

Python and Scientific Computing

Notes (John D. Blum) Fernando Perez

Contents

Chapter 1. Why python?	5
------------------------	---

CHAPTER 0. CONTENTS

9.1. weave	61
9.2. swig	61
9.3. f2py	61
9.4. Others	61
Bibliography	63

CHAPTER 1

Why python?

CHAPTER 2

2^{200} is a huge number!

```
>>> 2**200  
1606938044258990275541962092341162602522202993782792835301376L
```

but python will blithely compute it and much larger numbers for you as long as you have CPU and


```
>>> last = 'Hunter'  
>>> last[0]  
'H'  
>>> last[1]  
'u'  
>>> last[-1]  
'r'
```

To access substrings, or generically in terms of the sequence protocol, slices, you use a colon to indicate a range

```
# string slicing  
>>> last[0:2]  
'Hu'  
>>> last[2:4]  
'nt'
```

As this example shows, python uses "one-past-the-end" indexing when defining a range; eg, in the range `indmin:indmax`, the element of `imax` is not included. You can use negative indices when slicing too; eg, to get everything before the last character

```
>>> last[0:-1]  
'Hunte'
```



```
# s is a single string and we split it into a list of strings
```


needed to compute the product of two numbers between 1 and 100 in an inner loop – you could use a dictionary to cache the cube of all odd of numbers < 100; if you were inteterested in all numbers, you might simply use a list to store the cached cubes – I am cacheing only the odd numbers to show you how a dictionary can be used to represent a sparse data structure

```
>>> cubes = dict([(i, i**3) for i in range(1,100,2)])
>>> cubes[5]
125
```

The last example is syntactically a bit challenging, but bears careful study. We are initializing a dictionary with a list comprehension. The list comprehension is made up of length 2 tuples (*i*, *i*^{**3}). When a dictionary is initialized with a sequence of length 2 tuples, it assumes the first element of the tuple *i* is the *key* and the second element *i*^{**3}is the *value*


```
[‘First’, ‘Last’, ‘Age’, ‘Weight’, ‘Height’, ‘Birthday’]
```

Notice how this works like a pipeline: `fh.readline` returns a line of text as a string; we call the string method `strip` which returns a string with all white space (spaces, tabs, newlines) removed from the left and right; we then call the `split` method on this stripped string to split it into a list of strings.

3.2. E ective interactive work

3.3. Customizing IPython

3.3.1. Basics. Flexible configuration system. It uses a configuration file which allows per-

CHAPTER 4

Numeric tut

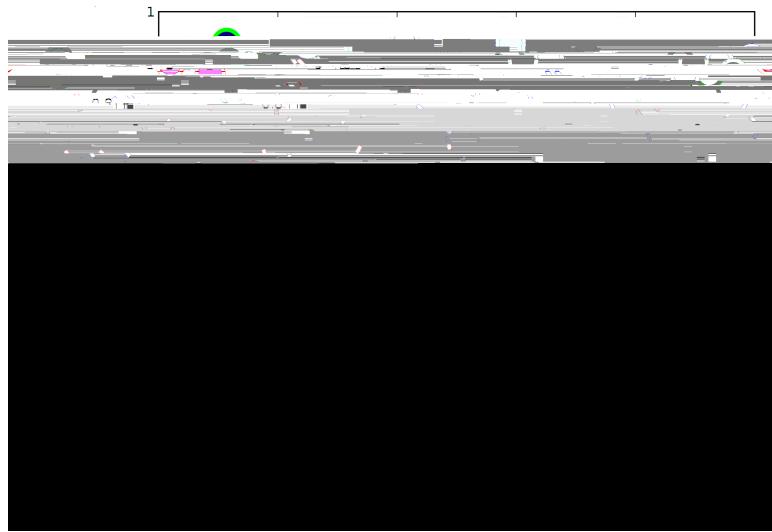


Figure 5.3.2. The default marker plot, before marker customization

```
fontproperties: a matplotlib.font_manager.FontProperties instance
horizontalalignment or ha: [ 'center' | 'right' | 'left' ]
label: any string
lod: [True | False]
multialignment: [ 'left' | 'right' | 'center' ]
name or fontname: string eg, [ 'Sans' | 'Courier' | 'Helvetica' ... ]
position: (x,y)
rotation: [ angle in degrees 'vertical' | '
```

```
from matplotlib import mean
x = n.arange(100)
y = n.take(x, range(10, 20))
print mean(y)
```

For the remainder of this manual, the term `numerix` is used to mean either the Numeric or numarray package. To select numarray or Numeric from the prompt, run your matplotlib script with

```
> python myscript.py --numarray # use numarray
> python myscript.py --Numeric # use Numeric
```

Typically, however, users will choose one or the other and make this setting in their rc file using either `numerix : Numeric` or `numerix : numarray`.

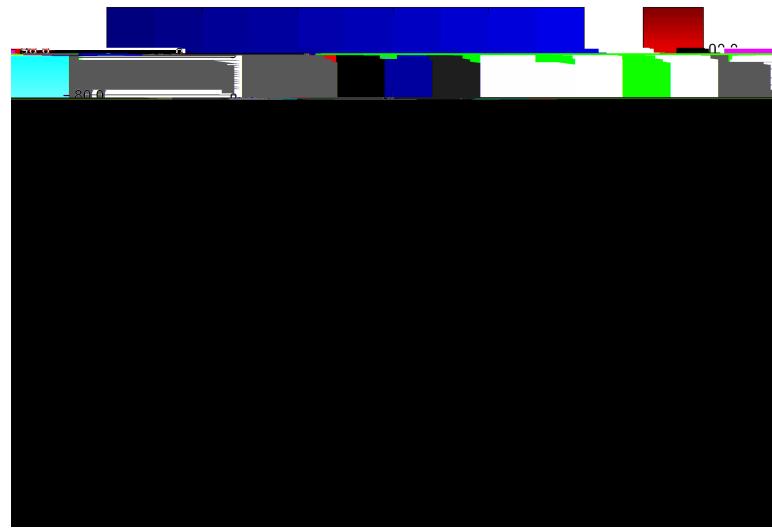


Figure 5.7.1. A simple image plot of a 2D matrix, using nearest neighbor interpolation and the jet colormap.

```
In [15]: Ix [15] changes(100,60) rpx. shape=(100,100) in([16]) i: 1(b)=1 (e)sh(a)(k(r) h(e)p6) ato e23. 9etate6  
which creates the image 1(magd)1((e)1(s)-358(B58(Ba63T7(i)1(c)gu(r)1(e)1(a63T)1(7.)-71)1-775(5)Y3(TPou357(cr
```


5.8. Customizing text and mathematical expressions

5.9. Event handling: Tracking the mouse and keyboard

CHAPTER 6

A tour of scipy

Purpose
Module overview
Some examples

CHAPTER 7

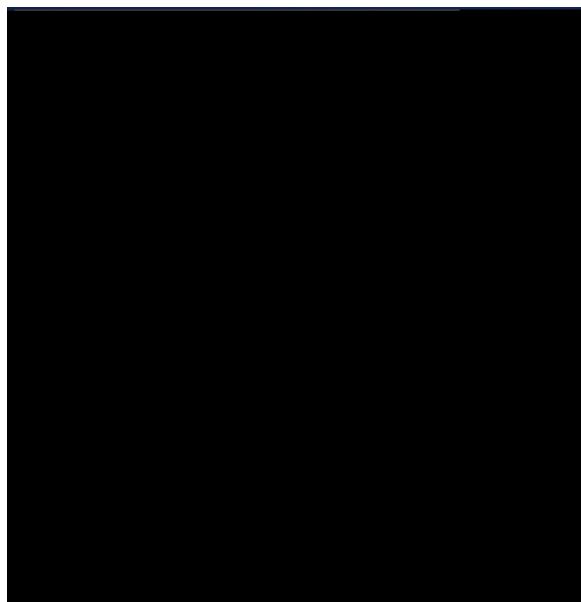
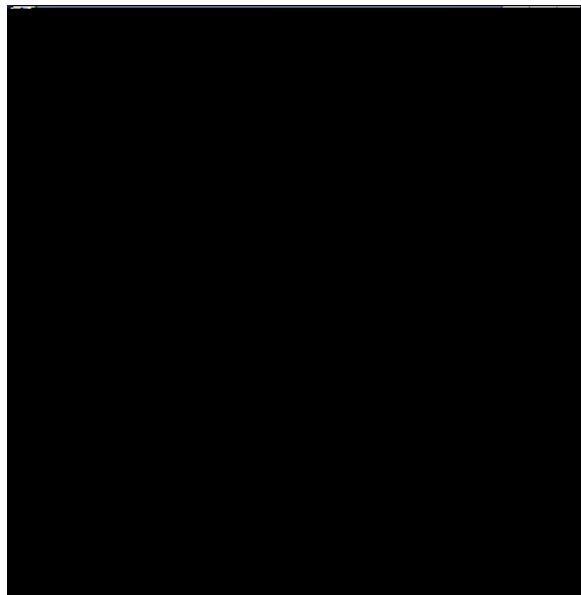


Figure 7.1.1. A Cube, brought to you by VTK

```
# Ready, set,
```







CHAPTER 8

3D visualization with MayaVi

8.1. Generalities

8.2. Scripted examples

Bibliography

- [1] D. Beasley.