                return self.comp1(wave) + self.comp2(wave)
            if self.operation == 'multiply':
                return self.comp1(wave) * self.comp2(wave)
    class BlackBody(SourceFunction):
        def __init__(self, temperature):
            '''Temperature in degrees Kelvin'''
            self.temperature=temperature
        def __call__(self, wave):
            BBCONST =6.625e-34 * 3e8/(1.38e-23 * 1.e-10)
            exparg = BBCONST/(n.array(wave)*self.temperature)
            exparg[exparg>600] = 600. # to prevent overflows
            return 1.e21/(wave**5 * (n.exp(exparg)-1.))

    class Gaussian(SourceFunction):
        def __init__(self, center, width):
            self.width=width
            self.center=center
        def __call__(self, wave):
            return n.exp(-(wave-self.center)**2/(2*self.width**2))
```

Again, we will start with an example of usage:

```
>>> spectrum = s.GaussianAbsorption(4000,20,0.8) * \
...     (s.Gaussian(3000,100)+2.*s.BlackBody(6000))
>>> plot(spectrum(wavelengths))
```



No really new object-oriented concepts are introduced in this example except perhaps the checking of object types. This is primarily an extension of the previous concepts to new operations and classes. Again it is useful to trace what happens for the usage example.

Three objects are initially created, two of them essentially identical to the previous example (though they have richer operator behavior now). The third is an instance of a new kind of wavelength function: `GaussianAbsorption` which is a concrete case of a general `TransmissionFunction`. The key thing to note is that these two kinds of functions have somewhat different rules about what can be done with them. Transmission functions are unitless. They can be multiplied with either transmission or source functions. But they cannot be added with each other (or anything else for that matter). Source functions have specific units. Thus they can be added with other source functions or multiplied by unitless functions, producing a new source function in the process. These rules are embodied in the definitions (or lack of them) for the operator methods for these classes. We'll get back to the details of these after following the example through to the end.

The first difference that shows up is when the `BlackBody` object is multiplied by a floating point constant. Since floating point constants don't know what to do with `SourceFunction` objects, it tells Python it can't deal with it which causes Python to then look to see if the `SourceFunction` object has a `__rmul__` method. It does, so it is called with the floating point value as its argument. Since multiplication is symmetric for this case, all that method does is call the `__mul__` method (don't duplicate code if you don't need to!). That method checks to see if the type of the other object is either a `TransmissionFunction` instance, an integer or float value (if none of these, it gives up). If it is a numeric constant, it turns it into a `ConstTransmission` object and then proceeds to create a composite source function (which now has been modified to accept both kinds of objects and to support addition and multiplication by saving the operation type as one of the object's attributes).

The resulting composite source function is added to the `GaussianSource` object the way it was before (but now it is necessary to indicate addition in the new composite source object (which has as one of it elements another composite source object). Finally this is multiplied by a Gaussian line absorption transmission function creating a third composite source object. In this case it is the `GaussianAbsorption` object's `__mul__` method that is called first. That returns the final composite source function object.

As in the previous case, calling the final object with a wavelength array is what evaluates the model by evaluating the components of each composite object in turn and then adding or multiplying the results as appropriate and returning those back in turn (notice that the `__call__` method for the composite source object checks to see which operation to perform).

## 5.3 Further enhancements to the spectrum model

At this point we'll stop presenting full implementations and instead discuss how one might go about enhancing the capabilities of code (we have only so much space and you have only so much patience). Each issue will show one or more examples of usage for the proposed mechanism.

### 5.3.1 Determining total flux

Very often the point of making such spectral source models is being able to determine the total flux expected. After all, imaging observations effectively integrate flux density over wavelengths, and one often wants to compare the observations with a model. Integrating the flux density of a model spectrum is an essential capability.

Fortunately, numerical integration is a well-studied subject. Unfortunately, no general algorithm is foolproof for all functions that must be integrated. The advantage of the approach chosen for modeling spectra is that it provides a means for avoiding these problems. Generally speaking, the problem with numerical integration is knowing where the function is changing rapidly. Since each source and transmission function is specially constructed, we can include as part of their behaviors (i.e., methods) a means of them telling us where we should sample the function for integration purposes. In other words we could define a method (with a specific implementation for each kind of function) called `waveset()` that returns an array of wavelengths that properly sample the structure of the function. For example, for the `GaussianSource` or `GaussianAbsorption` objects, it would ensure that it returned enough points within the main part of the Gaussian profile. It possibly could take an optional parameter that indicated sampling frequency or what amount of percent change was permitted in the function between samples. The integration routine would use these wavelengths to evaluate the function for integration purposes.

But what about composite objects? What are their wavelength sets? Simple, when one calls `.waveset()` for a composite object, it calls `.waveset()` on the two components and joins them (i.e., the union of the returned wavelengths. If either of those objects are composite, the same process is repeated until it hits endpoint spectrum objects (just like addition).

The integration routine would be defined in the abstract class (it should have no dependencies on the specific functions) and would first call the `.waveset()` method to get the wavelengths it will use for doing the numerical integration. Possibly several integration methods could be used, either as options to the main method or as different methods. In this way, it should be possible to make the integration relatively robust against a wide variety of model parameters.

An example of use:

```
>>> source = GaussianAbsorption(4000,20,0.8) * \
...          (Gaussian(3000,100) + 1.e10*BlackBody(6000))
>>> source.integrate() # returns integrated flux
```

### 5.3.2 Handling empirical spectra

A means of modeling spectra that could not accept empirical spectra would be very limited. The example given only addressed analytical models. How could one combine the two approaches? If one grants that it will be necessary to resample the empirical spectra (and it is–e.g., combining it with a very narrow line analytical feature that is smaller than the spacing in the empirical model), then one may treat the empirical spectra as an extreme form of analytical spectra. The interpolation behavior is then embodied in the evaluation behavior (i.e., the `__call__` method). The initialization of the `SourceFunction` object saves the arrays that define the wavelengths for the fluxes and the fluxes themselves. Likewise, the `.waveset()` method returns the specific wavelengths for the fluxes used. Constructed that way, empirical spectra fit very well within this object framework. Likewise, empirical transmission functions can be handled the same way.

An example:

```
>>> data = pyfits.getdata('fuse.fits')
>>> source = TableSource(flux=data.field('flux'),
...                      wavelength=data.field('wave'))
```

### 5.3.3 Valid wavelength ranges

In many instances, particularly with empirical data, it may be necessary to indicate what the valid wavelength range of the component and the net spectrum model is. This is fairly easy to add. Each component may add as part of its initialization what the valid range is for that component (even for analytical models) as an optional parameter. Empirical components would, by default, take their valid range from the range of wavelengths for the flux values. The net valid range would be obtained from a method called `waverange()`, defined for the base class to use the values saved for basic components, and it would be overridden for composite objects to call `waverange()` for each of its components and take the intersection of those ranges to obtain the net range for that composite. A value of `None` at either end would mean no limit. For example, using the previous table data and a black body:

```
>>> source.waverange()
[985., 1085.]
>>> BlackBody(6000).waverange()
[None, None]
```

It may also make sense to provide a method to greatest extents of ranges present (the union of all ranges).

A secondary use of wavelength ranges is to bound integration of analytic components that no intrinsic limits to their range. For example, if the net range of a given model is unbounded, then a default range may be used or an exception may be generated.

### 5.3.4 Component normalization

Frequently it is necessary to define the scaling factor for a given component based on the integrated flux of that component, often through a different transmission function than being used in the given model (say a V filter). One way to incorporate this capability into the proposed scheme is to add a scale factor to all function objects (including composite objects) that defaults to 1.0. Then a `.normalize()` method would be added to the base class which takes one mandatory argument (the integrated flux expected) and an optional transmission function (.e.g., a filter transmission curve) to be applied to the source function before integration. Since this is generic to all source functions there need be only one version defined for the base class. This method then does the integration on the net source function, and takes the ratio of the integration result with the desired value to set the scale factor. The scale factor must of course be used by the `__call__` method to apply it to the computed fluxes. Some examples (units are addressed later):

```
>>> source = BlackBody(6000).normalize(VMag(23.3))
>>> source = (Gaussian(3000,50) +
...         1.e10*BlackBody(6000)).normalize(Jy(3.1),
...                    trans=JohnsonV)
```

### 5.3.5 Redshifts

Handling redshifts is straightforward as well. Any function component (source or transmission) can take an optional $z$ parameter at initialization and save it as an attribute. This works for concrete components but not so conveniently for composite ones. These can be handled either by defining a method to set the $z$ for the composite object, or a function that does the equivalent. The effect of a nonzero $z$ is to transform the intrinsic wavelengths being used and divide $F_\lambda$ by $(1+z)$. The flux is computed at the 'rest' wavelength for the model. Thus all methods that deal with wavelengths (`__call__`, `waverange`, `waveset`, etc.) need to apply the appropriate transformation to the wavelengths. For example, in the `__call__` method, the wavelengths given as an argument would be redshifted to the source's rest frame, and then the model applied to that set of wavelengths and the resulting fluxes returned. For things that return wavelengths apply the inverse transformation. Both these transformations can be handled as standard functions used by all the relevant routines. In fact, it is likely that a common interface routine for all these methods can be defined for the base classes that then call the component-specific version that doesn't worry about $z$ at all. This isolates the redshift handling code to a small number of locations. The following snippets of code illustrate how this would be accomplished.

```
class SourceFunction:
[...]
    def __call__(self, wavelengths):
        return self.resteval(invZ(wavelengths, self.z))/(1.+self.z)
    def waveset(self):
        return Z(self.restwaveset(), self.z)
```

What had previously been defined as `__call__` and `waveset` in the concrete function classes now are renamed `resteval` and `restwaveset` respectively. Since `validrange` is only defined for the base class, there is little reason to depend on such indirection.

The following shows how redshift would be used.

```
>>> source = BlackBody(6000,z=1.3) # or
>>> source = BlackBody(6000).z(1.3)
>>> source = (Gaussian(3000,20)+Blackbody(6000)).z(1.3) # or
>>> source = Z(Gaussian(3000,20)+Blackbody(6000), 1.3)
>>> source = (GaussianAbsorption(3000,20,0.8,z=.3)* \
              BlackBody(6000,.5)).z(.8)
```

The last case shows two components with individual redshifts and then with a subsequent redshift applied to the combination (cumulatively). Note that it is possible to define a function `Z` that actually performs a transformation of wavelengths when given a scalar or array, and sets the `z` attribute of source functions when those appear as arguments. Not everyone may think that it would be good to share the same function for both uses.

### 5.3.6 Different unit systems

Any practical modeling system would have to handle many different units, both for the wavelengths, and the fluxes. The approach taken here is to use only one for internal representation (a common approach) and deal with other units only for conversion to and from other representations. At first glance units appear deceptively simple, but unfortunately, they are anything but. This is partly because there is context involved (e.g., electron volts can be interpreted as wavelengths or energies), and because there may be dependencies on other values such as exists between$F_\lambda$ and $F_\nu$ (depends on the wavelengths or frequencies used). The first problem can be solved by confining our context to spectra (electron volts is presumed to be a wavelength). The second is trickier since it needs more than the flux to transform. It would be nice to have transformation functions that only took scalar or arrays as arguments and applied the appropriate scaling factor to generate the values in the appropriate units. It usually is important to have things like unit transformations have a consistent interface so that one does not need a lot of code checking whether the conversion function is this type or that before applying it. So a pragmatic solution is to just allow for an optional wavelength argument to the unit conversion functions that is mandatory for conversions between frequency and wavelength representations. Allowing the specification of the units for the `__call__` method avoids having to again specify the wavelength in the unit conversion function since the wavelength is already present as a argument. Dealing with this problem is not necessary for wavelength unit conversions. For example:

```
>>> asJy(BlackBody(6000)(NM(300)) # evaluate at 300 nm, return in Janskys
>>> source = GaussianSource(EV(.5), EV(.1)) # centered at .5 electron volts
>>> source(NM(10), funits=Fnu) # or
>>> asFnu(source(NM(10), NM(10))
```

## 5.4 The upside to object-oriented programs

A major goal of Object-Oriented Languages is achieving as much decoupling of dependencies as possible. The more one can isolate code dependencies and make it more modular, the fewer problems you will generally have when changes are needed. When you must make changes in many places to add a new feature, you are much more likely to break something. Having to deal with many modules and locations at once makes it difficult to really understand what is going on; it is far easier to get confused.

This is done by trying bring the code that manipulates data as close to the data as possible. A mindset that is focused on functions primarily (as C and Fortran are) forces one to do a lot of bookkeeping to keep track of the data. Where is it? What things can I do with it? Typically it leads to lots of conditional code that says if it is this kind of data do this, if that, do that, and so forth. Add a new kind of data or variant, and you must go and change many functions so that they can deal with it. Very Bad.

With objects, the code is kept with the object. Each object knows how to do what's required of it. These may vary from object to object or may not. To add a new object that is supposed to 'play nicely' with others, usually doesn't require making changes to the code of all the others. Often it doesn't require any.

The spectrum model example is a good illustration of that. To add a new model doesn't require handling integration, units, redshift, or many other common effects. Most of the code for the model is that focused on what the model is all about: determining the flux at a given wavelength. And that's primarily it. Secondarily it is giving hints about where the model changes the most. And very little else. The cost to add models is about as minimal as it could be. Likewise, the general algorithms such as that doing the composite evaluation or integration, don't need to know anything about the specifics of any of the models. This is generally a Good Thing. (This is referred to as 'data hiding' or 'encapsulation' in the OO biz.)

Despite the simplicity of the model code, it is quite capable of generating quite complex networks of sources and transmission functions. The simplicity of organization does not prevent it from being used for complex cases. Given the operator overloading features (something not available in Java), it is possible to make these networks correspond very closely to their mathematical equivalent. Unlike synphot, it isn't necessary to form an expression as a string and write a program to parse and evaluate it. The code is the definition! (Lest those who say that this is bad, Python makes it trivial to evaluate strings containing such code, so it's just as easy to do it the other way).

Much of the power of Object-Oriented Programming comes from what is called 'polymorphism'. What it means is having several objects that share some common behavior and attributes, but possibly have much that is different as well. The spectral components example very much makes use of this. They all must be able to evaluate themselves at requested wavelengths (how they do so is entirely up to them). They must give a set of wavelengths that sample them well. They must handle redshifts, normalization, and integration. They must support basic addition and multiplication. Some of these behaviors are handled by the parent class, some by the child classes. But they all must meet these standard behaviors. They may have other nonstandard methods and attributes. There is nothing wrong with that. But the point is that it allows one to write very general software that takes a wide variety of components and handles them uniformly. They handle their specific differences internally.

If you find you are writing a lot of functional code that has many tests for the kind of data it is working on, particularly the same set of tests in different functions, that is usually a sign that the problem is a good candidate for polymorphic objects.

Notice that most of the enhancements did not require a great reworking of the architecture. Given a properly designed framework, quite powerful enhancements are possible without extensive reworking.

The nice thing about Python is that it doesn't force you to put everything in an object-oriented framework. You can make it entirely functional or a hybrid. A good example of a hybrid approach is numpy where many operations are handled by functions, not methods, primarily since it is a better match to mathematical convention.

## 5.5 The downside

Invariably there is some bad with the good. Object-oriented technology has its downside. One is that although it is very good at reducing dependencies, the manner in how that is done can make it more difficult to follow what actually is happening as time progresses. This can make debugging more involved if there are many objects involved, and many jumps from one object to another. Those used to procedural programming (which by its nature is more time-oriented) can find this more frustrating to understand. Taking this specific example, one sees the flow of program control jump from child class to parent and back, and from one object's method to another that it refers to. The flow is just not as linear through the file as many procedural programs would be.

This is partly because objects rely heavily on indirection, either through the objects they link to, or the classes they inherit from. Indirection is an indication of greater abstraction, more power, and a correspondingly greater power to confuse.

Some problems don't lend themselves to object orientation. The example does, but there are cases that are hard to frame this way. It is a mistake to try to force all problems into one approach.

Those that are experienced at procedural programming tend to have a harder adjustment to an object-oriented approach. It's quite easy to fall into a pattern of using classes in a mostly procedural way. The best guard against that is by reading good examples of OO design (in real projects) or have others that have that kind of experience review your code.

The previous section glibly asserted that example showed how flexible the OO architecture was given a proper framework. Achieving the proper framework is often not trivial. The ability to do so comes with experience and some analysis of the problem. Typically, OO design puts more emphasis on the analysis and design phase than does a procedural approach. A good design makes it easy to extend and maintain, a bad design not. The same certainly can be said for any approach (including procedural), but an OO approach is more sensitive to the quality of the design. Having said that, Python is so productive that one should particularly avoid becoming paralyzed by the analysis and design phase. Experimentation is an important part of the design process and Python makes that comparatively easy. Do not make the mistake of trying to figure everything out before starting. Think a little, try something, start over.

## 5.6 Loose ends

Taking a case study approach to OO programming in Python means some mechanical details have been passed over. It's not possible to cover them all, but some of the basics will be elaborated.

### 5.6.1 Method inheritance and overloading

When you use a method for an object Python will search for the method definition up the inheritance chain. It sees if the method exists for the specific class that is being used. If it doesn't exist there, it looks at the class that it inherits from to see if that class defines it. If not and that class inherited from yet another, that one will be searched for the method until there are no further inherited classes (then an exception is raised). Overloading a method means that it exists in an inherited class and it is redefined in a descendant class. Generally speaking, overloading a method means that the method should support the same argument interface that the original method does (nothing enforces that), though it usually is considered permissible to allow extra optional arguments and keywords.

### 5.6.2 Object initialization

One thing to realize is that, unlike some other OO languages, Python requires fairly explicit instructions regarding objects. One such area is in their creation. All classes have an implicit default definition of `__init__` that exists if they do not define one. So it is not necessary to define `__init__` (even if inheritance is not used). But realize that no attributes can be created at initialization if `__init__` is not defined since that is where they must be set (it is always possible to add them any time later if you don't use special features to prohibit them). If you inherit from a class that does define its own `__init__` and you don't define `__init__` in the subclass, then the original `__init__` will be used. If you wish to define a new `__init__` for the subclass and invoke the parent class `__init__` you must do so explicitly (as shown in the example in section 5.1.5). Or you may completely ignore the parent class `__init__` if you are replacing its functionality entirely. You have full control, but you must be explicit about what initializations you wish to be done.

#### 5.6.3 Multiple inheritance

Python permits classes to inherit from more than one class. When these parent classes share the same method names, Python has clear (but involved) rules about determining the search order for which one it uses (called "method resolution order"). It is considered good practice to use multiple inheritance as sparingly as possible. See http://www.python.org/2.3/mro.html.

#### 5.6.4 New-style vs old-style classes

With version 2.2 Python introduced "new-style" classes that provided many more capabilities for classes. For most beginners, these distinctions are not relevant since they involve fairly advanced concepts. All Python data types are now "new-style" classes. Old-style classes were retained for compatibility purposes. If your class definition does not inherit from "object" or a built-in Python data type (lists, strings, etc.) it is an old-style class, otherwise it is a new style class. Again, you are not likely to need to know or care yet; this explanation is to explain why you may see these two variants:

```
class Class: # old style
class Class(object): # new style
```

When Python 3.0 shows up, it will only support new style classes and then inheriting from object will be optional. (ref. http://www.python.org/2.2.2/descrintro.html)

#### 5.6.5 Duck typing

Making use of polymorphism does not require that the objects inherit from a common class. It is a common idiom in Python to allow objects that may have no common parent to be used in the same context so long as they support the needed behaviors. For example, there are many things that expect a 'file-like' object. Something that can be written to and read from as though it were a file. So long as you provide an object that has the needed methods and attributes, that's good enough. Likewise, when writing your own classes and code, be careful not to try to be too specific on the types of arguments. It is usually better to enclose attempts to use them in try/except blocks rather than enforce that they be a certain type or class. In this way the code will be much more flexible.

And the phrase "Duck typing"? It derives from the philosophy that if something quacks like a duck, walks like a duck, looks like a duck, etc., as far as you are concerned, it is a duck. It doesn't actually have to be of type "Duck" for it to be acceptable. Use of this phrase indicates that this approach is being used.

## 5.7 What you haven't learned about Python (so if you are interested, go look it up)

#### 5.7.1 iterators

Iterators are a powerful extension to the language. They are objects that can be iterated over in that one can ask for the next item until the end is reached. They are like sequences in some respects but cannot be indexed arbitrarily. They can be infinite. Many things in Python that used to return lists now are iterators. Iterators can be used in `for` statements.
See http://www-106.ibm.com/developerworks/library/l-pycon.html?n-l-9271.

#### 5.7.2 generators

Generators are similar to iterators except they allow one to write functions that repeatedly return values and retain the state of where they last left off.
See http://www-128.ibm.com/developerworks/linux/library/l-pycon.html.

### 5.7.3 list comprehensions

These are a convenient way of creating lists. An example explains best:

```
>>> newlist = [i**2 for i in range(10)]
```

creates a list of all squares of 0 through 9.
See http://www.secnetix.de/~olli/Python/list_comprehensions.hawk for the full details.

### 5.7.4 sets

Python has recently introduced a set data type (otherwise known as unordered collections).
See http://www.python.org/doc/2.4/whatsnew/node2.html.

### 5.7.5 metaclasses

New-style classes provide some very powerful capabilities, particularly with regard to 'metaclass' capabilities. These generally are quite advanced aspects, considered 'brain-exploding' by many.
See http://www.python.org/2.2.2/descrintro.html#metaclass if you are fearless.

## 5.8 The Zen of Python

(author: Tim Peters, a Python legend)

- Beautiful is better than ugly.
- Explicit is better than implicit.
- Simple is better than complex.
- Complex is better than complicated.
- Flat is better than nested.
- Sparse is better than dense.
- Readability counts.
- Special cases aren't special enough to break the rules.
- Although practicality beats purity.
- Errors should never pass silently.
- Unless explicitly silenced.
- In the face of ambiguity, refuse the temptation to guess.
- There should be one– and preferably only one –obvious way to do it.
- Although that way may not be obvious at first unless you're Dutch.
- Now is better than never.
- Although never is often better than *right* now.
- If the implementation is hard to explain, it's a bad idea.
- If the implementation is easy to explain, it may be a good idea.
- Namespaces are one honking great idea – let's do more of those!

## Exercises

1. Complete the dictionary inheritance example by completing new versions of the `has_key`, `update`, `get`, and `setdefault` methods.

2. Add support for tabular source and transmission spectra to the spectrum example

# 6 Interfacing C & C++ programs

This tutorial will start with an overview of all the approaches to interfacing with C and C++ (or otherwise trying to get performance improvements), followed by examples of manually writing wrappers for C functions, ending with an example that uses numpy arrays as arguments to the C function.

## 6.1 Overview of different tools

There are, fortunately or unfortunately depending on your view, many ways to interface Python to C and C++ code (or achieve equivalent performance). A single tutorial cannot hope to cover all of them. Or even two. But a short overview of many (but not all!) of the possibilities and what factors should be considered in choosing them will be given. The following link gives a good example of using the different approaches and the speedups that resulted (be careful not to overgeneralize from the one example though): http://www.scipy.org/documentation/weave/weaveperformance.html

**Manual wrapping:** This is the case of explicitly using the Python C-API. In many respects this is the most work, but also has the least dependencies on other tools and is generally the most portable solution. One advantage of this approach is that you will learn what goes on under the hood (compared to using the more automatic tools described below), and learn something about Python internals. This is also a disadvantage. This is the method that this tutorial will cover.

**SWIG:** SWIG stands for Simplified Wrapper Interface Generator. This is a mostly automated tool for computer generating the interfacing code between C functions and Python. It generally avoids needing to learn as much about the Python C-API (though customizations may require some use of the Python C-API). Although it avoids having to learn about the Python API, it means learning about how to use SWIG, which has its own learning curve. It generally is most useful if one is trying to interface a large, existing C library for which writing Python wrappers would be very tedious. Another advantage of SWIG is that the SWIG software does not need to be distributed with the C libraries. One can generate the wrapper code on a build machine and distribute the code it generates. In this respect it is as portable as manual wrapping. (http://www.swig.org)

**weave:** Weave is a tool that allows one to: 1) write 'in-line' C code (written as strings within Python source files) that can be automatically wrapped, built, and imported on the fly, 2) Turn array expressions into corresponding C++ code, also wrapped, built and imported on the fly, or 3) wrap existing C extensions. It requires installing scipy. It does not currently work with numarray for the array facilities (though we are close to porting weave to work with numarray). It's array facility allows one to write Python syntax code for arrays that may not be very efficient, and then, without change, have the same code converted to C++ and run much faster (e.g., where you must iterate over array elements in an explicit loop). It generally avoids much of the pain of writing wrappers (and even C code for array expressions), but it is not as good a tool as SWIG is for wrapping existing C libraries, and its dependence on scipy is a drawback (currently). Using weave limits C code to the Python context (i.e., the C code is not usable in other C programs) It requires a C++ compiler as well. (http://www.scipy.org/documentation/weave)

**PyCXX:** This is explicitly a tool for wrapping C++ code and to make the interface between C++ objects and Python OO facilities more transparent and convenient (matplotlib makes use of it). SWIG used to support C++ poorly, but has improved greatly recently so it could also be considered for wrapping C++ code. (http://cxx.sourceforge.net)

**Boost.Python:** Another means of wrapping C++ code. (http://www.boost.org/libs/python/doc/)

**ctypes:** A module that allows access to existing sharable modules (not the kind written explicitly for Python) to execute functions present in the module. The conversion of data types is handled by the module as well as handling pointers and structures. In effect it lets you do the wrapping at the Python level. The advantage of this approach is that it allows direct access to existing libraries without needing to generate C wrapping code. But there are limitations to what it can do, and it forces dealing with platform specifics of sharable libraries to the 'wrapping' Python code. (http://starship.python.net/crew/theller/ctypes/)

**Pyrex:** Allows writing code in a pseudo Python syntax that will be turned into C code. How much faster it is depends on how you write the pseudo Python (the more specific one can be about types, for example, the more likely the speed will improved), though it usually is slower than code written directly in C. Doesn't do anything special about numeric arrays (and thus not particularly convenient to use in the array context). Generally much easier to write than the manual method. Code so written is inextricably bound to the Python context. (http://www.cosc.canterbury.ac.nz/~greg/python/Pyrex/)

**Psyco:** A special implementation of Python for Intel processors. that does special optimizations internally. This does not require recoding in any way except to give directives about optimization. Can be very fast in some cases; however it doesn't do much for numeric arrays, particularly if you must operate on non-Python numeric types (anything but float doubles, long ints, and complex doubles). Not at all portable since it only works on Intel processors and requires a special version of Python. (http://psyco.sourceforge.net)

### 6.1.1 Summary

If you are adverse to writing C at all, try Pyrex or weave (in mode 2), or psyco if you don't mind binding your solution to Intel processors. If you want to minimize the work of wrapping new C code, use weave (if installing scipy is not an issue). If you wish to interface an existing C library of a significant size (i.e., large number of functions), consider SWIG. Use PyCXX, Boost.Python, weave, or SWIG to wrap C++ code (which depends on what features of C++ you are using and how you wish to interface to Python). Use ctypes if wrapping an existing library is not feasible (e.g., you don't have a compiler available). If you just have a small number of C functions to wrap, you may find manual interfacing easiest to do, particularly if one of the examples is close to what you need to do and will serve as a template.

## 6.2 Overview of manual interfacing

This guide is intended to give a basic overview of how to call C functions from Python by hand. Even if you end up using some of the alternatives to writing extensions, it still is good to understand what is going on underneath between Python and C.

There is already documentation in the Python distribution on how to interface C programs (*Extending and Embedding the Python Interpreter* & *Python/C API Reference Manual*); but its size is imposing and difficult for many to get started with. That documentation is quite useful once you get the basic idea of how the Python C API works.

This tutorial will not cover calling Python from C, nor will it describe how to develop a new Python type or class in C.

## 6.3 A few basic concepts before getting started

### 6.3.1 How Python finds and uses C extensions

The vast majority of C extensions use the dynamic loading feature of all modern operating systems. Suppose you want to write a C extension that you wish to import as `bozo`. Python will first search directories in its path for a bozo package directory, then for an extension module. (Each directory is searched for each possible form of a module before proceeding to the next directory in the path.) The acceptable extension module names are: `bozo.`*xxx* or `bozomodule.`*xxx*, where the filename extension .*xxx* is generally `.so` for Unix (including Mac OS X) and `.pyd` or `.dll` for Windows. (If neither a package or extension module is found then it looks for a Python module in its various forms.) When it finds `bozomodule.so`, it will then make a system call to examine all public symbols in that dynamically loadable module. It is looking for only one, called `initbozo`). From that it finds everything else (more details later). The important point is that it is rare that one needs to statically link Python with an extension. The module may not even have been in existence when you started your Python session (indeed, this is what allows some tools to compile and load new extensions on the fly from an existing Python session).

### 6.3.2 Compiling and Linking C Extensions

The details of compiling and linking C extensions vary from platform to platform. These are given in detail in the *Extending and Embedding the Python Interpreter* reference. It is usually far easier is to use distutils to handle the details of building C extensions

### 6.3.3 A Simple Example

```
[bozo.c]

#include <Python.h>

static PyObject *
times_two(PyObject *self, PyObject *args)
{
    int val;
    if (!PyArg_ParseTuple(args, "i", &val)) \
        return NULL;
    return Py_BuildValue("i", 2*val);
}
static PyMethodDef bozoMethods[] = {
    {"times_two", times_two, METH_VARARGS, "Double any integer"},
    {NULL, NULL, 0, NULL} /* Sentinel */
};
PyMODINIT_FUNC
initbozo(void)
{
    (void) Py_InitModule("bozo", bozoMethods);
    if (PyErr_Occurred())
}
[setup.py]
from distutils.core import setup, Extension
setup(name="bozo", version="1.0",
      ext_modules=[Extension("bozo", ["bozo.c"])])
# To build type "python setup.py build"
# The sharable will appear in one of the build subdirectories
# of the source directory.
# To install: "python setup.py install"
```

This represents a new C extension module which will, when built, end up as `bozomodule.so`, be imported as `bozo`, contain one and only one function, called `times_two`, that takes an integer argument and returns that integer value multiplied by two. That is,

```
>>> import bozo
>>> bozo.times_two(2)
4
```

**Line-by-line Explanation**

All Python C extension functions have one of two possible signatures, namely, they either take two or three `PyObject*` arguments, and return a `PyObject*` (this example only takes two). `PyObject*` is the generic type used for all Python values whether they are built-in types or objects. The function is declared as `static` so that it is not exposed as a public symbol (Python is able to access it through the mechanism described later). The first argument is a reference to `self` when it is used as a method call (and because this is not a method definition, is not used). The second is expected to be a Python tuple that contains all of the arguments provided when calling the function at the Python level.

There are many specialized functions to obtain the contents of Python tuple objects. Since all function calls at the C level must unpack the arguments from this tuple, there are some standard higher-level functions provided to handle the tedium of doing so in one call. In this case it is `PyArg_ParseTuple` (there are other variants, e.g., if keyword arguments are expected). `PyArg_ParseTuple` takes the tuple argument as its first argument, a format string as its second argument, and pointers to variables that are to receive the values unpacked from the tuple as the rest of the arguments. The format string indicates how many and what kinds of values are expected. In this particular case, `"i"` tells it to expect an integer value (correspondingly `"ifs"` tells it to expect 3 values, an integer, float, and string). Here the integer value will be put into the variable `val`, thus a pointer to `val` is passed.

Since Python has no type checking this seems very risky. What if someone passed a different type, such as a string? This is why it is imperative to check the return value of the `PyArg_ParseTuple` function. If the values are compatible with the format string, then the function will return with a nonzero value, otherwise it returns with a zero value. Hence in the example, the return value is checked to see if it is zero. If it is, the function returns with a NULL value. C extension functions called by Python that return NULL values indicate that Python should raise an exception.

The function `Py_BuildValue` effectively does the reverse; it returns a Python object suitable for returning to Python, built from the format string and a corresponding number of arguments that provide the values (which may be a single value or a tuple depending on whether one or more values are provided). Here there is only one value, an integer (the original value multiplied by 2).

The rest of the module contains the mechanism used to expose this function to Python. The next item is an array of structs that contains a record for each function defined. Each entry contains the Python name for the function, a reference to the function itself, some information about the argument conventions (`METH_VARARGS` means that it takes two arguments; `METH_KEYWORDS` means that it takes three), the last argument being the keyword dictionary provided by Python). The NULL values in the last entry indicate the end of the struct array (note that this function table is also declared `static` to make it private).

Finally, there is one public symbol in the module. Python expects to see a symbol of the form `init`*name*, in this case `initbozo`. This function calls a Python module initialization function with the method table defined just before as the second argument (the name of the module is the first argument). When Python imports the module, it will check to see if there were any errors on initialization; there is no need to check for an error on the `Py_InitModule` call unless one intends to print a more descriptive error message as to why it failed.

So when Python opens this module, it seeks a function named `initbozo` and executes it. By doing so it obtains a reference to all the functions defined in `bozoMethods` which it will use to call the functions when needed.

### 6.3.4 So what about more complicated examples?

Rather than wade through complex examples, we will discuss the issues involved with more complex cases and refer the reader to the documentation for the full details. The main point is to put these issues into context. A more complex example is annotated in section 6.5.

### 6.3.5 But what about using arrays?

Those impatient to see arrays used in a C extension may jump ahead to Section 6.6. Except for the part dealing with reference counting (explained in 6.4.4) it should be understandable.

## 6.4 General Pointers

The simplest interfaces are generally when only simple objects (i.e., values close to primitive types such as ints, floats, and strings) need to be passed to and from C functions. In those cases one needs little more than `PyArg_ParseTuple` (or `PyArg_ParseTupleAndKeywords`), and `Py_BuildValue` to accomplish the task. Realistically, if that is all one needed to pass and receive, it is likely one didn't need to write a C extension in the first place. For numerical processing, it will often be true that the only other complex object that must be handled is a numpy array object (ndarray), and perhaps lists, tuples, and dictionaries. Accessing ndarrays will be addressed in the next section.

Accessing other kinds of Python objects is accomplished by using the Python C API. Lists, tuples, strings and dictionaries have many functions to create, modify and access these objects. For example, there are calls to get the $i$th element from a list. Function calls to access definite types such as these are considered part of the concrete protocol; functions part of the abstract protocol allow accessing more abstract types such as sequences, mappings or Python objects without forcing the object to be a specific type. There are many calls to manipulate Python objects, for example, to get object attributes or make method calls. Generally one can perform the same operations on Python types and objects in C that one can in Python. It's just a lot more tedious. You must make sure that types are correct, and handle error cases. Not to mention reference counting (more on that later).

It is usually a good idea to separate the C code into a wrapper part (the component that handles extracting all the information from Python to pass to another C function that is generic, i.e., has no particular dependence on Python). If one is trying to interface to existing C functions, this approach is the only sensible one. When one is writing a new type for Python or is performing very intricate operations on Python objects, this is not possible at all; the whole extension is interwoven with the Python API.

### 6.4.1 Handling Calling Arguments

`PyArg_ParseTuple()` and its variants have a number of options to make handling calling arguments more convenient. In particular, you may associate a converter function with an argument to automatically call it to convert the argument to another type (see the `O&` option). One can use `|` in the format string to separate the required arguments from the optional arguments and end the format string with `:`<*functionname*> to indicate that any error in the calling sequence should use the given name. See section 5.5 of the *C-API* reference for full details.

### 6.4.2 Returning None

Returning Python `None` values is fairly simple (i.e., a return value that is interpreted as `None` within Python; note, this is quite different than returning NULL values that signal that Python should raise an exception):

**Method** 1:

```
return Py_BuildValue("");
```

**Method** 2:

```
Py_INCREF(Py_None); # Explained in section on reference counting
return Py_None;
```

### 6.4.3 Exceptions

As previously mentioned, exceptions are signaled by returning a NULL value. More work is required if an associated string and exception type are desired. A number of functions are provided to handle exceptions. The most useful for simple cases are:

```
PyErr_SetString(PyObject *exc, char *msg);
```

This sets the string used by Python to report the exception. The first argument is given an exception value. Any Python exception type can be used; the corresponding name in C for a Python exception generally has `PyExc_` prepended to the corresponding name (e.g., `PyExc_ArithmeticError` for `ArithmeticError`). The following illustrates:

```
PyErr_SetString(PyExc ValueError, "zero value not permitted");
```

To check whether errors have occurred in a series of Python API calls (as opposed to errors detected by your own C code):

```
PyObject *PyErr_Occurred()
```

Which returns the current exception object if one did occur and NULL otherwise.

```
PyErr Clear()
```

Will clear any error states.

```
PyErr_Format(PyObject *exc, const char *format...)
```

A convenience function that sets the error string using the format string and extra arguments provided (a la `printf`) and returns NULL, See Chapter 4 in the *C API* reference for full details.

### 6.4.4 Reference Counting

Without a doubt, the most error-prone aspect of writing more complex C extensions is handling reference counts properly. Reference counting is how Python manages memory. Every time an object references another, the reference count of that object is incremented. Every time a reference is removed, the reference count is decremented. After being decremented, if the count reaches 0, Python frees the memory associated with that object (and calls its destructor if necessary). When you write a C extension that relies on Python objects persisting past that call, then it is essential to ensure that the reference counts are appropriately adjusted. Not doing so may result in segfaults or other catastrophic failures.

If you are lucky, such errors only result in memory leaks. Like many other C problems, such problems may be erratic and hard to reproduce and debug. Unfortunately, the Python API is not entirely consistent in its reference counting conventions. Pay attention to the API documentation regarding this issue rather than assuming!

Python API calls may return two kinds of references to Python Objects (i.e., a `PyObject*` pointer): "owned" and "borrowed". An owned reference is one for which the Python API has incremented the reference count for you; a borrowed reference is when the reference count has not been incremented for you. In the latter case, the C code cannot depend on that object remaining available at a later time (either by returning to Python and being called again, or by calling Python API functions that may change the state of Python objects).

These concepts are better illustrated with some examples. Typically API calls that create new Python objects return an owned reference. An example is the `PyString_FromString` function. This function takes an ordinary C string and returns a Python string object. This string object is an owned reference meaning that the function has increased the reference count in the expectation that the calling program needs to keep the object around until it explicitly wants to release it. The calling C function (i.e., your code) can do one of two things with that owned reference. It can do various processing steps with that Python string, and then decrement the reference count when finished (in effect, giving up ownership). The object will then be freed from memory if nothing else has obtained ownership in the meantime. The other option is to return that string to Python without decrementing its reference count.

If your C function returns a Python object back to Python as a return value, then it must be an owned reference since Python is assuming that everything you return is an owned reference (it has assumed that you've appropriately had the reference count incremented, either directly or indirectly). In the case of the Python string just mentioned, if you explicitly return that string (e.g., return `PyString_FromString("Hello World");`) then that object is presumed to be owned. In this example it is since the API call has implicitly obtained ownership for you. It would be a great mistake to decrement the reference count to the object before returning it (it would likely result in a segmentation fault or similarly nasty ending).

Many API calls return borrowed references. For example, if you use `PyTuple_GetItem` to obtain a reference to an item in a tuple you will get a borrowed reference. There is no need to decrement the reference count if the item is no longer needed after the next call to a Python API function or return from the C function to Python. On the other hand, if you wish to return that object to Python, you must increment the reference count to make it owned or suffer a horrible fate.

Incrementing reference counts when you aren't supposed to or neglecting to decrement reference counts when you are supposed to will lead to memory leaks.

The macros `Py_INCREF()` and `Py_DECREF()` are used to manipulate reference counts of the `PyObject*` pointer supplied as an argument. Note that it is necessary to obtain ownership of `Py_None` before returning it explicitly (`Py_BuildValue("")` does that implicitly). There are corresponding macros (`Py_XINCREF()` and `Py_XDECREF()`)that will appropriately handle the case when the argument is a NULL pointer (when nothing is done)

See section 1.2.1 of the *C API* reference for full details.

One can build Python with some special options to make help debugging reference count problems in extensions easier. Consult `Misc/SpecialBuilds.txt` in the Python source tree for instructions on how to do this. The most useful (and simplest) option is probably the first, `Py_REF_DEBUG`, which shows the total number of reference counts after each interactive command.

### 6.4.5 Using debuggers on Python C Extensions

To make using debuggers easier, use the "`./configure --with-pydebug`" configuration option to configure the Python source tree for debug mode before installing Python. Such "debug Pythons" are generally easier to use in an extension debugging context since they configure distutils to compile and link extensions for debugging.

### 6.4.6 How to Make Your Module Schizophrenic

Significant C extension modules often contain functions useful for other writers of C extensions (numpy is a good example of such a case). However, the usual style for Python extensions is that they only expose one public symbol, they can't be used in the usual way to link other C libraries or extensions to (actually, the reasons have more to do with finding portable ways of making extension modules linkable rather than requiring private function). The clever Python developers have developed a highly portable solution, albeit somewhat obscure and ugly. If you don't need to do this yet, ignore this section!

The short explanation is that the solution is centered on developing an include file for your extension module that exposes the private functions through a function jump table (an array of function pointers to the private functions) and macros (to make the awful syntax of referencing a function pointer array appear as a simple function call). This approach requires code that uses the extension as a library to call an initialization function that fills in a pointer to the jump table before any attempt to use the API functions.

For the details read *Providing a C API for an Extension Module* in the *Extending and Embedding the Python Interpreter* reference. Read it a few times ;-).

## 6.5 A More Complex Example

*[dp wrap.c]*

```
/* Separation into wrapper code artificial since called function
** has Python API calls too */
/* Lacking some error checking */

#include <Python.h>
extern PyObject * dp(PyObject *);
extern PyObject * add_spam(PyObject *);

static PyObject *
print_wrap(PyObject *self, PyObject *args)
{
    PyObject *obj, *rval;
    if (!PyArg_ParseTuple(args, "O", &obj))
        return NULL;
    rval = dp(obj);
    if (rval)
        return Py_BuildValue("O", rval);
    else
        return NULL;
}

static PyObject *
add_spam_wrap(PyObject *self, PyObject *args)
{
    PyObject *obj;
    if (!PyArg_ParseTuple(args, "O", &obj))
        return NULL;
    return add_spam(obj); /* note PyBuild_Value not used since:
                          ** 1) returned object is already owned
                          ** 2) single value doesn't need tuple
                          */
}

static PyMethodDef dpMethods[] = {
{"dpprint", print_wrap, METH_VARARGS,
    "Returns all numeric values in a dictionary in a list"},
{"add_spam", add_spam_wrap, METH_VARARGS,
    "appends ', and spam' to given string representation of object"},
{NULL, NULL, 0, NULL} /* Sentinel */
};

PyMODINIT_FUNC
initdp(void)
{
    /* Note use of alternate module init that allows defining
    ** Docstring for Module xs
    */
    (void) Py_InitModule3("dp", dpMethods, "Two silly and useless functions");
}
```

*[dp.c]*

```
#include <Python.h>
#include <string.h>
#include <stdlib.h>

PyObject* dp(PyObject *dict)
{
    /*
    ** Extract all numeric values in a dictionary and return as a list.
    ** Raise exception if not a dictionary
    */
    int dictsize, i;
    PyObject *dlist, *dkeys, *key, *ditem;
    if (!PyDict_Check(dict))
    {
        PyErr_SetString(PyExc_TypeError,
                 "Argument must be dictionary");
        return NULL;
    }
    dictsize = PyDict_Size(dict);
    dlist = PyList_New(0);
    dkeys = PyDict_Keys(dict);
    for (i=0; i<dictsize; i++)
    {
        key = PyList_GetItem(dkeys, i); /* borrowed reference */
        ditem = PyDict_GetItem(dict, key); /* borrowed reference */
        if (PyNumber_Check(ditem))
        {
            Py_INCREF(ditem); /* Important! */
            PyList_Append(dlist, ditem);
        }
    }
    /* Free up remaining unneeded owned python object before returning */
    Py_DECREF(dkeys);
    return dlist;
}

PyObject* add_spam(PyObject *obj)
{
    /*
    ** Add the string ', and spam' to the string representation of the object
    */
    PyObject *pystr, *newstr;
    char *str1, *str2;
    int csize;
    pystr = PyObject_Str(obj); /* should check for success */
    str1 = PyString_AsString(pystr);
    csize = PyString_Size(pystr);
    str2 = (char *) malloc(csize + 20); /* leave space for ', and spam' */
    strcpy(str2, str1);
    strcat(str2, ", and spam");
    newstr = PyString_FromString(str2);
    free(str2);
    Py_DECREF(pystr);
    return newstr;
}
```

*[setup.py]*

```
from distutils.core import setup, Extension
setup(name="dp", version="1.0",
ext_modules=[Extension("dp", ["dp_wrap.c", "dp.c"])])
```

*[dp_test.py]*

```
"""Doctest module for dp extension
>>> dp.__doc__
'Two silly and useless functions'
>>> dp.dpprint.__doc__
'Returns all numeric values in a dictionary in a list'
>>> dp.dpprint({1:"hello","bozo":2})
[2]
>>> dp.dpprint([2])
Traceback (most recent call last):
File "<stdin>", line 1, in ?
TypeError: Argument must be dictionary
```

```
>>> dp.dpprint()
Traceback (most recent call last):
File "<stdin>", line 1, in ?
TypeError: function takes exactly 1 argument (0 given)
>>> dp.dpprint({1:None, 2:3, 5:3, 6:1, 9:"None"})
[3, 3, 1]
>>> dp.add_spam([1,2])
'[1, 2], and spam'
>>> dp.add_spam.__doc__
"appends ', and spam' to given string representation of object" """

def _test():
    import doctest, dp_test
    return doctest.testmod(dp_test)

if __name__ == "__main__":
    print _test()
```

## 6.6 numpy example

In principle, using numpy from C is handled in a similar way. The primary difference is that numpy has its own C-API (much like each of the Python data objects do) that gives the programmer full access to the contents of arrays. The *Guide to Numpy* book very completely documents the numpy C-API. This tutorial should give you the foundation to understand the explanations in that book.

First we write the function to be wrapped; in particular a 1-d convolution function:

```
[convolve.c]
#include "Python.h"
#include "numpy/arrayobject.h"
static void Convolve1d(long ksizex, npy_float64 *kernel,
    long dsizex, npy_float64 *data, npy_float64 *convolved)
{
    long xc; long halfk = ksizex/2;
    for(xc=0; xc<halfk; xc++)
        convolved[xc] = data[xc];
    for(xc=halfk; xc<dsizex-halfk; xc++) {
        long xk; double temp = 0;
        for (xk=0; xk<ksizex; xk++)
            temp += kernel[xk]*data[xc-halfk+xk];
        convolved[xc] = temp;
    }
    for(xc=dsizex-halfk; xc<dsizex; xc++)
        convolved[xc] = data[xc];
}
```

Notice that this function has no explicit dependencies on numpy or Python (well, it does make use of the `npy_float64` typedef that the numpy include file (arrayobject.h) provides, but double could have been used as well). It is a straightforward C function that takes 2 pointers to double precision 1-d arrays, along with corresponding sizes for the arrays, and a pointer to the output array of the same type and size as the input array (not kernel).

The following begins the wrapper part of the file.

```
static PyObject *
Py_Convolve1d(PyObject *obj, PyObject *args)
{
    PyObject *okernel, *odata;
    PyArrayObject *kernel=NULL, *data=NULL, *convolved=NULL;
    if (!PyArg_ParseTuple(args, "OO", &okernel, &odata)) {
        PyErr_SetString(PyExc_ValueError,
               "Convolve1d: Invalid number of parameters.");
        goto _fail;
    }
```

Two PyObject pointers are defined for the two expected arguments, and the object pointers for those arguments are obtained.

```
    kernel = (PyArrayObject *) PyArray_ContiguousFromAny(
             okernel, NPY_FLOAT64, 1, 1);
    data = (PyArrayObject *) PyArray_ContiguousFromAny(
            odata, NPY_FLOAT64, 1, 1);
    if (!kernel || !data) goto _fail;
```

What happens in this part of the code needs some background explanation. Typically a C programmer expects arrays to be a simple, contiguous array of values in memory, and in the C context, this is the normal convention. But what numpy considers arrays may not be this simple. Arrays may not be contiguous since a sliced, strided view of an array defines an array to be to be non-contiguous series of values. What's more, the values in the array may be byte-swapped from the native representation of the processor, and it may not even be properly memory-aligned. Dealing with such arrays places a large burden on the programmer to iterate through all the values in the array (something numpy handles behind the scenes).

The two calls to PyArray_ContiguousFromAny for each of the respective arguments first ensures that the argument is an array or a Python object that can be cast into an array (e.g., a Python list). If not, a NULL value is returned. If the argument is an array which is not contiguous, properly byte-ordered, or aligned, then a copy of the array will be generated that is. If the type specified in the function call is different than the type of the array (the presence of NPY_DOUBLE indicates that a float64 array is being requested), a copy will also be made. The 3rd and 4th arguments specify the minimum and maximum acceptable values for the number of dimensions. If the input array is the right type and satisfies the other conditions, the function simply returns the input argument, otherwise it returns the pointer to the new array copy. In short, these function calls ensure you get data in an easily used form and of the type requested.

```
    convolved = (PyArrayObject *) PyArray_FromDims(
                data->nd, data->dimensions, NPY_FLOAT64);
    if (!convolved) goto _fail;
```

The PyArray_FromDims function call creates a new array from scratch given the specified shape and type. At this point it is worth pointing out that the 'array' pointers are not themselves pointers to C arrays but instead pointers to Python data structures. This data structure contains information about the array such as where the actual array data are located, the type, number of dimensions, the size of each dimension, strides, and other information. This information is outlined in the previously referenced numpy chapters (xxx). We will only refer to those structure members necessary for this simple example. So the member nd refers to the number of dimensions and the member dimensions is a pointer to an array of data dimensions (of length nd). After this preparation, we are ready to call the function that we wrote to actually do the computation, now using the properly cast data member of the array structure that points to the data array.

```
    Convolve1d(kernel->dimensions[0], (npy_float64 *) kernel->data,
               data->dimensions[0], (npy_float64 *) data->data,
               (npy_float64 *) convolved->data);
```

After processing the arrays, they should be DECREF'ed if no longer used. After this completes successfully, we can clean up (handling reference counts appropriately for the normal and error cases) and return the result to Python.

```
    Py_DECREF(kernel);
    Py_DECREF(data);
    return PyArray_Return(convolved);
_fail:
    Py_XDECREF(kernel);
    Py_XDECREF(data);
    Py_XDECREF(convolved);
    return NULL;
}
```

Finally, the rest of the code needed by Python to see the new function:

```
static PyMethodDef convolveMethods[] = {
{"convolve1d", convolve1d, METH_VARARGS,
    "convolve 1-d array"},
{NULL, NULL, 0, NULL} /* Sentinel */
};

PyMODINIT_FUNC
initconvolve(void)
{
    import_array() /* Note essential initialization call for numpy! */
    (void) Py_InitModule("convolve", convolveMethods);
}
[setup.py]
import numpy
def configuration(parent_package='',top_path=None):
    from numpy.distutils.misc_util import Configuration
    config = Configuration('convolve',parent_package,top_path)
    config.add_extension('convolve',
                         sources=["convolve.c"],
                         include_dirs = [numpy.get_include()])
    return config
if __name__ == "__main__":
    from numpy.distutils.core import setup
    config = configuration(top_path='').todict()
    setup(author='Smooth Operator',
          author_email = 'con@stsci.edu',
          description = '1D array convolution function',
          version = '1.0',
          **config)
```

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# Appendix A: Python Books, Tutorials, and On-line Resources

The Python web site (www.python.org) contains pointers to a great deal of information about Python including its standard documentation, conferences, books, tutorials, etc. In particular, the following links will contain up-to-date lists of books and tutorials:

- Books: www.python.org/moin/PythonBooks
- Tutorials: www.python.org/doc/Intros.html (all online)

Books of note for beginners that have some programming experience:

- *Learning Python* (2nd ed) Lutz & Ascher: Probably the standard introductory book
- *The Quick Python Book* by Harms & McDonald: some prefer the style of this one
- *Python: Visual QuickStart Guide* by Fehily: and others this one
- *Dive Into Python: Python for Experienced Programmers* by Pilgrim (free on-line version also available)

On-line tutorials or books:

- *An Introduction to Python* by van Rossum: The original tutorial
- *A Byte of Python by Swaroop*: essentially an on-line book.
- *A Quick Tour of Python* by Greenfield and White:
  http://stsdas.stsci.edu/pyraf/doc/python_quick_tour (A bit dated but comparatively brief). PDF also available.

Reference books:

- *Python Essential Reference* (2nd ed.) by Beazley
- *Python in a Nutshell* by Martelli
- Python Library Documentation (available free on-line)

Mailing lists:

- astropy: For astronomical packages (e.g. PyRAF, PyFITS, numdisplay):
  http://www.scipy.net/mailman/listinfo/astropy
- numpy: http://sourceforge.net/mail/?group_id=1369
- matplotlib: http://sourceforge.net/mail/?group_id=80706
- ipython: http://www.scipy.net/pipermail/ipython-user/

Numpy: The most complete reference for numpy is the Guide to Numpy book written by Travis Oliphant. While it is not free (it will eventually be so), it has a wealth of information about numpy, particularly about the more advanced features and inner workings. It can be obtained from: http://www.tramy.us/. Free documentation and tutorials can be found at: http://www.scipy.org/Documentation

Manuals for numpy, PyFITS, PyRAF, ipython, and matplotlib are all available. Google PyFITS, numpy or PYRAF with "manual" to find those. The matplotlib User Guide is available on a link from the home page (Google "matplotlib"). The ipython manual is available from ipython.scipy.org. The numdisplay instructions are available at: http://stsdas.stsci.edu/numdisplay/doc/numdisplay_help.html

# Appendix B: Why would I switch from IDL to Python (or not)?

We do not claim that all, or even most, current IDL users should switch to using Python now. IDL suits many people's needs very well and we recognize that there must be a strong motivation for starting to use Python over IDL. This appendix will present the pros and cons of each so that users can make a better informed decision about whether they should consider using Python. At the end we give a few cases where we feel users should give serious consideration to using Python over IDL.

## Pros and Cons of each

These are addressed in a comparative sense. Attributes that both share, e.g.., that they are interpreted and relatively slow for very simple operations, are not listed.

**Pros of IDL:**

- Mature many numerical and astronomical libraries available
- Wide astronomical user base
- Numerical aspect well integrated with language itself
- Many local users with deep experience
- Faster for small arrays
- Easier installation
- Good, unified documentation
- Standard GUI run/debug tool (IDLDE)
- Single widget system (no angst about which to choose or learn)
- SAVE/RESTORE capability
- Use of keyword arguments as flags more convenient

**Cons of IDL:**

- Narrow applicability, not well suited to general programming
- Slower for large arrays
- Array functionality less powerful
- Table support poor
- Limited ability to extend using C or Fortran, such extensions hard to distribute and support
- Expensive, sometimes problem collaborating with others that don't have or can't afford licences.
- Closed source (only RSI can fix bugs)
- Very awkward to integrate with IRAF tasks
- Memory management more awkward
- Single widget system (useless if working within another framework)
- Plotting:
  - Awkward support for symbols and math text
  - Many font systems, portability issues (v5.1 alleviates somewhat)
  - not as flexible or as extensible
  - plot windows not intrinsically interactive (e.g., pan & zoom)

**Pros of Python:**

- Very general and powerful programming language, yet easy to learn. Strong, but optional, Object Oriented programming support
- Very large user and developer community, very extensive and broad library base
- Very extensible with C, C++, or Fortran, portable distribution mechanisms available
- Free; non-restrictive license; Open Source
- Becoming the standard scripting language for astronomy
- Easy to use with IRAF tasks
- Basis of STScI application efforts
- More general array capabilities
- Faster for large arrays, better support for memory mapping
- Many books and on-line documentation resources available (for the language and its libraries)
- Better support for table structures
- Plotting
  - framework (matplotlib) more extensible and general
  - Better font support and portability (only one way to do it too)
  - Usable within many windowing frameworks (GTK, Tk, WX, Qt...)
  - Standard plotting functionality independent of framework used
  - plots are embeddable within other GUIs
  - more powerful image handling (multiple simultaneous LUTS, optional resampling/rescaling, alpha blending, etc)
- Support for many widget systems
- Strong local influence over capabilities being developed for Python

**Cons of Python:**

- More items to install separately
- Not as well accepted in astronomical community (but support clearly growing)
- Scientific libraries not as mature:
  - Documentation not as complete, not as unified
  - Not as deep in astronomical libraries and utilities
  - Not all IDL numerical library functions have corresponding functionality in Python
- Some numeric constructs not quite as consistent with language (or slightly less convenient than IDL)
- Array indexing convention "backwards"
- Small array performance slower
- No standard GUI run/debug tool
- Support for many widget systems (angst regarding which to choose)

- Current lack of function equivalent to SAVE/RESTORE in IDL
- matplotlib does not yet have equivalents for all IDL 2-D plotting capability (e.g., surface plots)
- Use of keyword arguments used as flags less convenient
- Plotting:
  - comparatively immature, still much development going on
  - missing some plot type (e.g., surface)
  - 3-d capability requires VTK (though matplotlib has some basic 3-d capability)

**Specific cases**

Here are some specific instances where using Python provides strong advantages over IDL

- Your processing needs depend on running a few hard-to-replicate IRAF tasks, but you don't want to do most of your data manipulation in IRAF, but would rather write your own IDL-style programs to do so (and soon other systems will be accessible from Python, e.g., MIDAS, ALMA, slang, etc)
- You have algorithms that cannot be efficiently coded in IDL. They likely won't be efficiently coded in Python either, but you will find interfacing the needed C or Fortran code easier, more flexible, more portable, and distributable. (Question: how many distributed IDL libraries developed by 3rd parties include C or Fortran code?) Or you need to wrap existing C libraries (Python has many tools to make this easier to do).
- You do work on algorithms that may migrate into STSDAS packages. Using Python means that your work will be more easily adapted as a distributed and supported tool.
- You wish to integrate data processing with other significant non-numerical processing such as databases, web page generation, web services, text processing, process control, etc.
- You want to learn object-oriented programming and use it with your data analysis. (But you don't need to learn object-oriented programming to do data analysis in Python.)
- You want to be able to use the same language you use for data analysis for most of your other scripting and programming tasks.
- Your boss makes you.
- You want to be a cool, with-it person.
- You are honked off at ITT Space Systems/RSI.

Obviously using a new language and libraries entails time spent learning. Despite what people say, it's never that easy, especially if one has a lot of experience and code invested in an existing language. If you don't have any strong motivations to switch, you should probably wait.

# Appendix C: IDL/numpy feature mapping

| **IDL** | **Python Equivalent** |
|---|---|
| `.run` | `import` (.py assumed)<br>`reload(module)` # to recompile/re-execute<br>ipython: `run` |
| `@<filename>` | `execfile('fileame')`<br>ipython: `run` |
| `exit` | control-D (MS windows: control-Z)<br>ipython: `Quit` or `Exit` |
| up-arrow (command recall) | up-arrow |
| **Operators** | |
| `<,> (clipping)` | Currently no operator equivalent. The functional |
| `a < 100.` | equivalent is `choose(a<100, (a, 100.))` |
| `a > 100.` | |
| `MOD` | `%` |
| `# (matrix multiply)` | `multiply.outer()` is equivalent for some applications, `matrixmultiply()` for others. |
| `^` | `**` |
| **Boolean operators** | |
| `and` | no operator equivalent<br>Python and operator is not the same! |
| `or` | no operator equivalent<br>Python or operator is not the same! |
| `not` | no operator equivalent<br>Python not operator is not the same! |
| **Comparison operators** | |
| `.EQ.` | `==` |
| `.NE.` | `!=` |
| `.LT.` | `<` |
| `.LE.` | `<=` |
| `.GT.` | `>` |
| `.GE.` | `>=` |
| **Bitwise operators** | |
| `and` | `&` |
| `or` | `\|` |
| `xor` | `^` |
| `not` | `~` |
| `ishift(a,1)` | `a<<1` |
| `ishift(a,-1)` | `a>>1` |
| **Slicing and indexing** | **Note: order of indices is opposite!**<br>`a(i,j)` (IDL) equivalent to `a[j,i]` (Python) |
| `i:j` | `i:j` (j element not part of slice) |
| `i:*` | `i:` |
| `*:i` | `:i` |
| `a(i,*)` | `a[:,i]` |
| `a(i:j:s)` | `a[i:j:s]` |

| | |
|---|---|
| | empty arrays and slices permitted (E.g., `a[0:0]` is an array of length 0) |
| | `-i` (indexing from end of array) |
| | `...` (fills in unspecified dimensions) |
| | `NewAxis` (add new axis to array shape as part of subscript to match shapes) |
| | Slicing does not create copy of data, but a new view of data. |
| **Index arrays** | |
| `newarr = arr(indexarr)` | `newarr = arr[indexarr]` |
| `arr(indexarr) = valuearr` | `arr[indexarr] = valuearr` |
| **Array Creation** | |
| `fltarr()` | `array(seq, [dtype])` to create from existing sequence |
| `dblarr()` | `zeros(shape, [dtype])` to create 0 filled array |
| `complexarr()` | `ones(shape, [dtype])` to create 1 filled array |
| `intarr()` | chararray for fixed length strings |
| `longarr()` | |
| `bytarr()` | |
| `make_arr()` | |
| `strarr()` | |
| `findgen()` | `arange(size, [dtype]))` |
| `dindgen()` | `arange(start, end, [dtype])` |
| `indgen()` | `arange(start, end, step, [dtype])` |
| `lindgen()` | no equivalent for strings |
| `sindgen()` | |
| `replicate()` | `repeat` (more general) |
| **Array Conversions** | |
| `byte(arrayvar)` | `arrayvar.astype(<dtype>)` |
| `fix(arrayvar)` | |
| `long(arrayvar)` | |
| `float(arrayvar)` | |
| `double(arrayvar)` | |
| `complex(arrayvar)` | |
| **Array Manipulation** | |
| `reform()` | `reshape()` [also `arrayvar.flat()` and `ravel()`, or changing the shape attribute] |
| `sort()` | `argsort() [i.e., indices needed to sort]` |
| `arr(sort(arr))` | `sort(arr) [i.e., sorted array]` |
| `max(arrayvar)` | `arrayvar.max()` |
| `min(arrayvar)` | `arrayvar.min()` |
| `where()` | `where()` |
| `arr(where(condition))` | `arr[where(condition)]` |
| `transpose()` | `transpose()` |
| `[a,b]` (array concatenation) | `concatenate()` |
| **Array shape behavior** | |
| shape mismatches result in the smaller of the two | If shapes do not follow broadcast rules, error generated. No shape truncation performed ever. |

| | |
|---|---|
| **Numeric types** | |
| `byte` | `int8` |
| | `uint8` (unsigned) |
| `int` | `int16` |
| `long` | `int32` |
| `float` | `float32` |
| `double` | `float64` |
| `complex` | `complex32` |
| | `complex64` |
| | `uint16` |
| | `uint32` |
| | `int64` |
| | `uint64` |
| **Math Functions** | |
| `abs()` | `abs()` |
| `acos()` | `arccos()` |
| `alog()` | `log()` |
| `alog10()` | `log10()` |
| `asin()` | `arcsin()` |
| `atan()` | `arctan()` |
| `atan(y,x)` | `arctan2()` |
| `ceil()` | `ceil()` |
| `conj()` | `conjugate()` |
| `cos()` | `cos()` |
| `cosh()` | `cosh()` |
| `exp()` | `exp()` |
| `floor()` | `floor()` |
| `imaginary()` | `complexarr.imag` (`.real` for real component) |
| `invert()` | Matrix module |
| `ishift()` | `right_shift()`, `left_shift()` |
| `round()` | `round()` |
| `sin()` | `sin()` |
| `sinh()` | `sinh()` |
| `sqrt()` | `sqrt()` |
| `tan()` | `tan()` |
| `tanh()` | `tanh()` |
| `fft()` | `fft` (fft module) |
| `convol()` | `convolve()` (convolve module) |
| `randomu()` | `random()`, `uniform()` (random module) |
| `randomn()` | `normal()` (random module) |
| **Programming** | |
| `execute()` | `exec()` |
| `n_elements(arrayvar)` | `arrayvar.nelements()` |
| `n_params()` | closest equivalent is `len(*args)`. Ability to supply default values for parameters replaces some uses of `n_params()` |
| `size()` | `.shape` attribute, `.dtype` attribute |
| `wait` | `time.sleep` (time module) |

# Appendix D: matplotlib for IDL Users

Author: Vicki Laidler

This is not a complete discussion of the power of matplotlib (the OO machinery) or pylab (the functional interface). This document only provides a translation from common IDL plotting functionality, and mentions a few of the additional capabilities provided by pylab. For a more complete discussion, you will eventually want to see the tutorial and the documentation for the pylab interface:
http://matplotlib.sourceforge.net/tutorial.html
http://matplotlib.sourceforge.net/matplotlib.pylab.html

## Setting up and customizing your Python environment:

Whether you use PyRAF, IPython, or the default python interpreter, there are ways to automatically import your favorite modules at startup using a configuration file. See the documentation for those packages for details. The examples in this document will explicitly import all packages used.

## Setting up and customizing matplotlib:

You will want to modify your `.matplotlibrc` plot to use the correct backend for plotting, and to set some default behaviors. (The STScI versions of the default `.matplotlibrc` have already been modified to incorporate many of these changes.) If there is a `.matplotlibrc` file in your current directory, it will be used instead of the file in your home directory. This permits setting up different default environments for different purposes. You may also want to change the default behavior for image display to avoid interpolating, and set the image so that pixel (0,0) appears in the lower left of the window.

```
image.interpolation  : nearest   # see help(imshow) for options
image.origin : lower             # lower | upper
```

I also wanted to change the default colors and symbols.

```
lines.marker      : None    # like !psym=0; plots are line plots
                              by  default
lines.color       : k       # black
lines.markerfacecolor  : k  # black
lines.markeredgecolor  : k  # black
text.color          : k     # black
```

Symbols will be solid colored, not hollow, unless you change `markerfacecolor` to match the color of the background.

### About overplotting behavior:

The default behavior for matplotlib is that every plot is a "smart" overplot, stretching the axes if necessary; and one must explicitly clear the axes, or clear the figure, to start a new plot. It's possible to change this behavior in the setup file, to get new plots by default

```
axes.hold           : False    # whether to clear the axes by
                                 default on
```

and override it by specifying the "hold" keyword in the plotting call. However I DO NOT recommend this; it takes a bit of getting used to, but I found it easier to completely change paradigms to "build up the plot piece by piece" than it is to remember which commands will decorate an existing plot and which won't.

**Some philosophical differences:**

Matplotlib tends towards atomic commands to control each plot element independently, rather than keywords on a plot command. This takes getting used to, but adds versatility. Thus, it may take more commands to accomplish something in matplotlib than it does in IDL, but the advantage is that these commands can be done in any order, or repeatedly tweaked until it's just right. This is particularly apparent when making hardcopy plots: the mode of operation is to tweak the plot until it looks the way you want, then press a button to save it to disk. Since the pylab interface is essentially a set of convenience functions layered on top of the OO machinery, sometimes by different developers, there is occasionally a little bit of inconsistency in how things work between different functions. For instance the `errorbar` function violates the principle in the previous paragraph: it's not an atomic function that can be added to an existing plot; and the scatter function is more restrictive in its argument set than the plot function, but offers a couple of different keywords that add power.

**Some syntactic differences:**

You can NOT abbreviate a keyword argument in matplotlib. Some keywords have had some shorthand versions programmed in as alternates - for instance `lw=2` instead of `linewidth=2` - but you need to know the shorthand. Python uses indentation for loop control; leading spaces will cause an error if you are at the interactive command line. To issue 2 commands on the same line, use a semicolon instead of an ampersand.

## The Rosetta Stone:

| | | |
|---|---|---|
| | `IDL` | `Matplotlib` |
| `Setup` | `(none needed if your paths are correct)` | `from numarray import *`<br>`from pylab import *`<br>`import pyfits`<br>`(Or, none needed if you set up your favorite modules in the configuration file for the Python environment you’re using.)` |
| `Some data sets:` | `foo = indgen(20)`<br>`bar = foo*2` | `foo = arange(20)`<br>`bar = foo*2` |
| `Basic plotting:` | `plot, foo` | `plot(foo)` |
| | `plot, foo, bar` | `plot(foo, bar)` |
| | `plot, foo, bar,`<br>`line=1, thick=2` | `plot(foo, bar, ’-’, lw=2)`<br>`***or spell out linewidth=2` |
| | `plot, foo, bar, ticklen=1` | `plot(foo, bar)`<br>`grid()` |
| | `plot, foo, bar, psym=1` | `plot(foo, bar, ’x’)`<br>`OR`<br>`scatter(foo, bar)` |
| | `plot, foo, bar, psym=-1,`<br>`symsize=3` | `plot(foo, bar, ’-x’, ms=5)`<br>`***or spell out markersize=5` |
| | `plot, foo, bar,`<br>`xran=[2,10], yran=[2,10]` | `plot(foo, bar)`<br>`xlim(2,10)`<br>`ylim(2,10)` |
| | `err=indgen(20)/10.` | `err = arange(20)/10.` |

| | | |
|---|---|---|
| | plot, foo, bar, psym=2<br>errplot, foo,<br>bar-err,bar+err | errorbar(foo, bar, err,<br>fmt='o')<br>errorbar(foo, bar, err, 2*err,<br>'o')<br>(error bars in x and y) |
| Overplotting with<br>default behaviour<br>changed (Not<br>recommended or<br>used in any other<br>examples | plot, foo, bar<br>oplot, foo, bar2 | plot(foo, bar)<br>plot(foo, bar2, hold=True) |
| Text, titles and<br>legends: | xyouts, 2, 25, 'hello' | text(2, 25, 'hello') |
| | plot, foo, bar,<br>title='Demo', xtitle='foo',<br>ytitle='bar' | plot(foo, bar)<br>title('Demo')<br>xlabel('foo')<br>ylabel('bar') |
| | plot, foo, bar*2, psym=1<br>oplot, foo, bar, psym=2 | plot(foo, bar*2, 'x',<br>label='double')<br>plot(foo, bar, 'o',<br>label='single') |
| | legend,['twicebar','bar'],<br>psym=[1,2],/upper,/right | legend(loc='upper right')<br>***legend will default to<br>upper right if no location<br>is specified.<br>Note the *space* in the<br>location specification string |
| | plot, foo, bar,<br>title=systime() | import time<br>plot(foo, bar)<br>label(time.asctime()) |
| Window Manipulation | erase | clf() OR cla() |
| | window, 2 | figure(2) |
| | wset, 1 | figure(1) |
| | wdelete, 2 | close(2) |
| | wshow | [no equivalent] |
| Log plotting | plot_oo, foo, bar | loglog(foo+1, bar+1) |
| | plot_io, foo, bar | semilogy (foo, bar) |
| | plot_oi, foo, bar | semilogx (foo, bar) |
| | | ***Warning: numbers that<br>are invalid for logarithms<br>(<=) will not be plotted, but<br>will silently fail; no warning<br>message is generated.<br>***Warning: you can't<br>alternate between linear plots<br>containing zero or negative<br>points, and log plots of valid<br>data, without clearing the<br>figure first - it will generate<br>an exception. |

| | | |
|---|---|---|
| Postscript output | set_plot, 'ps'<br>device,<br>file='myplot.ps',/land<br>plot, foo, bar<br>device,/close | plot(foo, bar)<br>savefig('myplot.ps',<br>orientation='landscape') |
| Viewing image<br>data: | im = mrdfits('myfile.fits',<br>1)<br><br>tv, im<br>loadct, 5<br>loadct, 0<br>contour, im<br>xloadct | f = pyfits.open('myfile.fits')<br>im = f[1].data<br>imshow(im)<br>jet()<br>gray()<br>contour(im)<br>[no equivalent] |
| Histograms | mu=100 & sigma=15 &<br>x=fltarr(10000)<br>seed=123132<br>for i = 0, 9999 do x[i] =<br>mu + sigma*randomn(seed)<br>plothist, x | mu, sigma = 10, 15<br>x = mu + sigma*randn(10000)<br>n, bins, patches = hist(x, 50) |
| | *** Note that histograms are specified a bit<br>differently and also look a bit different:  bar chart<br>instead of skyline style | |
| Multiple plots on a<br>page | !p.multi=[4,2,2]<br>plot, foo, bar<br>plot, bar, foo<br>plot, foo, 20*foo<br>plot, foo, bar*foo | <br>subplot(221) ; plot(foo, bar)<br>subplot(222) ; plot(bar, foo)<br>subplot(223) ; plot(foo,<br>20*foo)<br>subplot(224) ; plot(foo,<br>bar*foo) |
| Erasing and<br>redrawing a<br>subplot: | [no equivalent] | subplot(222)<br>cla()<br>scatter(bar, foo) |
| plotting x, y, color<br>and size: | [no obvious equivalent] | scatter(foo, bar, c=foo+bar,<br>s=10*foo) |
| Adding a colorbar | [no obvious equivalent] | colorbar() |

## Some comparisons:

### Some additional functionality:

- modify axes without replotting
- add labels, generate hardcopy, without replotting
- colored lines and points, many more point styles
- smarter legends
- TEX-style math symbols supported
- interactive pan/zoom

**Some functionality that is not yet conveniently wrapped:**

(These are items that are available through the OO machinery, but are not yet wrapped into convenient functions for the interactive user. We welcome feedback on which of these would be most important or useful!)

- subtitles
- `loadct` - to dynamically modify or flick through colortables
- `tvrdc,x,y` - to read the xy position of the cursor (will soon be available)
- histogram specification by bin interval rather than number of bins

**Some still-missing functionality:**

(These are items for which the machinery has not yet been developed.)

- surface plots
- save - to save everything in an environment
- journal - to capture commands & responses. (ipython can capture commands.)

**Symbols, line styles, and colors:**

`!psym` equivalences:

**0** line `-`

**1** plus `+`

**2** asterisk unsupported; overplotting `+` with `x` is close

**3** dot `.`

**4** diamond `d`

**5** triangle `^`

**6** square `s`

**7** cross `x`

**10** histogram `ls='steps'`

`!linestyle` equivalences:

**1** solid `-`

**2** dotted `:`

**3** dashed `--`

**4** dash-dot `-.`

The following line styles are supported:

`-` : 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

The following color strings are supported

`b` : blue

`g` : green

`r` : red

`c` : cyan

`m` : magenta

`y` : yellow

`k` : black

`w` : white

Matplotlib also accepts rgb and colorname specifications (eg hex rgb, or "white").

Approximate color table equivalences:

**loadct,0** gray()

**loadct,1** almost bone()

**loadct,3** almost copper()

**loadct,13** almost jet()

Color tables for images:

**autumn**

**bone**

**cool**

**copper**

**flag**

**gray**

**hot**

**hsv**

**jet**

**pink**

**prism**

**spring**

**summer**

**winter**

# Appendix E: Editors and Integrated Development Environments

## Editors

Python is easier to use with a good editor. Since indentation is important in Python, use of an editor that supports block indentation (indenting and undoing indentation for a block of lines) is very handy. Also important is using an editor that can automatically convert tabs to spaces (the recommended means of indenting). Fortunately, a great variety of editors handle both these requirements. Many editors provide many more features that make Python easier to code including syntax highlighting, code folding, auto-completion, etc. See http://wiki.python.org/moin/PythonEditors for a list of editors that have good support for Python.

## Integrated Development Environments

The use of IDEs with Python is not as widespread as it is for other languages (particularly Java). Some would explain that by saying that Python doesn't require IDE's as much (or doesn't benefit as much) as other languages. It may be the culture, and certainly it is at least partly due to the fact that the user base is smaller than more widely used languages (thus fewer resources available to devote to IDEs on either the open source or commercial front). Nevertheless, there are IDE's available for Python, both open source and commercial. Generally speaking, IDEs provide class browsing features, a debugger, code completion as well as more advanced editing features. It is questionable whether these sorts of features are worth the effort expended on learning how to use them if your use of Python is not heavy, especially if you are not developing complex projects.

IDLE is one that is distributed with Python. Pythonwin is one that is also open source, but only runs under Microsoft windows. In many respects emacs serves as an IDE if you willing to learn how to use it. BoaConstrictor and Eric3 are the other best known. Wing IDE, BlackAdder, and Komodo are the most well known commercial IDE's for Python; these generally have many more features than the opensource IDEs. Wing IDE is significantly cheaper for educational institutions (~$100 per developer per platform). All three are very inexpensive for students and individual (non-work, non-commercial) use (~$30). Google any of these names (with Python also in the search box) to get more information.

## Appendix F: numpy vs Numeric vs numarray

In the beginning there was Numeric, which was the first array package available for Python. Because of various shortcomings that made it more awkward to use for larger arrays, STScI developed numarray. Since each has advantages over the other, there has not been any clear indication that all Numeric users are willing to move to numarray (primarily because numarray is slower for small arrays than Numeric). This situation led to a schism in library support where many useful libraries were available for one or the other. Travis Oliphant decided to merge the two communities by merging the best features of both Numeric and numarray into a new package called numpy. The work on numpy has matured to the point that there are few reasons to use either Numeric or numarray, particularly if you are just starting to use Python.

We strongly recommend using numpy; STScI has converted all its software to use numpy. Numeric is no longer being maintained, and STScI will end all support for numarray by mid-2008.

# Appendix G: Multidimensional Array Indexing Order

What is the right way to index multi-dimensional arrays? Before you jump to conclusions about the one and true way to index multi-dimensional arrays, it pays to understand why this is a confusing issue. This appendix will try to explain in detail how numpy indexing works and why we adopt the convention we do for images, and when it may be appropriate to adopt other conventions.

The first thing to understand is that there are two conflicting conventions for indexing 2-dimensional arrays. Matrix notation uses the first index to indicate which row is being selected and the second index to indicate which column is selected. This is opposite the geometrically oriented-convention for images where people generally think the first index represents $x$ position (i.e., column) and the second represents $y$ position (i.e., row). This alone is the source of much confusion; matrix-oriented users and image-oriented users expect two different things with regard to indexing.

The second issue to understand is how indices correspond to the order the array is stored in memory. In Fortran the first index is the most rapidly varying index when moving through the elements of a two dimensional array as it is stored in memory. If you adopt the matrix convention for indexing, then this means the matrix is stored one column at a time (since the first index moves to the next row as it changes). Thus Fortran is considered a "Column-major" language. C has just the opposite convention. In C, the last index changes most rapidly as one moves through the array as stored in memory. Thus C is a "Row-major" language. The matrix is stored by rows. Note that in both cases it presumes that the matrix convention for indexing is being used, i.e., for both Fortran and C, the first index is the row. Note this convention implies that the indexing convention is invariant and that the data order changes to keep that so.

But that's not the only way to look at it. Suppose one has large two-dimensional arrays (images or matrices) stored in data files. Suppose the data are stored by rows rather than by columns. If we are to preserve our index convention (whether matrix or image) that means that depending on the language we use, we may be forced to reorder the data if it is read into memory to preserve our indexing convention. For example if we read row-ordered data into memory without reordering, it will match the matrix indexing convention for C, but not for Fortran. Conversely, it will match the image indexing convention for Fortran, but not for C. For C, if one is using data stored in row order, and one wants to preserve the image index convention, the data must be reordered when reading into memory.

In the end, which you do for Fortran or C depends on which is more important, not reordering data or preserving the indexing convention. For large images, reordering data is potentially expensive, and often the indexing convention is inverted to avoid that.

The situation with numpy makes this issue yet more complicated. The internal machinery of numpy arrays is flexible enough to accept any ordering of indices. One can simply reorder indices by manipulating the internal stride information for arrays without reordering the data at all. Numpy will know how to map the new index order to the data without moving the data.

So if this is true, why not choose the index order that matches what you most expect? In particular, why not define row ordered images to use the image convention? (This is sometimes referred to as the Fortran convention vs the C convention, thus the 'C' and 'FORTRAN' order options for array ordering in numpy.) The drawback of doing this is potential performance penalties. It's common to access the data sequentially, either implicitly in array operations or explicity by looping over rows of an image. When that is done, then the data will be accessed in non-optimal order. As the first index is incremented, what is actually happening is that elements spaced far apart in memory are being sequentially accessed, with usually poor memory access speeds. For example, for a two dimensional image `'im'` defined so that `im[0, 10]` represents the value at `x=0`, `y=10`. To be consistent with usual Python behavior then `im[0]` would represent a column at `x=0`. Yet that data would be spread over the whole array since the data are stored in row order. Despite the flexibility of numpy's indexing, it can't really paper over the fact basic operations are rendered inefficient because of data order or that getting contiguous subarrays is still awkward (e.g., `im[:,0]` for the first row, vs `im[0]`), thus one can't use an idiom such as `for row in im`; `for col in im` does work, but doesn't yield contiguous column data.

As it turns out, numpy is smart enough when dealing with ufuncs to determine which index is the most rapidly varying one in memory and uses that for the innermost loop. Thus for ufuncs there is no large intrinsic advantage to either approach in most cases. On the other hand, use of `.flat` with an FORTRAN-ordered array will lead to non-optimal memory access as adjacent elements in the flattened array (iterator, actually) are not contiguous in memory.

Indeed, the fact is that Python indexing on lists and other sequences naturally leads to an outside-to-inside ordering (the first index gets the largest grouping, the next the next largest, and the last gets the smallest element). Since image data are normally stored by rows, this corresponds to position within rows being the last item indexed.

For astronomy, we've concluded that it is more important to leave the data order unchanged rather than the indexing order since the data arrays may be so large. When this is rarely the case, then using the Fortran convention for indexing may make sense. If you do want to use Fortran ordering realize that there are two approaches to consider: 1) accept that the first index is just not the most rapidly changing in memory and have all your I/O routines reorder your data when going from memory to disk or visa versa, or use numpy's mechanism for mapping the first index to the most rapidly varying data. We recommend the former if possible. The disadvantage of the latter is that many of numpy's functions will yield arrays without Fortran ordering unless you are careful to use the 'order' keyword. Doing this would be highly inconvenient.

Otherwise we recommend simply learning to reverse the usual order of indices when accessing elements of an array. Granted, it goes against the grain, but it is more in line with Python semantics and the natural order of the data.