Python Workshop
Numpy Arrays

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What is Numpy

- Numpy is the main package for scientific computing using Python
- Provides an array object of type ndarray
- Many functions and methods available for fast array operations

Numpy Version

- Numpy can be obtained at `http://docs.scipy.org/doc/`
- Current version is 1.6.
- To determine the installed version

```
In [10]: import numpy

In [11]: print numpy.__version__
1.6.1
```

Data Types (dtype)

bool	Boolean (True or False) stored as a byte
int	Platform integer (normally either int32 or int64)
int8	Byte (-128 to 127)
int16	Integer (-32768 to 32767)
int32	Integer (-2147483648 to 2147483647)
int64	Integer (9223372036854775808 to 9223372036854775807)
uint8	Unsigned integer (0 to 255)
uint16	Unsigned integer (0 to 65535)
uint32	Unsigned integer (0 to 4294967295)
uint64	Unsigned integer (0 to 18446744073709551615)
float	Shorthand for float64.
float16	Half precision float: sign bit, 5 bits exponent, 10 bits mantissa
float32	Single precision float: sign bit, 8 bits exponent, 23 bits mantissa
float64	Double precision float: sign bit, 11 bits exponent, 52 bits mantissa
complex	Shorthand for complex128.
complex64	Complex number, represented by two 32-bit floats (real and imaginary components)
complex128	Complex number, represented by two 64-bit floats (real and imaginary components)

`http://docs.scipy.org/doc/numpy-1.6.0/user/basics.types.html`

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Creating an Array

- Using the built-in *array* function

```
In [18]: import numpy

In [19]: a1d = numpy.array([0, 1, 2, 3, 4])

In [20]: a1d
Out[20]: array([0, 1, 2, 3, 4])

In [21]: a2d = numpy.array([ [1, 1, 1, 1], [2, 2, 2, 2] ])

In [22]: a2d
Out[22]:
array([[1, 1, 1, 1],
       [2, 2, 2, 2]])
```

- Using the built-in *arange* function

```
In [25]: a = numpy.arange(10)

In [26]: a
Out[26]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

In [27]: a = numpy.arange(0, 100, 10)

In [28]: a
Out[28]: array([ 0, 10, 20, 30, 40, 50, 60, 70, 80, 90])
```

Creating an Array

- Using the built-in *empty* function

```
In [27]: a = empty( (2,2) )

In [28]: a
Out[28]:
array([[  2.16777011e-313,   1.78514665e-296],
       [  2.28748514e-296,   2.43212233e-296]])
```

- Using the built-in *zeros* function

```
In [29]: a = zeros( (2,2) )

In [30]: a
Out[30]:
array([[ 0.,  0.],
       [ 0.,  0.]])
```

- Using the built-in *ones* function

```
In [33]: a = ones( (2,2), dtype=int)

In [34]: a
Out[34]:
array([[1, 1],
       [1, 1]])
```

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Creating an Array

- Using the built-in linspace function

```
In [29]: a = numpy.linspace(0, 1, 7)

In [30]: a
Out[30]:
array([ 0.        ,  0.16666667,  0.33333333,  0.5       ,  0.66666667,
        0.83333333,  1.        ])
```

- Universal functions operate elementwise on an array and produce a new array as a result

```
In [16]: import numpy

In [17]: x = numpy.linspace(0, 2 * numpy.pi, 20)

In [18]: y = numpy.sin(x)

In [19]: plot(x, y)
Out[19]: [<matplotlib.lines.Line2D object at 0x04A7B8B0>]

In [20]: show()
```

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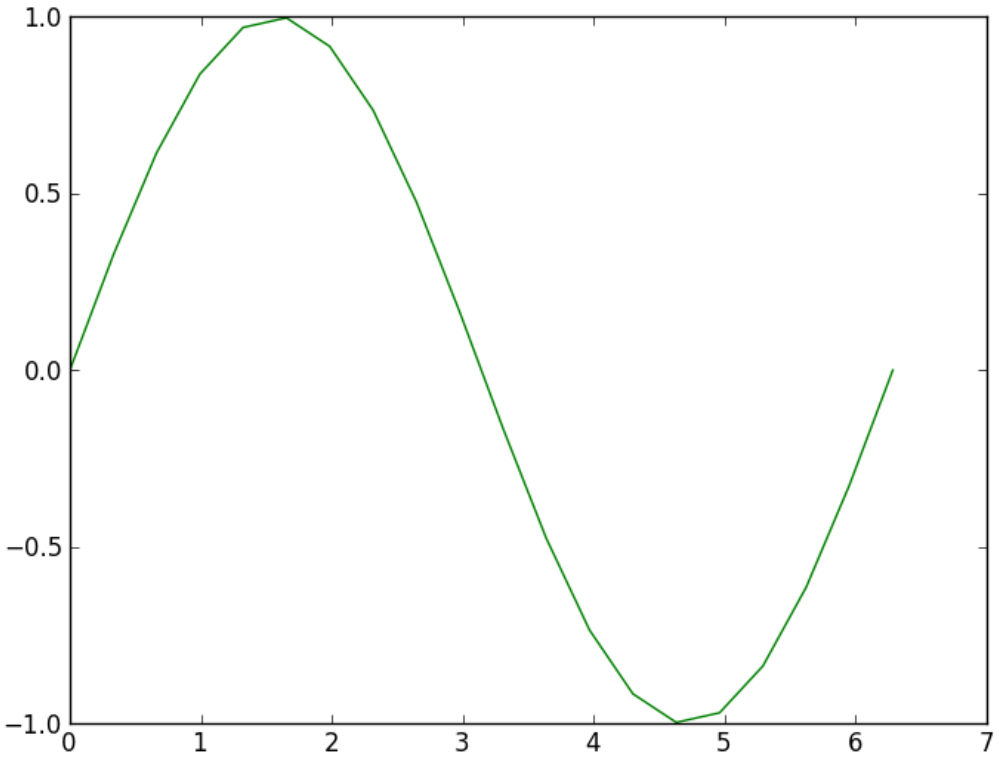
Loading an Array from a File



Loading an Array from a File

- If we have the following table stored in an ascii text file

  1 3 6 9
  12 15 18 21
  23 26 29 31
  77 78 79 2

- The table can be loaded into a numpy array using the numpy loadtxt function

```
In [28]: a = numpy.loadtxt('data\\4by4array.txt')

In [29]: a
Out[29]:
array([[  1.,   3.,   6.,   9.],
       [ 12.,  15.,  18.,  21.],
       [ 23.,  26.,  29.,  31.],
       [ 77.,  78.,  79.,   2.]])
```

Array Indexing

- Indexing is the term used to access elements in an array
- One of the biggest gotchas is that numpy arrays are zero-based, which means that the first element of the array is in position zero

```
In [9]: a = numpy.arange(1,10)

In [10]: a
Out[10]: array([1, 2, 3, 4, 5, 6, 7, 8, 9])

In [11]: a[0]
Out[11]: 1
```

- Negative indices can be used to go backward through an array

```
In [12]: a[-1]
Out[12]: 9

In [13]: a[-2]
Out[13]: 8
```

Array Slicing

- Slicing is the process of extracting multiple array elements
- Slicing returns an array

```
In [14]: a
Out[14]: array([1, 2, 3, 4, 5, 6, 7, 8, 9])

In [15]: a[2:5]
Out[15]: array([3, 4, 5])

In [16]: a[:2]
Out[16]: array([1, 2])

In [17]: a[5:]
Out[17]: array([6, 7, 8, 9])
```

- Format for slicing is *array[start:end:increment]*
- Note that the slice is up to the end but not including it

Array Slicing Examples

- Every third value

```
In [42]: arange(99)[::3]
Out[42]:
array([ 0,  3,  6,  9, 12, 15, 18, 21, 24, 27, 30, 33, 36, 39, 42, 45, 48,
       51, 54, 57, 60, 63, 66, 69, 72, 75, 78, 81, 84, 87, 90, 93, 96])
```

- Every third value up to, but not including position 50

```
In [43]: arange(99)[:50:3]
Out[43]: array([ 0,  3,  6,  9, 12, 15, 18, 21, 24, 27, 30, 33, 36, 39, 42, 45,
48])
```

Views Verus Copies

- Slicing produces a view of an array, not a copy!

```
In [44]: a = arange(10)

In [45]: b = a[7:]

In [46]: a
Out[46]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

In [47]: b
Out[47]: array([7, 8, 9])

In [48]: a[-1] = 1000

In [49]: a
Out[49]: array([   0,    1,    2,    3,    4,    5,    6,    7,    8, 1000])

In [50]: b
Out[50]: array([   7,    8, 1000])

In [51]: a is b
Out[51]: False

In [52]: a is b.base
Out[52]: True
```

Shape Manipulation

- The shape of an array is stored with the array and can be accessed by a.shape

```
In [61]: a = numpy.empty( (2, 3, 4) )

In [62]: a.shape
Out[62]: (2, 3, 4)
```

- The *reshape* method can be used to reshape an array provided a valid shape is given

```
In [58]: a = arange(81).reshape(9,9)

In [59]: a
Out[59]:
array([[ 0,  1,  2,  3,  4,  5,  6,  7,  8],
       [ 9, 10, 11, 12, 13, 14, 15, 16, 17],
       [18, 19, 20, 21, 22, 23, 24, 25, 26],
       [27, 28, 29, 30, 31, 32, 33, 34, 35],
       [36, 37, 38, 39, 40, 41, 42, 43, 44],
       [45, 46, 47, 48, 49, 50, 51, 52, 53],
       [54, 55, 56, 57, 58, 59, 60, 61, 62],
       [63, 64, 65, 66, 67, 68, 69, 70, 71],
       [72, 73, 74, 75, 76, 77, 78, 79, 80]])
```

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Helpful Methods and Functions

- min, max, mean, sum

```
In [76]: import numpy.random

In [77]: a = numpy.random.random( (50) )

In [78]: a
Out[78]:
array([ 0.55414299,  0.3271058 ,  0.31632925,  0.47979442,  0.25520635,
        0.80985775,  0.81492243,  0.85632766,  0.09273485,  0.56799651,
        0.04924593,  0.51993142,  0.60822579,  0.24912596,  0.06104689,
        0.29200259,  0.42240031,  0.4868186 ,  0.35386243,  0.70139757,
        0.07047982,  0.40676585,  0.1478561 ,  0.42732459,  0.11536969,
        0.50936407,  0.01519514,  0.484014  ,  0.81256495,  0.61565382,
        0.31964842,  0.41620434,  0.13149336,  0.60968828,  0.93935494,
        0.7523049 ,  0.56316456,  0.51333611,  0.03416447,  0.70446818,
        0.57875077,  0.78433295,  0.14120873,  0.99182476,  0.10675879,
        0.99531427,  0.66518705,  0.29422553,  0.26866666,  0.3063704 ])

In [79]: a.min()
Out[79]: 0.015195139324459928

In [80]: a.max()
Out[80]: 0.99531427387945004

In [81]: a.mean()
Out[81]: 0.45079062017573351

In [82]: a.sum()
```

Helpful Methods and Functions

- *where* can be used to find the indices where some condition is true

```
In [109]: ibound
Out[109]:
array([[1, 1, 1, 1, 1, 1, 1, 0, 0, 0],
       [1, 1, 1, 1, 1, 1, 1, 0, 0, 0],
       [1, 1, 1, 1, 1, 1, 1, 0, 0, 0],
       [1, 1, 1, 1, 1, 1, 1, 1, 1, 1],
       [1, 1, 1, 1, 1, 1, 1, 1, 1, 1],
       [1, 1, 1, 1, 1, 1, 1, 1, 1, 1],
       [1, 1, 1, 1, 1, 1, 1, 1, 1, 1],
       [1, 1, 1, 1, 1, 1, 1, 1, 1, 1],
       [1, 1, 1, 1, 1, 1, 1, 1, 1, 1],
       [1, 1, 1, 1, 1, 1, 1, 1, 1, 1]])

In [110]: idx_active = numpy.where(ibound > 0)

In [111]: idx_active
Out[111]:
(array([0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 3, 3,
       3, 3, 3, 3, 3, 3, 3, 4, 4, 4, 4, 4, 4, 4, 4, 4, 4, 5, 5, 5, 5, 5,
       5, 5, 5, 5, 5, 6, 6, 6, 6, 6, 6, 6, 6, 6, 6, 7, 7, 7, 7, 7, 7, 7, 7,
       7, 7, 8, 8, 8, 8, 8, 8, 8, 8, 8, 8, 9, 9, 9, 9, 9, 9, 9, 9, 9, 9]),
 array([0, 1, 2, 3, 4, 5, 6, 0, 1, 2, 3, 4, 5, 6, 0, 1, 2, 3, 4, 5, 6, 0, 1,
       2, 3, 4, 5, 6, 7, 8, 9, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 0, 1, 2, 3, 4,
       5, 6, 7, 8, 9, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 0, 1, 2, 3, 4, 5, 6, 7,
       8, 9, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 0, 1, 2, 3, 4, 5, 6, 7, 8, 9]))
```

Helpful Methods and Functions

- The indices can be used to access array elements

```
In [136]: head = numpy.random.random( (10, 10) ) * 100.

In [137]: head
Out[137]:
array([[  4.26240427e+01,   1.57995831e+01,   2.99365654e+01,
          6.33632715e+01,   3.94482417e+01,   1.49308627e+01,
          8.60771838e+01,   6.28894526e+01,   2.12602996e+01,
          1.89363873e+01],
...
       [  4.42445323e+01,   9.66760310e+01,   2.61880066e+01,
          5.00637180e+01,   7.34959659e+01,   3.57624988e+01,
          2.09579933e+00,   2.37504240e+01,   7.04080247e+01,
          8.49936631e+01]])

In [138]: print head.min(), head.max(), head.sum()
0.0629813630584 99.6093486525 4859.4605162

In [139]: print head[idx_active].min(), head[idx_active].max(), head[idx_active]
.sum()
0.0629813630584 99.6093486525 4339.2850813
```

Helpful Methods and Functions

- The indices can be used to assign values to array elements

```
In [140]: idx_inactive = where(ibound == 0)

In [141]: head[idx_inactive] = -999.

In [142]: head
Out[142]:
array([[  4.26240427e+01,   1.57995831e+01,   2.99365654e+01,
          6.33632715e+01,   3.94482417e+01,   1.49308627e+01,
          8.60771838e+01,  -9.99000000e+02,  -9.99000000e+02,
         -9.99000000e+02],
...
       [  4.42445323e+01,   9.66760310e+01,   2.61880066e+01,
          5.00637180e+01,   7.34959659e+01,   3.57624988e+01,
          2.09579933e+00,   2.37504240e+01,   7.04080247e+01,
          8.49936631e+01]])
```

Helpful Methods and Functions

- *where* can also be used to build a new array
- *where(condition, [x, y])*: x is inserted where the condition is true and y where the condition is false

```
In [143]: where( ibound == 0, -999, head)
Out[143]:
array([[  4.26240427e+01,   1.57995831e+01,   2.99365654e+01,
          6.33632715e+01,   3.94482417e+01,   1.49308627e+01,
          8.60771838e+01,  -9.99000000e+02,  -9.99000000e+02,
         -9.99000000e+02],
...
       [  4.42445323e+01,   9.66760310e+01,   2.61880066e+01,
          5.00637180e+01,   7.34959659e+01,   3.57624988e+01,
          2.09579933e+00,   2.37504240e+01,   7.04080247e+01,
          8.49936631e+01]])
```

Summary

- Numpy provides a great way to work with arrays. Its capabilities make it very useful for groundwater modeling
- The number of functions and methods can be overwhelming. The best way to become proficient is to start using it. Lots of information available on the internet.

Putting it all together: Theis Example

theis.py

```
1  import numpy as np
2  from scipy.special import expn
3
4  def theis(Q, T, S, t, r):
5      return Q / 4. / np.pi / T * expn(1, r ** 2 * S / 4. / T / t)
6
7  T = 1.; S = 0.001; t = 10.; rw = 0.01
8  xmin = -200; xmax = 200; nx = 100; ymin = -200; ymax = 200; ny = 100
9  x, y = np.meshgrid(np.linspace(xmin, xmax, nx), np.linspace(ymin, ymax, ny))
10 wells = [ [25, 30, 3], [50, 50, 3], [75, 30, 3] ]
11 ddn = np.zeros( x.shape, dtype=float)
12 for xw, yw, Qw in wells:
13     print 'Processing Well: x={0}, y={1}, Q={2}'.format(xw, yw, Qw)
14     r = np.sqrt((x - xw) ** 2 + (y - yw) ** 2)
15     r = np.where(r > rw, r, rw)
16     ddn = ddn + theis(Qw, T, S, t, r)
17
18 from matplotlib.pyplot import *
19 try:
20     close('all')
21 except:
22     pass
23 subplot(1, 1, 1, aspect='equal')
24 contourf(x, y, ddn)
25 colorbar(shrink=0.5)
26 show()
```