Introduction to Scientific Computing

Adjusted from:
http://www.nanohub.org/resources/?id=99
Original Authors are: Eric Jones and Travis Oliphant

Many excellent resources on the web
>> google: "learn python"
some good example:
http://www.diveintopython.org/toc/index.html
http://www.scipy.org/Documentation

Topics

- Introduction to Python
- Numeric Computing
- SciPy and its libraries

What Is Python?

ONE LINER

Python is an interpreted programming language that allows you to do almost anything possible with a compiled language (C/C++/Fortran) without requiring all the complexity.

PYTHON HIGHLIGHTS

- Automatic garbage collection
- Dynamic typing
- Interpreted and interactive
- Object-oriented
- "Batteries Included"
- Free
- Portable
- Easy to Learn and Use
- Truly Modular

Who is using Python?

RUTGERS

NATIONAL SPACE TELESCOPE LABORATORY

Data processing and calibration for instruments on the Hubble Space Telescope.

INDUSTRIAL LIGHT AND MAGIC

Digital Animation

PAINT SHOP PRO 8

Scripting Engine for JASC PaintShop Pro 8 photo-editing software

CONOCOPHILLIPS

Oil exploration tool suite

LAWRENCE LIVERMORE NATIONAL LABORATORIES

Scripting and extending parallel physics codes. pyMPI is their doing.

WALT DISNEY

Digital animation development environment.

REDHAT

Anaconda, the Redhat Linux installer program, is written in Python.

ENTHOUGHT

Geophysics and Electromagnetics engine scripting, algorithm development, and visualization

Language Introduction

Interactive Calculator

```
# adding two values
>>> 1 + 1
2
# setting a variable
>>> a = 1
>>> a
1
# checking a variables type
>>> type(a)
<type 'int'>
# an arbitrarily long integer
>>> a = 1203405503201
>>> a
1203405503201L
>>> type(a)
<type 'long'>
>>>> type(a).__name__=='long'
True
>>>> print type.__doc__
type(name, bases, dict)
```

```
# real numbers
>>> b = 1.2 + 3.1
>>> b
4.2999999999999998
>>> type(b)
<type 'float'>
# complex numbers
>>> c = 2+1.5j
>>> c
(2+1.5j)
```

The four numeric types in Python on 32-bit architectures are:
- **integer** (4 byte)
- **long integer** (any precision)
- **float** (8 byte like C's double)
- **complex** (16 byte)

The Numeric module, which we will see later, supports a larger number of numeric types.

Complex Numbers

CREATING COMPLEX NUMBERS

```
# Use "j" or "J" for imaginary
# part. Create by "(real+imagj)",
# or "complex(real, imag)" .
>>> 1j * 1J
(-1+0j)
>>> 1j * complex(0,1)
 (-1+0j)
>>> (1+2j)/(1+1j)
(1.5+0.5j)
```

EXTRACTING COMPONENTS

```
# to extract real and im
# component
>>> a=1.5+0.5j
>>> a.real
1.5
>>> a.imag
0.5
```

ABSOLUTE VALUE

```
>>> a=1.5+0.5j
>>> abs(a)
1.5811388
```

Strings

CREATING STRINGS

```
# using double quotes
>>> s = "hello world"
>>> print s
hello world
# single quotes also work
>>> s = 'hello world'
>>> print s
hello world
```

STRING OPERATIONS

```
# concatenating two strings
>>> "hello " + "world"
'hello world'

# repeating a string
>>> "hello " * 3
'hello hello hello '
```

STRING LENGTH

```
>>> s = "12345"
>>> len(s)
5
```

FORMAT STRINGS

```
# the % operator allows you
# to supply values to a
# format string.  The format
# string follows
# C conventions.
>>> s = "some numbers:"
>>> x = 1.34
>>> y = 2
>>> s = "%s %f, %d" %
(s,x,y)
>>> print s
some numbers: 1.34, 2
```

The strings

```
>>> s = "hello world"
>>> s.split()↰
['hello', 'world']

>>> ' '.join(s.split())
hello world

>>> s.replace('world' ,'Mars')
'hello Mars'

# strip whitespace
>>> s = "\t    hello    \n"
>>> s.strip()↰
'hello'
```

```
Regular expressions:
re.match(regex,subject)
re.search(regexp,subject)↰
re.group()↰
re.groups()↰
re.sub(regex, replacement,sub)↰

>>import re
>>s="The time is 12:30pm!"
>>m=re.match(".*time is (.*)pm", s))
>>m.group(1)↰
'12:30'
>>m.groups()↰
↰),'12:30'(
>>m=re.search(r'time.*(\d+:\d+)pm',s
>>m.group(1)↰
'12:30'
>>re.sub(r'\d+:\d+','2:10',s)↰
'The time is 2:10pm!'
```

Multi-line Strings

```
# triple quotes are used
# for mutli-line strings
>>> a = """hello
... world"""
>>> print a
hello
world

# multi-line strings using
# "\" to indicate
continuation
>>> a = "hello " \
...       "world"
>>> print a
hello world
```

```
# including the new line
>>> a = "hello\n" \
...       "world"
>>> print a
hello
world
```

List objects

LIST CREATION WITH BRACKETS

```
>>> l = [10,11,12,13,14]
>>> print l
[10, 11, 12, 13, 14]
```

CONCATENATING LIST

```
# simply use the + operator
>>> [10, 11] + [12,13]
[10, 11, 12, 13]
```

REPEATING ELEMENTS IN LISTS

```
# the multiply operator
# does the trick.
>>> [10, 11] * 3
[10, 11, 10, 11, 10, 11]
```

range(start, stop, step)

```
# the range method is helpful
# for creating a sequence
>>> range(5)
[0, 1, 2, 3, 4]

>>> range(2,7)
[2, 3, 4, 5, 6]

>>> range(2,7,2)
[2, 4, 6]
```

Indexing

RETRIEVING AN ELEMENT

```
# list
# indices: 0  1  2  3  4
  >>>  l = [10,11,12,13,14]
  >>>  l[0]
  10
```

SETTING AN ELEMENT

```
>>> l[1] = 21
>>> print l
[10, 21, 12, 13, 14]
```

OUT OF BOUNDS

```
>>> l[10]
Traceback (innermost last):
File "<interactive input>",line 1,in ?
IndexError: list index out of range
```

NEGATIVE INDICES

```
# negative indices count
# backward from the end of
# the list.
#
# indices: -5 -4 -3 -2 -1
  >>>   l = [10,11,12,13,14]

  >>> l[-1]
  14
  >>> l[-2]
  13
```

The first element in an array has index=0 as in C. *Take note Fortran programmers!*

More on list objects

LIST CONTAINING MULTIPLE TYPES

```
# list containing integer,
# string, and another list.
>>> l = [10,'eleven',[12,13]]
>>> l[1]
'eleven'
>>> l[2]
[12, 13]

# use multiple indices to
# retrieve elements from
# nested lists.
>>> l[2][0]
12
```

LENGTH OF A LIST

```
>>> len(l)
3
```

DELETING OBJECT FROM LIST

```
# use the del keyword
>>> del l[2]
>>> l
[10,'eleven']
```

DOES THE LIST CONTAIN x ?

```
# use in or not in
>>> l = [10,11,12,13,14]
>>> 13 in l
1
>>> 13 not in l
0
```

Slicing

`var[lower:upper]`

Slices extract a portion of a sequence by specifying a lower and upper bound. The extracted elements start at lower and go up to, *but do not include*, the upper element. Mathematically the range is [lower,upper).

SLICING LISTS

```
# indices: 0  1  2  3  4
   >>> l = [10,11,12,13,14]
   # [10,11,12,13,14]
   >>> l[1:3]
   [11, 12]

# negative indices work also
>>> l[1:-2]
[11, 12]
>>> l[-4:3]
[11, 12]
```

OMITTING INDICES

```
# omitted boundaries are
# assumed to be the beginning
# (or end) of the list.

# grab first three elements
>>> l[:3]
[10,11,12]
# grab last two elements
>>> l[-2:]
[13,14]
```

A few methods for list objects

some_list.append(x)

Add the element x to the end of the list, `some_list`.

some_list.count(x)

Count the number of times x occurs in the list.

some_list.index(x)

Return the index of the first occurrence of x in the list.

some_list.remove(x)

Delete the first occurrence of x from the list.

some_list.reverse( )

Reverse the order of elements in the list.

some_list.sort(cmp)

By default, sort the elements in ascending order. If a compare function is given, use it to sort the list.

List methods in action

```
>>> l = [10,21,23,11,24]

# add an element to the list
>>> l.append(11)
>>> print l
[10,21,23,11,24,11]

# how many 11s are there?
>>> l.count(11)
2

# where does 11 first occur?
>>> l.index(11)
3
```

```
# remove the first 11
>>> l.remove(11)
>>> print l
[10,21,23,24,11]

# sort the list
>>> l.sort()
>>> print l
[10,11,21,23,24]

# reverse the list
>>> l.reverse()
>>> print l
[24,23,21,11,10]
```

Mutable vs. Immutable

MUTABLE OBJECTS

```
# Mutable objects, such as
# lists, can be changed
# in-place.

# insert new values into list
>>> l = [10,11,12,13,14]
>>> l[1:3] = [5,6]
>>> print l
[10, 5, 6, 13, 14]
```

The cStringIO module treats strings like a file buffer and allows insertions. It's useful when working with large strings or when speed is paramount.

IMMUTABLE OBJECTS

```
# Immutable objects, such as
# strings, cannot be changed
# in-place.

# try inserting values into
# a string
>>> s = 'abcde'
>>> s[1:3] = 'xy'
Traceback (innermost last):
File "<interactive input>",line 1,in ?
TypeError: object doesn't support
          slice assignment

# here's how to do it
>>> s = s[:1] + 'xy' + s[3:]
>>> print s
'axyde'
```

Dictionaries

Dictionaries store *key/value* pairs. Indexing a dictionary by a *key* returns the *value* associated with it.

DICTIONARY EXAMPLE

```
# create an empty dictionary using curly brackets
>>> record = {}
>>> record['first'] = 'Jmes'
>>> record['last'] = 'Maxwell'
>>> record['born'] = 1831
>>> print record
{'first': 'Jmes', 'born': 1831, 'last': 'Maxwell'}
# create another dictionary with initial entries
>>> new_record = {'first': 'James', 'middle':'Clerk'}
# now update the first dictionary with values from the new one
>>> record.update(new_record)
>>> print record
{'first': 'James', 'middle': 'Clerk', 'last':'Maxwell', 'born':
1831}
```

A few dictionary methods

some_dict.clear( )

Remove all key/value pairs from the dictionary, `some_dict`.

some_dict.copy( )

Create a copy of the dictionary

some_dict.has_key(x)

Test whether the dictionary contains the key `x`.

some_dict.keys( )

Return a list of all the keys in the dictionary.

some_dict.values( )

Return a list of all the values in the dictionary.

some_dict.items( )

Return a list of all the key/value pairs in the dictionary.

Dictionary methods in action

```
>>> d = {‘cows’: 1,’dogs’:
5,  ...       ‘cats’: 3}

# create a copy.
>>> dd = d.copy()
>>> print dd
{'dogs':5,'cats':3,'cows': 1}

# test for chickens.
>>> d.has_key(‘chickens’)
0


# get a list of all keys
>>> d.keys()
[‘cats’,’dogs’,’cows’]
```

```
# get a list of all values
>>> d.values()
[3, 5, 1]


# return the key/value pairs
>>> d.items()
[('cats', 3), ('dogs', 5),
 ('cows', 1)]

# clear the dictionary
>>> d.clear()
>>> print d
{}
```

Tuples

Tuples are a sequence of objects just like lists. Unlike lists, tuples are immutable objects. While there are some functions
and statements that require tuples, they are rare. A good rule of thumb is to use lists whenever you need a generic sequence.

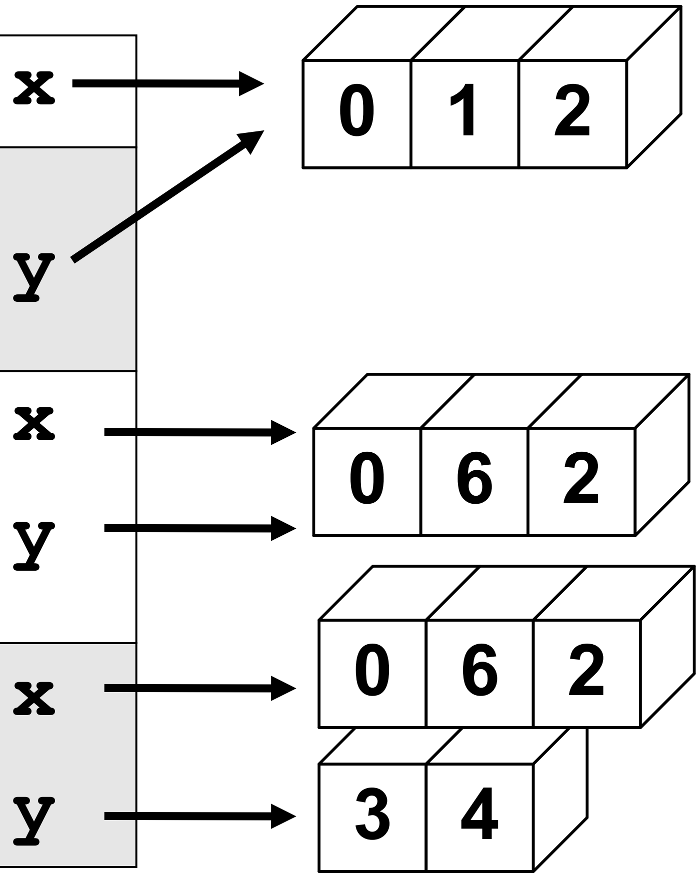
TUPLE EXAMPLE

```
# tuples are built from a comma separated list enclosed by ( )↰
>>> t = (1,’two’)↰
>>> print t
(1,‘two’)↰
>>> t[0]
1
# assignments to tuples fail
>>> t[0] = 2
Traceback (innermost last):
File "<interactive input>", line 1, in ?
TypeError: object doesn't support item assignment
```

Assignment

Assignment creates object references.

```
>>> x = [0, 1, 2]

# y = x cause x and y to point
# at the same list
>>> y = x

# changes to y also change x
>>> y[1] = 6
>>> print x
[0, 6, 2]

# re-assigning y to a new list
# decouples the two lists
>>> y = [3, 4]
```



Multiple assignments

```
# creating a tuple without
()↰
>>> d = 1,2,3
>>> d
↰)3 ,2 ,1(
```

```
# multiple assignments
>>> a,b,c = 1,2,3
>>> print b
2
```

```
# multiple assignments from a
# tuple
>>> a,b,c = d
>>> print b
2
```

```
# also works for lists
>>> a,b,c = [1,2,3]
>>> print b
2
```

If statements

`if/elif/else` provide conditional execution of code blocks.

IF STATEMENT FORMAT

```
if <condition>:
    <statements>
elif <condition>:
    <statements>
else:
    <statements>
```

IF EXAMPLE

```
# a simple if statement
>>> x = 10
>>> if x > 0:
...     print 1
... elif x == 0:
...     print 0
... else:
...     print -1
... < hit return >
1
```

Test Values

- True means any non-zero number or non-empty object
- False means not true: zero, empty object, or **`None`**

EMPTY OBJECTS

```
# empty objects evaluate false
>>> x = []
>>> if x:
...       print 1
... else:
...       print 0
... < hit return >
0
```

For loops

For loops iterate over a sequence of objects.

```
for <loop_var> in <sequence>:
    <statements>
```

TYPICAL SCENARIO

```
>>> for i in range(5):
...     print i,
... < hit return >
0 1 2 3 4
```

LOOPING OVER A STRING

```
>>> for i in 'abcde':
...     print i,
... < hit return >
a b c d e
```

LOOPING OVER A LIST

```
>>> l=['dogs','cats','bears']
>>> accum = ''
>>> for item in l:
...     accum = accum + item
...     accum = accum + ' '
... < hit return >
>>> print accum
dogs cats bears
```

While loops

While loops iterate until a condition is met.

```
while <condition>:
    <statements>
```

WHILE LOOP

```
# the condition tested is
# whether lst is empty.
>>> lst = range(3)
>>> while lst:
...print lst
...lst = lst[1:]
... < hit return >
[0, 1, 2]
[1, 2]
[2]
```

BREAKING OUT OF A LOOP

```
# breaking from an infinite
# loop.
>>> i = 0
>>> while 1:
...if i < 3:
...     print i,
...     else:
...         break
...     i = i + 1
... < hit return >
0 1 2
```

Anatomy of a function

The keyword **def** indicates the start of a function.

Function arguments are listed separated by commas. They are passed by *assignment*. More on this later.

```
def add(arg0, arg1):
    a = arg0 + arg1
    return a
```

Indentation is used to indicate the contents of the function. It is *not* optional, but a part of the syntax.

A colon (**:**) terminates the function definition.

An optional return statement specifies the value returned from the function. If return is omitted, the function returns the special value **None**.

Our new function in action

```
# We'll create our function
# on the fly in the
# interpreter.
>>> def add(x,y):
...     a = x + y
...     return a

# test it out with numbers
>>> x = 2
>>> y = 3
>>> add(x,y)
5
```

```
# how about strings?
>>> x = 'foo'
>>> y = 'bar'
>>> add(x,y)
'foobar'

# functions can be assigned
# to variables
>>> func = add
>>> func(x,y)
'foobar'
```

```
# how about numbers and strings?
>>> add('abc',1)
Traceback (innermost last):
File "<interactive input>", line 1, in ?
File "<interactive input>", line 2, in add
TypeError: cannot add type "int" to string
```

More about functions

```
# Every function returns
# a value (or NONE)
# but you don't need to
# specify returned type!

# Function documentation
>>> def add(x,y):
...     """this function
...     adds two numbers"""
...     a = x + y
...     return a

# You can always retrieve
# function documentation
>>> print add.__doc__

this function
adds two numbers
```

```
# FUNCTIONAL PROGRAMMING:
# "map(function, sequence)"
>>> def cube(x): return
x*x*x ...
>>> map(cube, range(1, 6))
[1, 8, 27, 64, 125]

# "reduce (function,
sequence)"
>>> def add(x,y): return x+y
...
>>> reduce(add, range(1, 11))
55
# "filter (function,
sequence)"
>>> def f(x): return x % 2 !=
0
...
>>> filter(f, range(2, 10))
[3, 5, 7, 9]
```

Even more on functions

```
# buld-in function "dir" is
# used to list all
# definitions in a module
>>> import scipy
>>> dir(scipy)
.........................
...<a lot of stuf>...
.........................
```

```
# Lambda function:
# Python supports one-line mini-
# functions on the fly.
# Borrowed from Lisp, lambda
# functions can be used anywhere
# a function is required.
>>> def f(x): return x*x
>>> map(f, range(5))
[0, 1, 4, 9, 16]
>> map(lambda x: x*x, range(5))
[0, 1, 4, 9, 16]
```

```
# more on lambda function:
>>> a=range(10)
>>> a.sort(lambda x,y: cmp(y,x))
>>> print a
 [9, 8, 7, 6, 5, 4, 3, 2, 1, 0]
>>> map(lambda x: x*2+10, range(5))
 [10, 12, 14, 16, 18]
>>> print reduce(lambda x,y: x+y, range(5))
 10
```

Modules

EX1.PY

```
# ex1.py

PI = 3.1416

def sum(lst):
    tot = lst[0]
    for value in lst[1:]:
        tot = tot + value
    return tot

l = [0,1,2,3]
print sum(l), PI
```

FROM SHELL

```
[ej@bull ej]$ python ex1.py
6, 3.1416
```

FROM INTERPRETER

```
# load and execute the module
>>> import ex1
6, 3.1416
# get/set a module variable.
>>> ex1.PI
3.1415999999999999
>>> ex1.PI = 3.14159
>>> ex1.PI
3.1415899999999999
# call a module variable.
>>> t = [2,3,4]
>>> ex1.sum(t)
9
```

Modules cont.

INTERPRETER

```
# load and execute the module
>>> import ex1
6, 3.1416
< edit file >
# import module again
>>> import ex1
# nothing happens!!!


# use reload to force a
# previously imported library
# to be reloaded.
>>> reload(ex1)
10, 3.14159
```

EDITED EX1.PY

```
# ex1.py version 2

PI = 3.14159

def sum(lst):
    tot = 0
    for value in lst:
        tot = tot + value
    return tot

l = [0,1,2,3,4]
print sum(l), PI
```

Modules cont. 2

Modules can be executable scripts or libraries or both.

EX2.PY

```
" An example module "

PI = 3.1416

def sum(lst):
    """ Sum the values in a
        list.
    """
    tot = 0
    for value in lst:
        tot = tot + value
    return tot
```

EX2.PY CONTINUED

```
def add(x,y):
    " Add two values."
    a = x + y
    return a

def test():
    l = [0,1,2,3]
    assert( sum(l) == 6)
    print 'test passed'

# this code runs only if this
# module is the main program
if __name__ == '__main__':
    test()
```

Classes

SIMPLE PARTICLE CLASS

```
>>> class particle:
... # Constructor method
...     def __init__(self,mass, velocity):
...     # assign attribute values of new object
...         self.mass = mass
...         self.velocity = velocity
... # method for calculating object momentum
...     def momentum(self):
...         return self.mass * self.velocity
... # a "magic" method defines object's string representation
...     def __repr__(self):
...    msg = "(m:%2.1f, v:%2.1f)" % (self.mass,self.velocity)
...         return msg
```

EXAMPLE

```
>>> a = particle(3.2,4.1)
>>> a
(m:3.2, v:4.1)
>>> a.momentum()
13.119999999999999
```

Reading files

FILE INPUT EXAMPLE

```
>>> results = []
>>> f = open('rcs.txt','r')

# read lines and discard header
>>> lines = f.readlines()[1:]
>>> f.close()

>>> for l in lines:
...     # split line into fields
...     fields = line.split()
...     # convert text to numbers
...     freq = float(fields[0])
...     vv = float(fields[1])
...     hh = float(fields[2])
...     # group & append to results
...     all = [freq,vv,hh]
...     results.append(all)
... < hit return >
```

PRINTING THE RESULTS

```
>>> for i in results: print i
[100.0, -20.30…, -31.20…]
[200.0, -22.70…, -33.60…]
```

EXAMPLE FILE: RCS.TXT

```
#freq (MHz)   vv (dB)   hh (dB)
  100          -20.3     -31.2
  200          -22.7     -33.6
```

More compact version

ITERATING ON A FILE AND LIST COMPREHENSIONS

```
>>> results = []
>>> f = open('rcs.txt','r')
>>> f.readline()
'#freq (MHz)  vv (dB)  hh (dB)\n'
>>> for l in f:
...     all = [float(val) for val in l.split()]
...     results.append(all)
... < hit return >
>>> for i in results:
...     print i
... < hit return >
```

EXAMPLE FILE: RCS.TXT

```
#freq (MHz)   vv (dB)   hh (dB)
  100          -20.3     -31.2
  200          -22.7     -33.6
```

Same thing, one line

OBFUSCATED PYTHON CONTEST...

```
>>> print [[float(val) for val in l.split()] for
...           l in open("rcs.txt","r")
...           if l[0] !="#"]
```

EXAMPLE FILE: RCS.TXT

```
#freq (MHz)   vv (dB)   hh (dB)
  100         -20.3     -31.2
  200         -22.7     -33.6
```

Sorting

THE CMP METHOD

```
# The builtin cmp(x,y)
# function compares two
# elements and returns
# -1, 0, 1
# x <  y --> -1
# x == y -->  0
# x >  y -->  1
>>> cmp(0,1)
-1

# By default, sorting uses
# the builtin cmp() method
>>> x = [1,4,2,3,0]
>>> x.sort()
>>> x
[0, 1, 2, 3, 4]
```

CUSTOM CMP METHODS

```
# define a custom sorting
# function to reverse the
# sort ordering
>>> def descending(x,y):
...     return -cmp(x,y)

# Try it out
>>> x.sort(descending)
>>> x
[4, 3, 2, 1, 0]
```

Sorting

SORTING CLASS INSTANCES

```
# Comparison functions for a variety of particle values
>>> def by_mass(x,y):
...     return cmp(x.mass,y.mass)
>>> def by_velocity(x,y):
...     return cmp(x.velocity,y.velocity)
>>> def by_momentum(x,y):
...     return cmp(x.momentum(),y.momentum())

# Sorting particles in a list by their various properties
>>> x = [particle(1.2,3.4),particle(2.1,2.3),particle(4.6,.7)]
>>> x.sort(by_mass)
>>> x
[(m:1.2, v:3.4), (m:2.1, v:2.3), (m:4.6, v:0.7)]
>>> x.sort(by_velocity)
>>> x
[(m:4.6, v:0.7), (m:2.1, v:2.3), (m:1.2, v:3.4)]
>>> x.sort(by_momentum)
>>> x
[(m:4.6, v:0.7), (m:1.2, v:3.4), (m:2.1, v:2.3)]
```

Criticism of Python

FUNCTION ARGUMENTS

```
# All function arguments are called by reference. Changing data in
# subroutine effects global data!
>>> def sum(lst):
...     tot=0
...     for i in range(0,len(lst)):
...         lst[i]+=1
...         tot += lst[i]
...     return tot
>>> a=range(1,4)
>>> sum(a)
9
>>> a
[2,3,4]
# Can be fixed by
>>> a=range(1,4)
>>> a_copy = a[:] # be careful: a_copy = a would not work
>>> sum(a_copy)
9
>>> a
[1,2,3]
```

Criticism of Python

FUNCTION ARGUMENTS

Python does not support something like "const" in C++. If users checks function declaration, it has no clue which arguments are meant as input (unchanged on exit) and which are output

COPYING DATA

User has "no direct contact" with data structures. User might not be aware of data handling. Python is optimized for speed -> references.

```
>>> a=[1,2,3,[4,5]]
>>> b=a[:]
>>> a[0]=2
>>> b
[1,2,3,[4,5]]
>>> a[3][0]=0
>>> b
[1,2,3,[0,5]]
```

```
# Can be fixed by
>>> import copy
>>> a=[1,2,3,[4,5]]
>>> b = copy.deepcopy(a)
>>> a[3][0]=0
>>> b
[1,2,3,[4,5]]
```

Criticism of Python

CLASS DATA

In C++ class declaration uncovers all important information about the class - class members (data and methods). In Python, data comes into
existence when used. User needs to read implementation of the class (much more code) to find class data and understand the logic of the class.
This is particularly important in large scale codes.

RELODING MODULES

If you import a module in command-line interpreter, but the module was later changed on disc, you can reload the module by typing
reload modulexxx
This reloads the particular modulexxx, but does not recursively reload modules that might also be changed on disc and are imported by the modulexxx.

NumPy

NumPy and SciPy

In 2005 Numarray and Numeric were merged into common project called "NumPy". On top of it, SciPy was build recently and spread very fast in scientific community.

Home: http://www.scipy.org/SciPy

IMPORT NUMPY AND SCIPY

```
>>> from numpy import *
>>> import numpy
>>> numpy.__version__
‘1.6.1’
        or better
>>> from scipy import *
>>> import scipy
>>> scipty.__version__
'0.12.0'
```

Array Operations

RUTGERS

SIMPLE ARRAY MATH

```
>>> a = array([1,2,3,4])
>>> b = array([2,3,4,5])
>>> a + b
array([3, 5, 7, 9])
```

NumPy defines the following constants:

```
pi = 3.14159265359
e  = 2.71828182846
```

MATH FUNCTIONS

```
# Create array from 0 to 10
>>> x = arange(11.)

# multiply entire array by
# scalar value
>>> a = (2*pi)/10.
>>> a
0.628318530718
>>> a*x
array([ 0.,0.628,…,6.283])

# apply functions to array.
>>> y = sin(a*x)
```

Introducing Numeric Arrays

SIMPLE ARRAY CREATION

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

CHECKING THE TYPE

```
>>> type(a)
<type 'numpy.ndarray'>
```

NUMERIC TYPE OF ELEMENTS

```
>>> a.dtype
dtype('int32')
```

BYTES IN AN ARRAY ELEMENT

```
>>>a.itemsize
4
```

ARRAY SHAPE

```
>>> a.shape
(4,)
>>> shape(a)
(4,)
```

CONVERT TO PYTHON LIST

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

ARRAY INDEXING

```
>>> a[0]
0
>>> a[0] = 10
>>> a
[10, 1, 2, 3]
```

Multi-Dimensional Arrays

MULTI-DIMENSIONAL ARRAYS

```
>>> a = array([[ 0, 1, 2, 3],
               [10,11,12,13]])
>>> a
array([[ 0, 1, 2, 3],
       [10,11,12,13]])
```

(ROWS,COLUMNS)

```
>>> shape(a)
(2, 4)
```

GET/SET ELEMENTS

```
>>> a[1,3]
13
```

column

row

```
>>> a[1,3] = -1
>>> a
array([[ 0, 1, 2, 3],
       [10,11,12,-1]])
```

ADDRESS FIRST ROW USING SINGLE INDEX

```
>>> a[1]
array([10, 11, 12, 13])
```

FLATTEN TO 1D ARRAY

```
>>> a.ravel()
array([0,1,2,3,10,11,12,13])
```

A.FLAT AND RAVEL() REFERENCE ORIGINAL MEMORY

```
>>> a.ravel()[7]=-1
>>> a
array([[ 0, 1, 2, 3],
       [10,11,12,-1]])
```

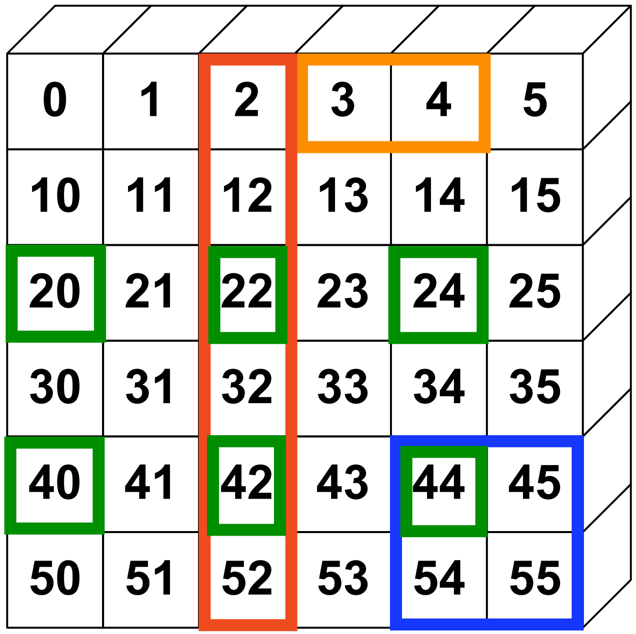
Array Slicing

SLICING WORKS MUCH LIKE STANDARD PYTHON SLICING

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

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

>>> a[:,2]
array([2,12,22,32,42,52])
```

STRIDES ARE ALSO POSSIBLE

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



Slices Are References

Slices are references to memory in original array. Changing values in a slice also changes the original array.

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

# create a slice containing only the
# last element of a
>>> b = a[2:3]
>>> b[0] = 10

# changing b changed a!
>>> a
array([ 1,  2, 10])
```

Array Constructor

```
array(object, dtype=None, copy=1,order=None, subok=0,ndmin=0)
```

`object` -any type of Python sequence. Nested list create multi-dimensional arrays.

`dtype` -character (string). Specifies the numerical type of the array. If it is None, the constructor makes its best guess at the numeric type.
dtype: integer, float, complex,...

`copy` -if **`copy=0`** and sequence is an array object, the returned array is a reference that data. Otherwise, a copy of the data in **`sequence`** is made.

`order` -'C': C-contiguous order, 'F': fortran contiguous, 'A': any order or maybe even non-contiguous

Array Constructor Examples

FLOATING POINT ARRAYS DEFAULT TO DOUBLE PRECISION

```
>>> a = array([0,1.,2,3])
>>> a.dtype
dtype('float64')
```

notice decimal

USE TYPECODE TO REDUCE PRECISION

```
>>> a = array([0,1.,2,3],'f')
>>> a.dtype
dtype('float32')
>>> len(ravel(a))*a.itemsize
16
```

BYTES FOR MAIN ARRAY STORAGE

```
# flat assures that
# multidimensional arrays
# work
>>>len(a.flat)*a.itemsize
32
```

ARRAYS REFERENCING SAME DATA

```
>>> a = array([1,2,3,4])
>>> b = array(a,copy=0)
>>> b[1] = 10
>>> a
array([ 1, 10,  3,  4])
```

32-bit Typecodes

Character	Bits (Bytes)	Identifier
D	128 (16)	**`Complex`**, `Complex64`
F	64 (8)	`Complex0`, `Complex8`, `Complex16`, `Complex32`
d	64 (8)	**`Float`**, `Float64`
f	32 (4)	`Float0`, `Float8`, `Float16`, `Float32`
l	32 (4)	**`Int`**
i	32 (4)	`Int32`
s	16 (2)	`Int16`
1 (one)	8 (1)	`Int8`
u	32 (4)	`UnsignedInt32`
w	16 (2)	`UnsignedInt16`
b	8 (1)	`UnsignedInt8`
O	4 (1)	`PyObject`

Highlighted typecodes correspond to Python's standard Numeric types.

Array Creation Functions

`arange([start,]stop[,step=1],dtype=None)`

Nearly identical to Python's `range()`. Creates an array of values in the range [`start,stop`) with the specified `step` value. Allows non-integer values for `start`, `stop`, and `step`. When not specified, `typecode` is derived from the `start`, `stop`, and `step` values.

```
>>> arange(0,2*pi,pi/4)
array([ 0.000, 0.785, 1.571, 2.356, 3.142,
    3.927, 4.712, 5.497])
```

`ones(shape,dtype=None,order='C')`
`zeros(shape,dtype=float,order='C')`

`shape` is a number or sequence specifying the dimensions of the array. If `typecode` is not specified, it defaults to float (in old versions `Int`)!!!

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

Array Creation Functions (cont.)

`identity(n,dtype='l')`

Generates an `n` by `n` identity matrix with `dtype=Int`.

```
>>> identity(4,dtype=int)
array([[1, 0, 0, 0],
       [0, 1, 0, 0],
       [0, 0, 1, 0],
       [0, 0, 0, 1]])
>>> identity(4,dtype=float)
array([[ 1.,  0.,  0.,  0.],
    [ 0.,  1.,  0.,  0.],
    [ 0.,  0.,  1.,  0.],
    [ 0.,  0.,  0.,  1.]])
```

Mathematic Binary Operators

```
a + b  →   add(a,b)
a - b  →   subtract(a,b)
a % b  →   remainder(a,b)
```

```
a * b   →   multiply(a,b)
a / b   →   divide(a,b)
a ** b  →   power(a,b)
```

MULTIPLY BY A SCALAR

```
>>> a = array((1,2))
>>> a*3.
array([3., 6.])
```

ELEMENT BY ELEMENT ADDITION

```
>>> a = array([1,2])
>>> b = array([3,4])
>>> a + b
array([4, 6])
```

ADDITION USING AN OPERATOR FUNCTION

```
>>> add(a,b)
array([4, 6])
```

IN PLACE OPERATION

```
# Overwrite contents of a.
# Saves array creation
# overhead
>>> add(a,b,a) # a += b
array([4, 6])
>>> a
array([4, 6])
```

Comparison and Logical Operators

```
equal          (==)    not_equal    (!=)    greater      (>)
greater_equal  (>=)    less         (<)     less_equal   (<=)
logical_and    (and)   logical_or   (or)    logical_xor
logical_not    (not)
```

2D EXAMPLE

```
>>> a = array(((1,2,3,4),(2,3,4,5)))
>>> b = array(((1,2,5,4),(1,3,4,5)))
>>> a == b
array([[1, 1, 0, 1],
       [0, 1, 1, 1]])
# functional equivalent
>>> equal(a,b)
array([[1, 1, 0, 1],
       [0, 1, 1, 1]])
```

Bitwise Operators

```
bitwise_and   (&)     invert         (~)     right_shift(a,shifts)
bitwise_or    (|)     bitwise_xor            left_shift (a,shifts)
```

BITWISE EXAMPLES

```
>>> a = array((1,2,4,8))
>>> b = array((16,32,64,128))
>>> bitwise_and(a,b)
array([ 17,   34,   68,  136])

# bit inversion
>>> a = array((1,2,3,4),UnsignedInt8)
>>> invert(a)
array([254, 253, 252, 251],'b')

# surprising type conversion
>>> left_shift(a,3)
array([ 8, 16, 24, 32],'i')
```

Changed from `UnsignedInt8` to `Int32`

Trig and Other Functions

TRIGONOMETRIC

```
sin(x)        sinh(x)
cos(x)        cosh(x)
arccos(x)

arccosh(x)
arctan(x)     arctanh(x)
arcsin(x)     arcsinh(x)
arctan2(x,y)
```

OTHERS

```
exp(x)            log(x)
log10(x)          sqrt(x)
absolute(x)       conjugate(x)
negative(x)       ceil(x)
floor(x)          fabs(x)
hypot(x,y)        fmod(x,y)
maximum(x,y)      minimum(x,y)
```

hypot(x,y)

Element by element distance calculation using

```
Equivalent to ``sqrt(x1**2 + x2**2)``,
element-wise.
```

SciPy

Overview

CURRENT PACKAGES

- Special Functions (scipy.special)
- Signal Processing (scipy.signal)
- Fourier Transforms (scipy.fftpack)
- Optimization (scipy.optimize)
- General plotting (scipy.[plt, xplt, gplt])
- Numerical Integration (scipy.integrate)
- Linear Algebra (scipy.linalg)
- Input/Output (scipy.io)
- Genetic Algorithms (scipy.ga)
- Statistics (scipy.stats)
- Distributed Computing (scipy.cow)
- Fast Execution (weave)
- Clustering Algorithms (scipy.cluster)
- Sparse Matrices* (scipy.sparse)

Basic Environment

CONVENIENCE FUNCTIONS

```
>>> info(linspace)
 linspace(start, stop, num=50, endpoint=1, retstep=0)

Evenly spaced samples.

Return num evenly spaced samples from start to stop.  If
endpoint=1 then
last sample is stop. If retstep is 1 then return the step value
used.
>>> linspace(-1,1,5)
array([-1. , -0.5,  0. ,  0.5,  1. ])
>>> logspace(0,3,4)
array([    1.,     10.,    100.,   1000.])
>>> info(logspace)
 logspace(start, stop, num=50, endpoint=1)

Evenly spaced samples on a logarithmic scale.

Return num evenly spaced samples from 10**start to 10**stop.  If
endpoint=1 then last sample is 10**stop.
```

`info` help system for scipy

similar to `dir` for the rest of python

`linspace` get equally spaced points.

`r_[]` also does this (shorthand)

`logspace` get equally spaced points in log10 domain

Basic Environment

CONVENIENT MATRIX GENERATION AND MANIPULATION

```
>>> A = mat('1,2,4;4,5,6;7,8,9')
>>> A=mat([[1,2,4],[4,5,6],[7,8,9]])
```

Simple creation of matrix with ";" meaning row separation

```
>>> print A
Matrix([[1, 2, 4],
        [2, 5, 3],
˥)]]9 ,8 ,7[
```

```
>>> print A**4
Matrix([[ 6497,  9580,  9836],
        [ 7138, 10561, 10818],
˥)]]27945 ,27220 ,18434[
```

Matrix Power

```
>>> print A*A.I
Matrix([[ 1.,  0.,  0.],
        [ 0.,  1.,  0.],
˥)]].1  ,.0  ,.0 [
```

Matrix Multiplication and Matrix Inverse

```
>>> print A.T
Matrix([[1, 2, 7],
        [2, 5, 8],
˥)]]9 ,3 ,4[
```

Matrix Transpose

More Basic Functions

TYPE HANDLING

iscomplexobj	real_if_close	isnan
iscomplex	isscalar	nan_to_num
isrealobj	isneginf	common_type
isreal	isposinf	cast
imag	isinf	typename
real	isfinite	

SHAPE MANIPULATION

squeeze	vstack	split
atleast_1d	hstack	hsplit
atleast_2d	column_stack	vsplit
atleast_3d	dstack	dsplit
apply_over_axes	expand_dims	apply_along_axis

OTHER USEFUL FUNCTIONS

select	unwrap	roots
extract	sort_complex	poly
insert	trim_zeros	any
fix	fliplr	all
mod	flipud	disp
amax	rot90	unique
amin	eye	extract
ptp	diag	insert
sum	factorial	nansum
cumsum	factorial2	nanmax
prod	comb	nanargmax
cumprod	pade	nanargmin
diff	derivative	nanmin
angle	limits.XXXX	

Input and Output

loadtxt, savetxt --- Reading and writing ASCII files

textfile.txt

```
Student Test1    Test2    Test3    Test4

Jane     98.3    94.2     95.3     91.3
Jon      47.2    49.1     54.2     34.7
Jim      84.2    85.3     94.1     76.4
```

Skip first two rows (default=0)

Read columns 1...5

```
>>> a = loadtxt('textfile.txt',skiprows=2,usecols=range(1,5))

>>> print a
[[ 98.3   94.2   95.3   91.3]
 [ 47.2   49.1   54.2   34.7]
 [ 84.2   85.3   94.1   76.4]]
>>> b = loadtxt('textfile.txt',skiprows=2,usecols=(1,-2))
>>> print b
[[ 98.3   95.3]
 [ 47.2   54.2]
 [ 84.2   94.1]]
```

Skip first two rows

Read columns 1 and -2

Few examples

Examples of SciPy use

Integration

Suppose we want to integrate Bessel function

$$\int_0^x \frac{J_1(t)}{t}\,dt$$

```
>>>from scipy import integrate, special
>>>info(integrate)
.....<documentation of integrate module>.....
>>> integrate.quad(lambda t: special.j1(t)/t,0,pi)
(1.062910971494,1.18e-14)
```

Creating a script j1int.py:

```
from scipy import *
from scipy import integrate, special
def fun(x):
    return integrate.quad(lambda t: special.j1(t)/t,0,x)

x=arange(1e-10,30,0.01)
print [fun(t)[0] for t in x]
```

Minimization

Suppose we want to minimize the function

$$(x-a)^2+(y-b)^2 = \min$$

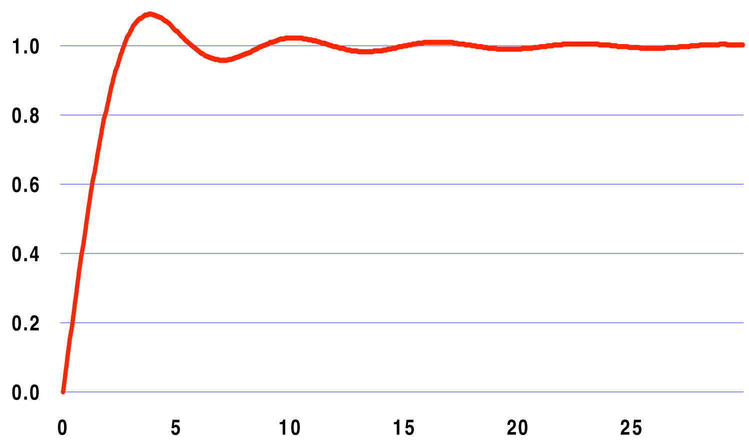
```
>>> from scipy import *
>>> import scipy
>>> info(scipy)
.... <documentation of all available modules>
>>> from scipy import optimize
>>> info(optimize)
>>> info(optimize.fmin_powell)

>>> def func(x,a): return (x[0]-a[0])**2+(x[1]-a[1])**2

>>> optimize.fmin_powell(func, [0,0], args=([5,6],))
Opimization terminated successfully,
     Current function value: 0.00000
     Iterations: 2
     Function evaluations: 38
array([5.,6.])
```

Starting guess

additional arguments

Root finding and integration

$$\int_0^x \frac{J_1(t)}{t} dt$$



The function $\int_0^x \frac{J_1(t)}{t} dt == 1$

has many solutions. Suppose we want to find all solution in the range [0:100]

Put it all together

```
from scipy import *
from scipy import integrate, optimize, special
""" Finds all solutions of the equation Integrate[j1(t)/t,{t,0,x}] == 1
    in the range x=[0,100]
"""

def func(x,a):
    " Computes Integrate[j1(t)/t,{t,0,x}] - a"
    return integrate.quad(lambda t: special.j1(t)/t, 0, x)[0] - a

# Finds approxiate solutions of the equation in the range [0:100]
x = arange(1e-10,100,0.2)                # creates an equaly spaced array
b = [func(t,1) for t in x]               # evaluates function on this array

z = [1e-10]                              # approximate solutions of the equation
for i in range(1,len(b)):                # if the function changes sign,
    if (b[i-1]*b[i]<0): z.append(x[i]) # the solution is bracketed


print "Zeros of the equation in the interval [0:100] are"
for j in range(1,len(z)):
    print j, optimize.brentq(func,z[j-1],z[j],args=(1,)) # calling root finder
```

It takes around 2 seconds to get

Zeros of the equation in the interval [0:100] are
0 2.65748482457
1 5.67254740317
2 8.75990144967
3 11.872242395
4 14.9957675329
5 18.1251662422
6 21.2580027553
7 24.3930147628
8 27.5294866728
9 30.666984016
10 33.8052283484
11 36.9440332549
12 40.0832693606
13 43.2228441315
14 46.362689668
15 49.5027550388
16 52.6430013038
17 55.7833981883
18 58.9239218038
19 62.0645530515
20 65.2052764808
21 68.3460794592
22 71.4869515584
23 74.6278840946
24 77.7688697786
25 80.9099024466
26 84.0509768519
27 87.1920884999
28 90.3332335188
29 93.4744085549
30 96.615610689
31 99.7568373684

Linear Algebra

scipy.linalg --- FAST LINEAR ALGEBRA

- Uses ATLAS if available --- very fast
- Low-level access to BLAS and LAPACK routines in modules `linalg.fblas`, and `linalg.flapack` (FORTRAN order)
- High level matrix routines
  - Linear Algebra Basics: `inv`, `solve`, `det`, `norm`, `lstsq`, `pinv`
  - Decompositions: `eig`, `lu`, `svd`, `orth`, `cholesky`, `qr`, `schur`
  - Matrix Functions: `expm`, `logm`, `sqrtm`, `cosm`, `coshm`, `funm` (general matrix functions)

Some simple examples

```
>>> A=matrix(random.rand(5,5))  # creates random matrix
>>> A.I
<inverse of the random matrix>
>>> linalg.det(A)
<determinant of the matrix>
>>> linalg.eigvals(A)
<eigenvalues only>
>>> linalg.eig(A)
<eigenvalues and eigenvectors>
>>> linalg.eigh(A)
<eigenvalues and eigenvectors for hermitian matrix>
>>> linalg.svd(A)
<SVD decomposition>
>>> linalg.cholesky(A)
<Cholesky decomposition for positive definite A>
>>> B=matrix(random.rand(5,5))
>>> linalg.solve(A,B)
<Solution of the equation A.X=B>
```

Special Functions

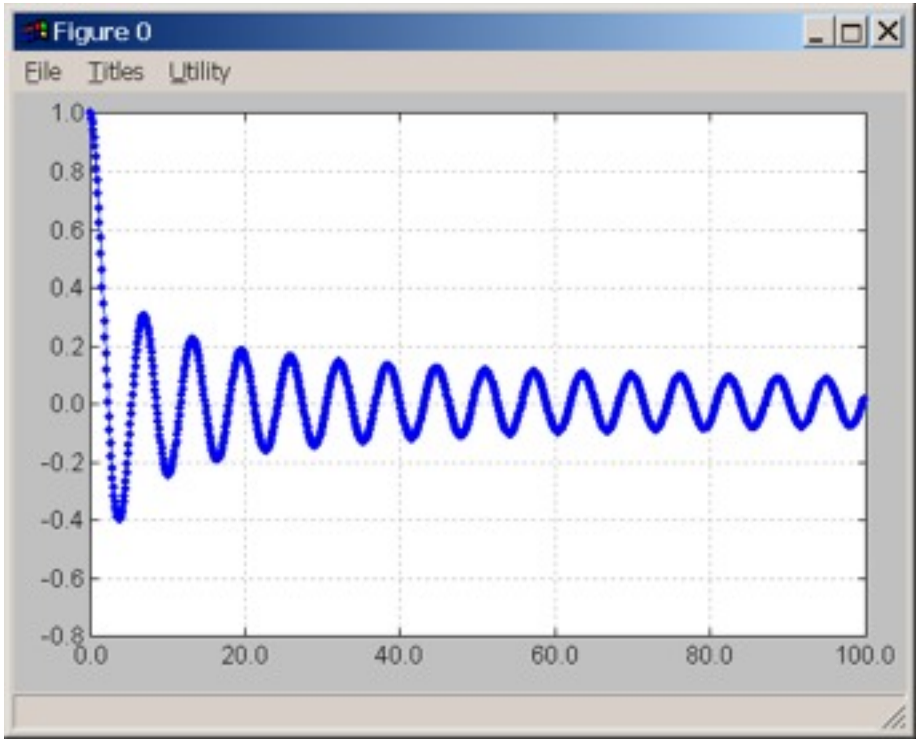
scipy.special

Includes over 200 functions:

Airy, Elliptic, Bessel, Gamma, HyperGeometric, Struve, Error, Orthogonal Polynomials, Parabolic Cylinder, Mathieu, Spheroidal Wave, Kelvin

FIRST ORDER BESSEL EXAMPLE

```
#environment setup
>>> from scipy import *
>>> from pylab import *
>>> from scipy import special


>>> x = arange(0,100,0.1)
>>> j0x = special.j0(x)
>>> plot(x,j0x,'o-')
>>> show()
```



Interpolation

scipy.interpolate --- General purpose Interpolation

- **1-d linear Interpolating Class**
  - Constructs callable function from data points
  - Function takes vector of inputs and returns linear interpolants
- **1-d and 2-d spline interpolation (FITPACK)**
  - Splines up to order 5
  - Parametric splines

Integration

scipy.integrate --- General purpose Integration

- **Ordinary Differential Equations (ODE)**

  `integrate.odeint`, `integrate.ode`

- **Samples of a 1-d function**

  `integrate.trapz` (trapezoidal Method), `integrate.simps` (Simpson Method), `integrate.romb` (Romberg Method)

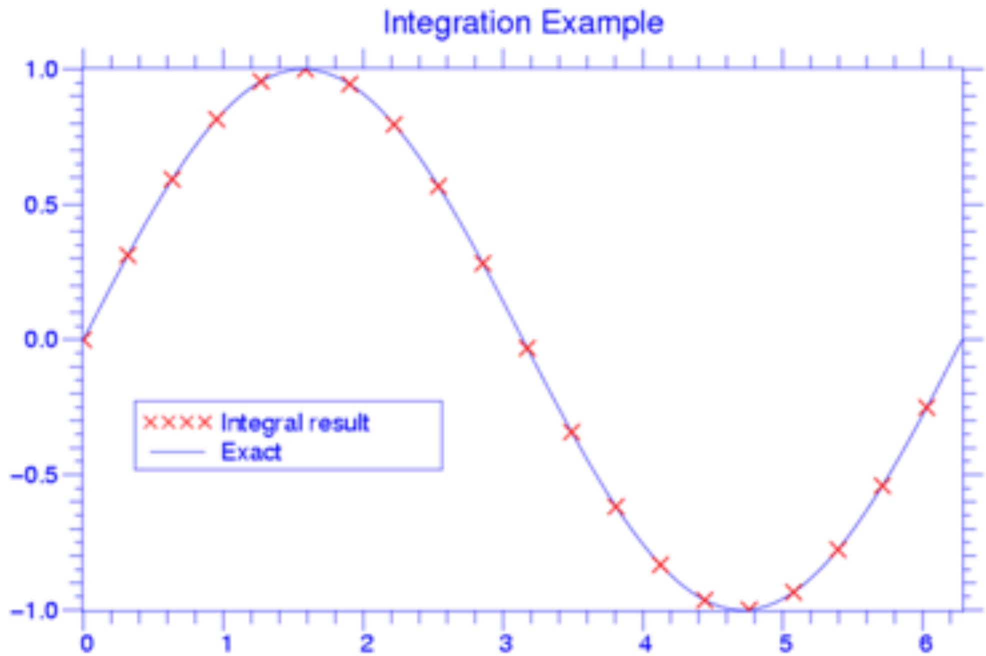
- **Arbitrary callable function**

  `integrate.quad` (general purpose), `integrate.dblquad` (double integration), `integrate.tplquad` (triple integration), `integrate.fixed_quad` (fixed order Gaussian integration), `integrate.quadrature` (Gaussian quadrature to tolerance), `integrate.romberg` (Romberg)

Integration

scipy.integrate --- Example

```
>>> def func(x):
    return integrate.quad(cos,0,x)[0]
>>> vecfunc = vectorize(func)

>>> x = r_[0:2*pi:100j]
>>> x2 = x[::5]
>>> y = sin(x)
>>> y2 = vecfunc(x2)
>>> xplt.plot(x,y,x2,y2,'rx')
```



Optimization

scipy.optimize --- unconstrained minimization and root finding

- **Unconstrained Optimization**

  fmin (Nelder-Mead simplex), **fmin_powell** (Powell's method), **fmin_bfgs** (BFGS quasi-Newton method), **fmin_ncg** (Newton conjugate gradient), **leastsq** (Levenberg-Marquardt), **anneal** (simulated annealing global minimizer), **brute** (brute force global minimizer), **brent** (excellent 1-D minimizer), **golden**, **bracket**

- **Constrained Optimization**

  fmin_l_bfgs_b, **fmin_tnc** (truncated newton code), **fmin_cobyla** (constrained optimization by linear approximation), **fminbound** (interval constrained 1-d minimizer)

- **Root finding**

  fsolve (using MINPACK), **brentq**, **brenth**, **ridder**, **newton**, **bisect**, **fixed_point** (fixed point equation solver)

Solving Hydrogen Atom

Schroedinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r}\right)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Ansatz for the solution:

$$\psi(\mathbf{r}) = Y_{lm}(\hat{\mathbf{r}})\frac{u(r)}{r}$$

Dimensionless variables:

$$x = \frac{r}{r_B} \qquad \varepsilon = \frac{E}{E_0} \qquad r_B = \frac{4\pi\epsilon_0\hbar^2}{me^2}$$

$$E_0 = \frac{\hbar^2}{2mr_B^2}$$

Ordinary differential Equation:

$$u''(x) - \left(\frac{l(l+1)}{x^2} - \frac{2Z}{x} - \varepsilon\right)u(x) = 0$$

Hydrogen Atom

First order system of equations
Can be solved by "integrate.odeint"

$$\begin{aligned} y &= (u(x), u'(x)) \\ \frac{dy}{dx} &= (u'(x), u''(x)) \end{aligned}$$

Boundary conditions

$$u(0) = 0 \rightarrow \psi(0) < \infty$$
$$u(\infty) = 0 \rightarrow \int |\psi(r)|^2 r^2 dr \propto \int u^2(r) dr < \infty$$

Boundary conditions given at the two ends → need shooting method

Shooting

- Suppose the two boundary conditions are given at a and b.
Choose u(a)=0 and u'(a)=c with c some small constant.
- Solve for u(x) to the other end and check if u(b)=0.
- Using root finding routine find energy E for which u(b)=0. This is a bound state.
- Continue with increasing E until sufficient number of bound states is found.

Solving radial Hydrogen atom

- It turns out that forward integration of radial Schroedinger equation is unstable. It is better to start integrating at infinity, and then continue down to zero.

- It is better to use logarithmic mesh for radial variable rather than linear. Radial functions need smaller number of points in logarithmic mesh.