Scientific Computing with Python numpy + matplotlib

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Review

Integers
Floating Point

Dynamic Typing – no declarations

```
x = 5
y = 6.3
```

Names start with a letter, cAsE SeNsiTiVe.
Long names OK.

Review Character Strings

Dynamic typing – no declaration
No memory allocation
Immutable

```
s = "Good Afternoon"

len(s)                  # length of string
```

Review String Slicing

```
s = “Good Afternoon”

s[0]  evaluates to “G”

s[5:10] selects “After”     # string slicing

s[:10] selects “Good After”
s[5:]  selects “Afternoon”

s[-4:] selects “noon”    # last 4 characters
```

String Methods

String is a Class with data & subroutines:

```
t = s.upper()
pos = s.find("A")
```

```
first = "George"
last = "Washington"
name = first + " " + last
                    # string concatenation
```

Review Lists

Ordered sequence of items

Can be floats, ints, strings, Lists

a = [16, 25.3, “hello”, 45]

a[0] contains 16

a[-1] contains 45

a[0:2] is a list containing [16, 25.3]

Create a List

```
days = [ ]
days.append(“Monday”)
days.append(“Tuesday”)

years = range(2000, 2014)
```

List Methods

List is a Class with data & subroutines:

```
d.insert(index, object)
d.remove(value)
d.sort( )                    # sort in place
```

Can concatenate lists with +

String split

```
s = “Princeton Plasma Physics Lab”

myList = s.split()   # returns a list of strings

print myList
 [ “Princeton”, “Plasma”, “Physics”, “Lab” ]

help(str.split)              # delimiters, etc.
```

Tuple

Designated by ( ) parenthesis

A List that can not be changed. Immutable.
No append.

Good for returning multiple values from a subroutine function.

Can extract slices.

Review math module

```
import math
dir(math)

math.sqrt(x)
math.sin(x)
math.cos(x)
```

```
from math import *
dir()

sqrt(x)
```

```
from math import pi
dir()

print pi
```

import a module

```
import math                # knows where to find it
```

```
import sys
sys.path.append("/u/efeibush/python")
import  cubic.py           # import your own code
```

```
if task == 3:
    import math            # imports can be anywhere
```

Looping with the range() function

```
for i in range(10):          # i gets 0 - 9
```

range() is limited to integers

numpy provides a range of floats

Summary

Integer, Float
String
List
Tuple

def function
Keywords: if elif else
while for in
import print

Indenting counts :

Run python as Interpreter

type()
dir()
help()

Programming = Problem Solving

Take a large problem and break it into a series of small problems.

Write an outline of the steps.

Relate each step to lines of code.

numpy module

ndarray *class*

Items are all the same type.

Contiguous data storage in memory of items.

Considerably faster than lists.

Class with data and methods (subroutines).

numpy module

ndarray *class*

```
import numpy

dir()
dir(numpy)
help(numpy)
help(numpy.ndarray)      # class
help(numpy.array)        # built-in function
```

numpy module

```
import numpy
dir(numpy)
help(numpy.zeros)
```

tuple

```
a = numpy.zeros( (3,5) )
                        # create 3 rows, 5 columns
      [   [0., 0., 0., 0., 0.],
          [0., 0., 0., 0., 0.],
          [0., 0., 0., 0., 0.] ]
                        # default type is float64
```

numpy Array Access

Access order corresponding to printed order:

[row] [column] index starts with 0

a[0][2] = 5

```
[     [ 0.,  0.,  5.,  0.,  0. ],
      [ 0.,  0.,  0.,  0.,  0. ],
      [ 0.,  0.,  0.,  0.,  0. ]  ]
```

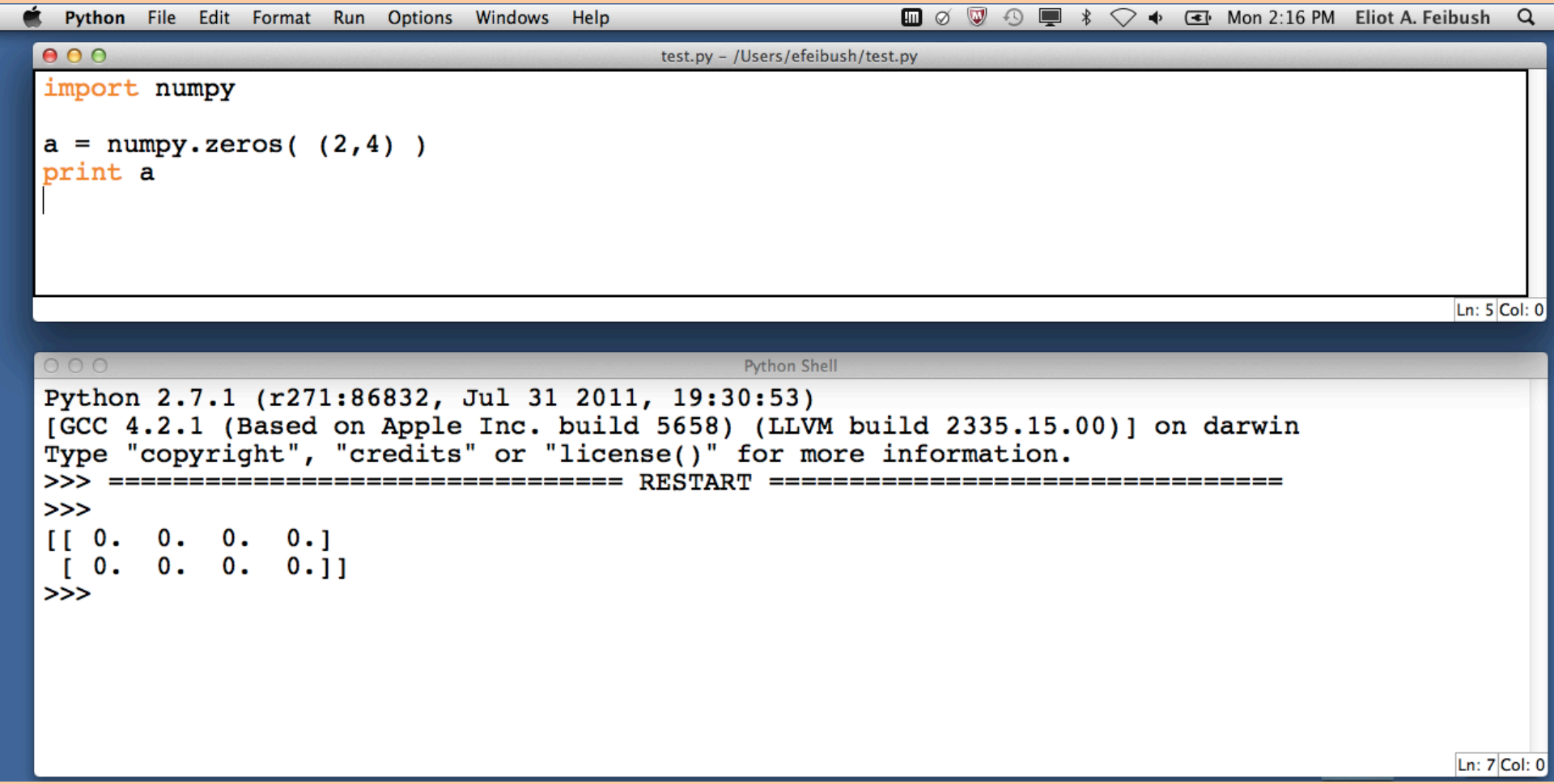
idle

Integrated Development Environment (IDE)

- Color-coded syntax
- statement completion
- debugger

Written in Python using tkinter GUI module

idle IDE



Can save text in interpreter window to a file.

control-p control-n to recall commands

Programming Exercise Prep

Mac: Editing source code

Textedit

Preferences

Format: Plain text

Open and Save

Uncheck: Add .txt extension

Save: File Format – Plain Text

Programming Exercise Prep

Mac: Run python from command line

Spotlight terminal

```
$ python myprogram.py
```

Anaconda: “The Distro”

Create your work environments

```
conda create –n proj1 python=2.7        # ~/proj1

conda create –p /home/efeibush/work/proj1 python=2.7

conda install package_name

pip install package_name


source activate /home/efeibush/proj1    # bash
```

Array Index Exercise

Write a python program:

Create an array (6, 3)

Set each element to rowIndex + columnIndex

print the array

edit index.py

python index.py

```
[ [ 0.  1.  2. ]
  [ 1.  2.  3. ]
  [ 2.  3.  4. ]
  [ 3.  4.  5. ]
  [ 4.  5.  6. ]
  [ 5.  6.  7. ] ]
```

1. Create Array

```
a = numpy.linspace(start, stop, nPoints, inclusive)
    # array of evenly spaced floats
    # begins with start
    # ends with stop
    # can include/exclude stop   True/False

        example: 0., 2.5, 101
                 0., 2.5, 100, False
```

Useful to make "range" of floats

```
for i in a:
```

ndarray has __iter__()

Arrays are iterable

1a. Create Array

```
alog = numpy.logspace(startExp,maxExp,nSteps)
```

Example: 2., 10., 9

2. Create Array

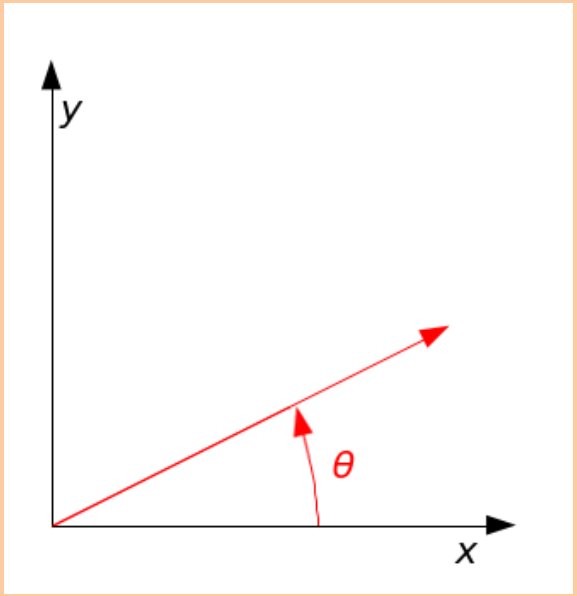
```
b = numpy.array( [ 2., 4., 6. ] )
    # 1-D from list

    # range(start, end, incr) returns a list so
b = numpy.array( range(10) )
    array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

b = numpy.array( ( 2., 4., 6. ) )
                        # 1-D from tuple
```

Rotation Matrix Exercise

Write a python program:

Create a 2 x 2 rotation matrix, 30 degrees:

$$\begin{bmatrix} \cos(30) & \sin(30) \\ -\sin(30) & \cos(30) \end{bmatrix}$$



radians = degrees * pi / 180.

Circle Exercise

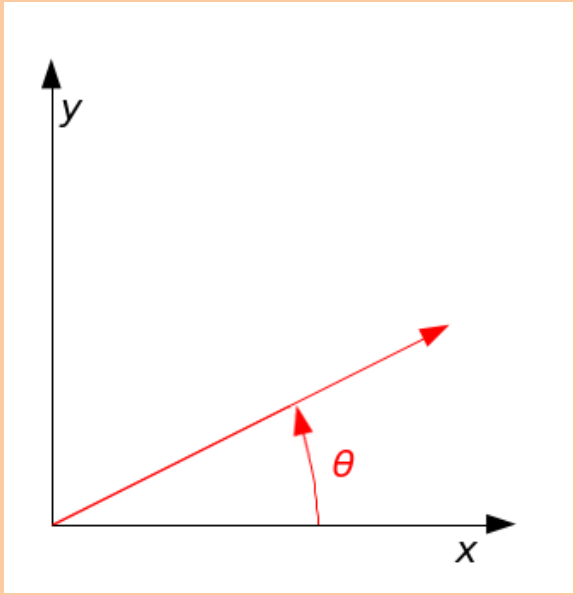
Add to your python program:

Create 18 *xy* points around unit circle

(18, 2) array

x = cosine(angle)

y = sine(angle)




```
print a.round(3)
```

Pointer vs. Deep Copy

```
a = numpy.zeros( (3, 3) )
b = a     # b is a pointer to a
c = a.copy()    # c is a new array

b is a     # True
c is a     # False
```

Views

base

Array Arithmetic

```
a = numpy.array( range(10, 20) )
```

a + 5
a – 3
a * 5
a / 3.14
a.sum() a.min() a.max()
a > 15
(a > 15).sum()

Array Arithmetic by Index

```
a = numpy.array( range(10) )
b = numpy.array( range(0, 1000, 100) )

a + b          # a[0] + b[0], a[1] + b[1] ...
a – b
a * b          # not row, column matrix product
a / b
```

The 2 arrays must be the same shape.

Row, Column Matrix Product

```
c = numpy.dot(a, b)
```

Dot product of 2 arrays.
Matrix multiplication for 2D arrays.

Transform Exercise

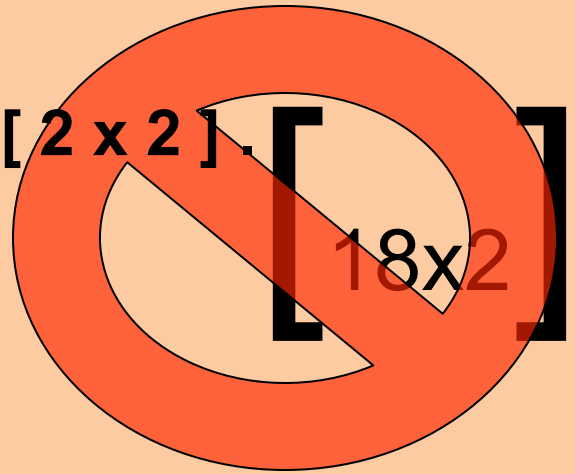
Add to your python program:

Transform 18 points by the rotation matrix.

Save in new array.

Scale up by factor of 2.

$$\begin{bmatrix} 18\text{x}2 \end{bmatrix} \cdot [\,2 \times 2\,]$$



Cross Product

```
zA = numpy.cross(xA, yA)
```

Note: we have been using *numpy.* functions

Array Shape

```
a = numpy.linspace(2, 32, 16)

a = a.reshape(4, 4)  # ndarray . method

a.shape              # ndarray attribute    tuple (4, 4)

a = numpy.linspace(2,32,16).reshape(8,2)

a.flatten()   # return a 1-D array
```

Methods have () Attributes do not.

Array Diagonals

```
a = numpy.linspace(1, 64, 64)

a = a.reshape(8, 8)

numpy.triu(a)       # upper triangle
numpy.tril(a)       # lower triangle

numpy.diag(a)       # main diagonal
numpy.diag(a, 1)    # 1 above
numpy.diag(a, -1)   # 1 below
```

numpy.array Order [row] [column]
vs.
Internal Storage Order

C is default, Fortran can be specified [contiguous] []

```
c = numpy.zeros( (2,4), dtype=numpy.int8)
f = numpy.zeros( (2,4), dtype=numpy.int8, order="F")
                    # show    c.flags    f.flags
c[0][1] = 5      # show    c.data[:]
f[0][1] = 5       # show   f.data[:]
```

numpy.array [][] access is the same regardless of internal storage order

ndarray.flags

Interpreter

Look at array flags

dir(a.flags)

Program

```
status = a.flags.c_contiguous
status = a.flags.f_contiguous
        # boolean True or False

ndarray.flatten()    # 'F' or 'C' (default)
```

Array Data Types

numpy.float64 is the default type

float32
int8, int16, int32, int64, uint8, uint16, uint32, uint64
complex64, complex128
bool - True or False

a.dtype shows type of data in array

```
>>> help(numpy.ndarray)  # Parameters
                         Attributes
```

Multi-Dimensional Indexing

```
a = numpy.array( range(12) )
a = a.reshape(2,6)      # 2 rows, 6 columns
```

a[1][5] contains 11

a[1, 5] is equivalent, more efficient

1. Array Slicing

```
a = numpy.array(range(0, 100, 10))
```

Array([0, 10, 20, 30, 40, 50, 60, 70, 80, 90])

a[2:4] contains 20, 30

a[-4 : -1] contains 60, 70, 80

Slicing returns ndarray

2. Array Slicing

```
a = numpy.array(range(64)).reshape(8,8)
```

a[3, 4] contains 28

```
asub = a[3:5,  4:6]
```

Very useful for looking at data & debugging.

```
a[:,2]     # all rows, column 2
a[3, 2:5]  # row 3, columns 2 and 3 and 4
```

Array Stuff

a.T
a.min()
a.max()
a.round()
a.var() - variance
a.std() – standard deviation

Organize Arrays

Make a list of arrays named a, b, and c:

```
w = [ a, b, c]

len(w)          # length of list is 3

w[1].max()      # use array method
```

numpy Tutorial

wiki.scipy.org/Tentative_Numpy_Tutorial

docs.scipy.org/doc/numpy/reference/routines.html

numpy for Matlab Users
wiki.scipy.org/NumPy_for_Matlab_Users

1. Plotting

matplotlib – designed to look like MATLAB plot

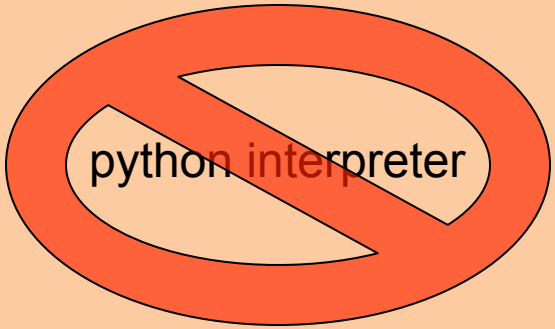
200 subroutines for various plots.

Generally available with Python

matplotlib.org
    gallery

Plotting on raleigh.princeton.edu

```
$ module load python/2.7
$ ipython --pylab
```



Bring up plot windows as separate threads, no blocking.
Draw commands are displayed sequentially.

```
ipython --pylab --classic --logfile mytype.txt
        dash dash pylab
```

```
import matplotlib.pyplot as plt
plt.plot( range(10), range(10) )
```

Plotting on raleigh.princeton.edu

```
$ ipython --pylab –i plot2.py
```

or

```
$ ipython --pylab
>>> import plot2
```

runs plot2.py from current directory

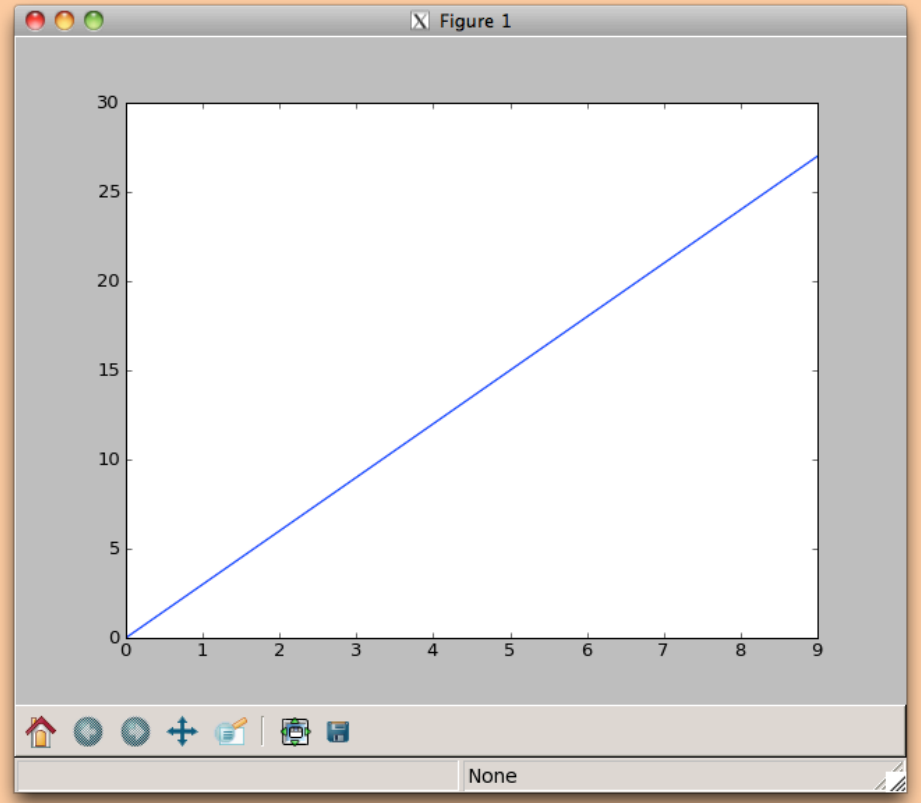
man ipython `--no-confirm-exit`

Plot Exercise

New python program:

Create a numpy array of ten ***X*** values.

Create a numpy array of ten ***Y*** values.




```
import matplotlib.pyplot as g
g.plot(x, y)
g.show()          # optional
```

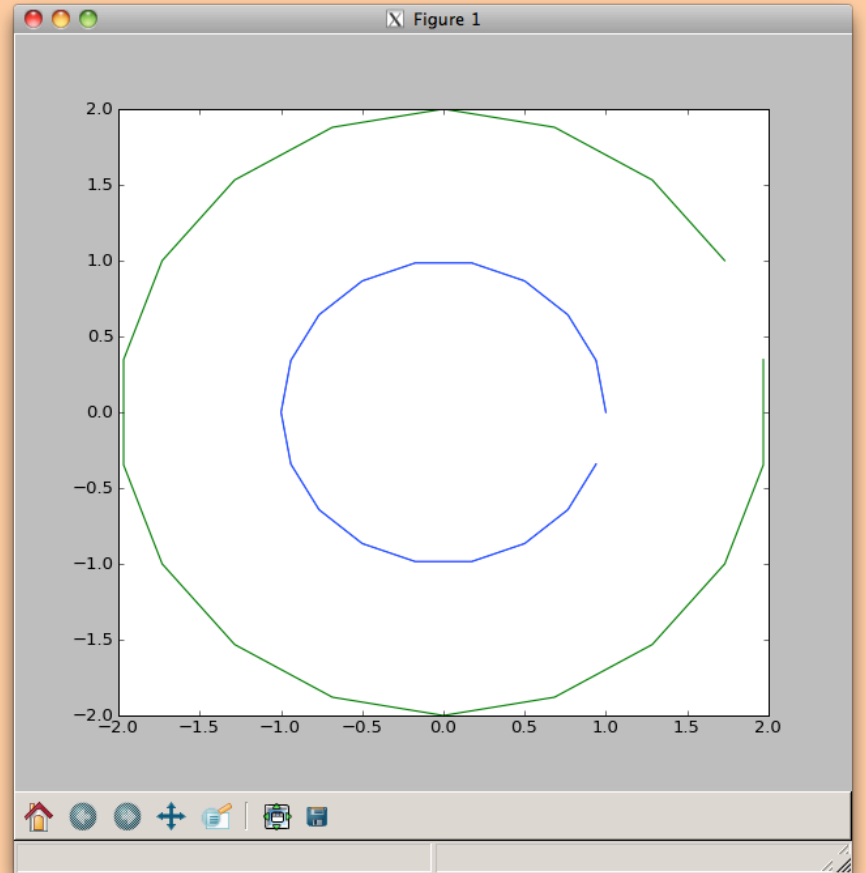
Plot Circles Exercise

Add to your python program:

Slice both (18, 2) arrays into:

x array

y array




```
g.plot(ax, ay)
g.plot(bx, by)
```

matplotlib Contour Plot

```
r = numpy.random.rand(10,10)

g.contour(r)      # contour line plot

fig2 = g.figure()     # start new window
fig2.canvas.manager.window.Move((648,20))

g.contourf(r)     # filled contour plot

clf()  # clear figure, erase
cla()    # clear axis
```

Review Defining a Function

Block of code separate from main.

Define the function before calling it.

```
def myAdd(a, b):        # define before calling
    return a + b

p = 25                  # main section of code
q = 30

r = myAdd(p, q)
```

Keyword Arguments

Provide default values for optional arguments.

```
def setLineAttributes(color="black",
    style="solid", thickness=1):
    ...

# Call function from main program
setLineAttributes(style="dotted")
setLineAttributes("red", thickness=2)
```

String Escape Sequence

```
s = '\n'      # interpreted as ASCII Linefeed

t = r'\n'     # raw string, t contains \n
```

matplotlib LaTeX

```
import matplotlib.pyplot as plt

plt.rc("text", usetex=True)
    # set config to draw text with Tex

plt.xlabel( r"\textbf{Time}" )
    # draw x label "Time" in bold font
    # compare to:   plt.xlabel("Time")
```

latex2.py example

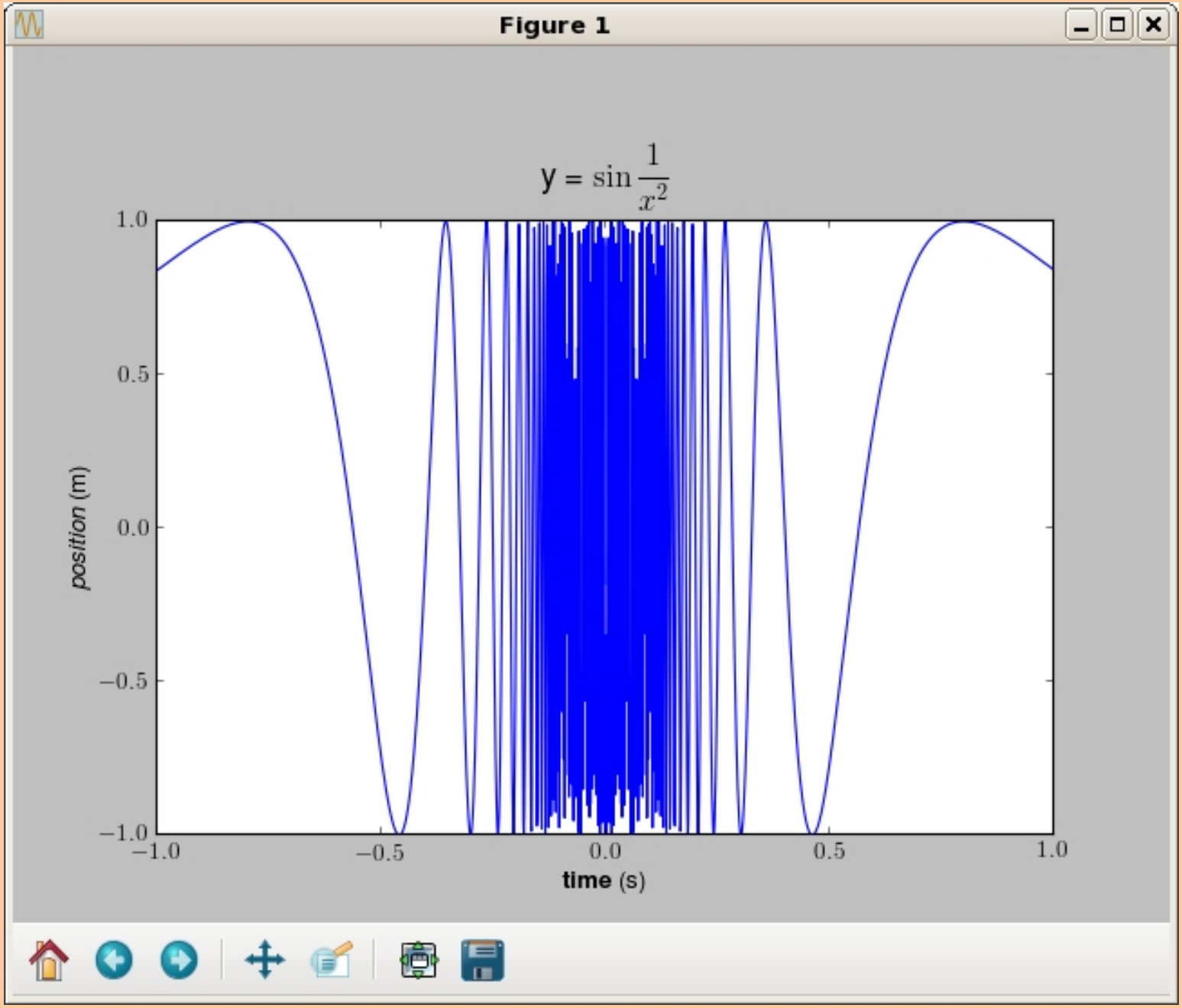


Figure 1
$y = \sin \frac{1}{x^2}$
1.0
0.5
0.0
−0.5
−1.0
position (m)
−1.0
−0.5
0.0
0.5
1.0
time (s)

matplotlib *f(x,y,t)*

raleigh.astro.princeton.edu

/u/efeibush/python/netcdf

readsteps.py

Display time steps from psiRZ

More Info & Resources

docs.scipy.org

princeton.edu/~efeibush/python/numpy

Princeton University Python Community

princetonpy.com