Intro to Research Computing with Python: NumPy & SciPy

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Today's class

Today we will discuss the following topics:

- NumPy: exciting features!
- SciPy: exciting features!

Lists aren't the ideal data type

Lists can do funny things that you don't expect, if you're not careful.

- Lists are just a collection of items, of any type.
- If you do mathematical operations on a list, you won't get what you expect.
- These are not the ideal data type for scientific computing.
- Arrays are a much better choice, but are not a native Python data type.

```
In [1]: a = [1, 2, 3, 4]

In [2]: a
Out[2]: [1, 2, 3, 4]

In [3]: b = [3, 5, 5, 6]

In [4]: b
Out[4]: [3, 5, 5, 6]

In [5]: 2 * a
Out[5]: [1, 2, 3, 4, 1, 2, 3, 4]

In [6]: a + b
Out[6]: [1, 2, 3, 4, 3, 5, 5, 6]
```

Arrays are what we want to use

Almost everything that you want to do starts with NumPy.

- Contains arrays of various types and forms: zeros, ones, linspace, *etc.*
- linspace takes 2 or 3 arguments, the default number of entries is 50.

```
In [7]: from numpy import zeros,
  ones, linspace

In [8]: zeros(5)
Out[8]: array([ 0., 0., 0., 0., 0.])

In [9]: ones(5, dtype = int)
Out[9]: array([ 1, 1, 1, 1, 1])
```

```
In [10]: zeros([2,2])
Out[10]:
array([[ 0., 0.],
       [ 0., 0.]])

In [11]: arange(5)
Out[11]: array([ 0, 1, 2, 3, 4])

In [12]: linspace(1,5)
Out[12]: array([ 1., 1.08163265,
1.16326531, 1.24489796,
.
.
4.67346939, 4.75510204,
4.83673469, 4.91836735, 5.  ])

In [13]: linspace(1, 5, 6)
Out[13]: array([ 1., 1.8, 2.6, 3.4,
  4.2, 5.])
```

Accessing array elements

Elements of arrays are accessed using square brackets.

- Python is *row major* (like C++, Mathematica), NOT *column major* (like Fortran, MATLAB, R).
- This means the first index is the row, not the column.
- Indexing starts at zero.

```
In [14]: zeros([2, 3])
Out[14]:
array([[ 0., 0., 0.],
       [ 0., 0., 0.]])

In [15]: a = zeros([2,3])
```

```
In [16]: a[1,2] = 1

In [17]: a[0,1] = 2

In [18]: a
Out[18]:
array([[ 0., 2., 0.],
       [ 0., 0., 1.]])

In [19]: a[2,1] = 1
-----------------------------------
IndexError Traceback
<ipython-input-21-83f146d6c508> in
<module>()
----> 1 a[2,1] = 1
IndexError:  index (2) out of range
(0<=index<2) in dimension 0

In [20]:
```

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Copying array variables

Use caution when copying array variables. There's a 'feature' here that is unexpected.

```
In [20]: a = 10; b = a; a = 20

In [21]: a, b
Out[21]: (20, 10)

In [22]: a = array([[1,2,3],[2,3,4]])

In [23]: b = a

In [24]: a[1,0] = -10

In [25]: a
Out[25]:
array([[1, 2, 3],
       [-10, 3, 4]])
```

```
In [26]: b
Out[26]:
array([[1, 2, 3],
       [-10, 3, 4]])

In [27]: b = a.copy()

In [28]: a[1,0] = 16

In [29]: a
Out[29]:
array([[1, 2, 3],
       [16, 3, 4]])

In [30]: b
Out[30]:
array([[1, 2, 3],
       [-10, 3, 4]])
```

vector-vector & vector-scalar multiplication

1-D arrays are often called 'vectors'.

- When vectors are multiplied you get element-by-element multiplication.
- When vectors are multiplied by a scalar (a 0-D array), you also get element-by-element multiplication.

```
In [31]: a = arange(4)

In [32]: a
Out[32]: array([0, 1, 2, 3])
```

```
In [33]: b = arange(4.) + 3

In [34]: b
Out[34]: array([ 3., 4., 5., 6.])

In [35]: c = 2

In [36]: c
Out[36]: 2

In [37]: a * b
Out[37]: array([ 0., 4., 10., 18.])

In [38]: a * c
Out[38]: array([0, 2, 4, 6])

In [39]: b * c
Out[39]: array([ 6., 8., 10., 12.])
```

matrix-vector multiplication

A 2-D array is sometimes called a 'matrix'.

- Matrix-scalar multiplication gives element-by-element multiplication.
- Matrix-vector multiplication DOES NOT give the standard result!

```
In [40]: a = array([[1,2,3],[2,3,4]])
In [41]: a
Out[41]:
array([[1, 2, 3],
       [2, 3, 4]])
In [42]: b = arange(3) + 1
In [43]: b
Out[43]: array([1, 2, 3])

In [44]: a * b
Out[44]:
array([[ 1, 4, 9],
       [ 2, 6, 12]])
```

Normal matrix-vector multiplication:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} * \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} a_{11} * b_1 + a_{12} * b_2 + a_{13} * b_3 \\ a_{21} * b_1 + a_{22} * b_2 + a_{23} * b_3 \\ a_{31} * b_1 + a_{32} * b_2 + a_{33} * b_3 \end{bmatrix}$$

matrix-matrix multiplication

Not surprisingly, matrix-matrix multiplication doesn't work as expected either, instead doing the same thing as vector-vector multiplication.

```
In [45]: a = array([[1,2,3],[2,3,4]])
In [46]: b = array([[1,2,3],[2,3,4]])
In [47]: a
Out[47]:
array([[1, 2, 3],
       [2, 3, 4]])
In [48]: a * b
Out[48]:
array([[ 1, 4, 9],
       [ 4, 9, 16]])
```

Normal matrix-matrix multiplication:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} * \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} =$$

$$\begin{bmatrix} a_{11} * b_{11} + a_{12} * b_{21} & a_{11} * b_{12} + a_{12} * b_{22} \\ a_{21} * b_{11} + a_{22} * b_{21} & a_{21} * b_{12} + a_{22} * b_{22} \end{bmatrix}$$

How to do matrix algebra?

There are two solutions to these matrix multiplication problems.

- The specially built-in array fixes (using 'array' types).
- The matrix module (using 'matrix' types).

The latter option is a bit clunkier, so we recommend the 'fixes'.

```
In [49]: from scipy import dot

In [50]: a = array([[1,2,3],[2,3,4]])
In [51]: b = array([[1,2,3],[2,3,4]])
In [52]: a
Out[52]:
array([[1, 2, 3],
       [2, 3, 4]])
```

```
In [53]: a.transpose()
Out[53]:
array([[1, 2],
       [2, 3],
       [3, 4]])

In [54]: dot(a.transpose(), b)
Out[54]:
array([[ 5, 8, 11],
       [ 8, 13, 18],
       [11, 18, 25]])

In [55]: dot(b, a.transpose())
Out[55]:
array([[14, 20],
       [20, 29]])

In [56]: c = arange(3) + 1
In [57]: dot(a,c)
Out[57]: array([14, 20])
```

The linalg module

The linalg module contains useful functions for matrix algebra.

- Typical matrix functions: inv, det, norm...
- More advanced functions: eig, SVD, cholesky...
- Both NumPy and SciPy have a linalg module. Use SciPy, because it is always compiled with BLAS/LAPACK support.

```
In [58]: from scipy import dot, linalg

In [59]: a = array([[1,2,3], [3,4,5], [1,1,2]])

In [60]: linalg.det(a)
Out[60]: -2.0

In [61]: dot(a, linalg.inv(a))
Out[61]:
array([[ 1.00000000e+00, 0.00000000e+00, 0.00000000e+00],
       [ 2.77555756e-16, 1.00000000e+00, 0.00000000e+00],
       [ 0.00000000e+00, 5.55111512e-17, 1.00000000e+00]])
```

Solving systems of equations

The linalg module comes with an important function: solve.

- linalg.solve is used to solve the system of equations $\boldsymbol{Ax} = \boldsymbol{b}$.

```
In [62]: a = array([[1,2,3], [3,4,5],
  [1,1,2]])

In [63]: a
Out[63]:
array([[ 1, 2, 3],
       [ 3, 4, 5],
       [ 1, 1, 2]])

In [64]: b = array([3, 4, 2])

In [65]: b
Out[65]: array([3, 4, 2])
```

```
In [66]: x = linalg.solve(a, b)

In [67]: x
Out[67]: array([-0.5, -0.5, 1.5])
```

$$\begin{bmatrix} \mathbf{1} & \mathbf{2} & \mathbf{3} \\ \mathbf{3} & \mathbf{4} & \mathbf{5} \\ \mathbf{1} & \mathbf{1} & \mathbf{2} \end{bmatrix} * \begin{bmatrix} \mathbf{-0.5} \\ \mathbf{-0.5} \\ \mathbf{1.5} \end{bmatrix} = \begin{bmatrix} \mathbf{3} \\ \mathbf{4} \\ \mathbf{2} \end{bmatrix}$$

Statistics

SciPy contains all of the statistical functions that you'll probably ever need.

- The scipy.stats module is based around the idea of a 'random variable' type.
- A whole variety of standard distributions are available:
  - Continuous distributions: Normal, Maxwell, Cauchy, Chi-squared, Gumbel Left-scewed, Gilbrat, Nakagami, ...
  - Discrete distributions: Poisson, Binomial, Geometric, Bernoulli, ...
- The 'random variables' have all of the statistical properties of the distributions built into them already: cdf, pdf, mean, variance, moments, ...

Statistics, continued

```
In [68]:
```

Statistics, continued

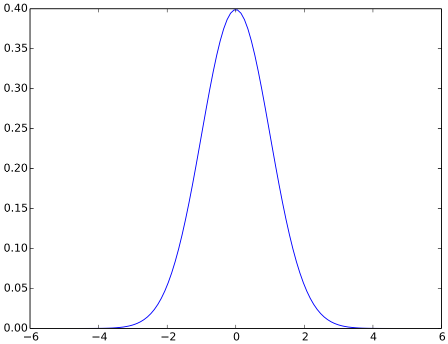
```
In [68]: from scipy.stats import norm

In [69]:
```

Statistics, continued

```
In [68]: from scipy.stats import norm

In [69]: x = linspace(-5, 5, 100)

In [70]:
```

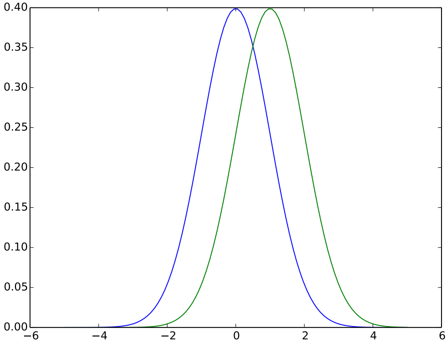
Statistics, continued

```
In [68]: from scipy.stats import norm

In [69]: x = linspace(-5, 5, 100)

In [70]: plot(x, norm.pdf(x))

In [71]:
```



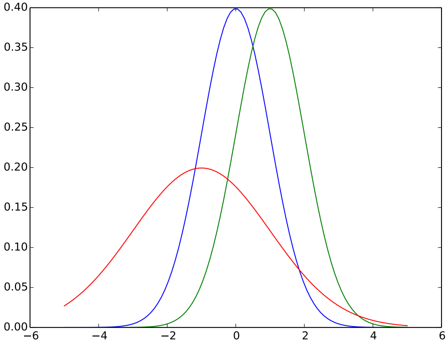
Statistics, continued

```
In [68]: from scipy.stats import norm

In [69]: x = linspace(-5, 5, 100)

In [70]: plot(x, norm.pdf(x))

In [71]: plot(x, norm.pdf(x, loc = 1))

In [72]:
```



Statistics, continued

```
In [68]: from scipy.stats import norm

In [69]: x = linspace(-5, 5, 100)

In [70]: plot(x, norm.pdf(x))

In [71]: plot(x, norm.pdf(x, loc = 1))

In [72]: plot(x, norm.pdf(x,
  loc = -1, scale = 2))
```



All continuous distributions take loc and $scale$ as keyword parameters to adjust the location and scale of the distribution. In general the distribution of a random variable X is obtained from $(X - loc)/scale$. The default values are $loc = 0$ and $scale = 1$.

Statistics, continued

```
In [73]:
```

Statistics, continued

```
In [73]: from pylab import hist

In [74]:
```

Statistics, continued

```
In [73]: from pylab import hist

In [74]: norm.mean(loc = -1,
  scale = 2)
Out[74]: -1.0

In [75]:
```

Statistics, continued

```
In [73]: from pylab import hist

In [74]: norm.mean(loc = -1,
  scale = 2)
Out[74]: -1.0

In [75]: norm.std(loc = -1, scale = 2)
Out[75]: 2.0

In [76]:
```

Statistics, continued

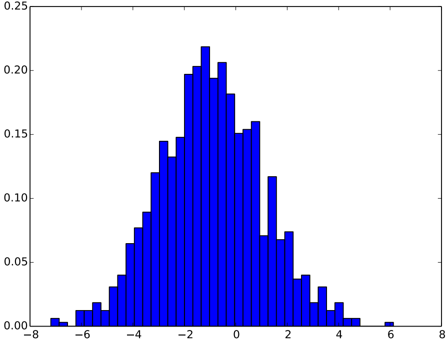
```
In [73]: from pylab import hist

In [74]: norm.mean(loc = -1,
  scale = 2)
Out[74]: -1.0

In [75]: norm.std(loc = -1, scale = 2)
Out[75]: 2.0

In [76]: norm.moment(3, loc = -1,
  scale = 2)
Out[76]: -13.0

In [77]:
```

Statistics, continued

```
In [73]: from pylab import hist

In [74]: norm.mean(loc = -1,
  scale = 2)
Out[74]: -1.0

In [75]: norm.std(loc = -1, scale = 2)
Out[75]: 2.0

In [76]: norm.moment(3, loc = -1,
  scale = 2)
Out[76]: -13.0

In [77]: samples = norm.rvs(
  size = 1000, loc = -1, scale = 2)

In [78]:
```

Statistics, continued

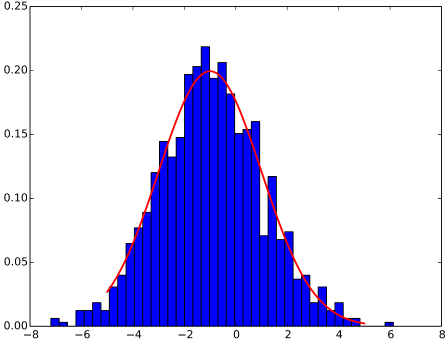
```
In [73]: from pylab import hist

In [74]: norm.mean(loc = -1,
  scale = 2)
Out[74]: -1.0

In [75]: norm.std(loc = -1, scale = 2)
Out[75]: 2.0

In [76]: norm.moment(3, loc = -1,
  scale = 2)
Out[76]: -13.0

In [77]: samples = norm.rvs(
  size = 1000, loc = -1, scale = 2)

In [78]: h = hist(samples, bins = 41,
  normed = True)
```




```
In [79]:
```

Statistics, continued

```
In [73]: from pylab import hist

In [74]: norm.mean(loc = -1,
  scale = 2)
Out[74]: -1.0

In [75]: norm.std(loc = -1, scale = 2)
Out[75]: 2.0

In [76]: norm.moment(3, loc = -1,
  scale = 2)
Out[76]: -13.0

In [77]: samples = norm.rvs(
  size = 1000, loc = -1, scale = 2)

In [78]: h = hist(samples, bins = 41,
  normed = True)
```




```
In [79]: plot(x, norm.pdf(x,
    loc = -1, scale = 2), 'r',
    linewidth = 2)
```

Statistics, a discrete example

```
In [80]:
```

Note that discrete distributions have Probability Mass Functions (PMF) instead of Probability Distribution Functions (PDF).

Statistics, a discrete example

```
In [80]: from scipy.stats import
  poisson

In [81]:
```

Note that discrete distributions have Probability Mass Functions (PMF) instead of Probability Distribution Functions (PDF).

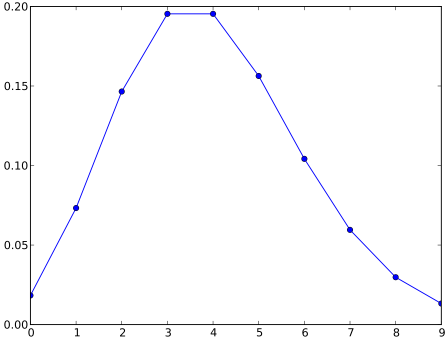
Statistics, a discrete example

```
In [80]: from scipy.stats import
  poisson

In [81]: x = arange(10)

In [82]:
```

Note that discrete distributions have Probability Mass Functions (PMF) instead of Probability Distribution Functions (PDF).

Statistics, a discrete example

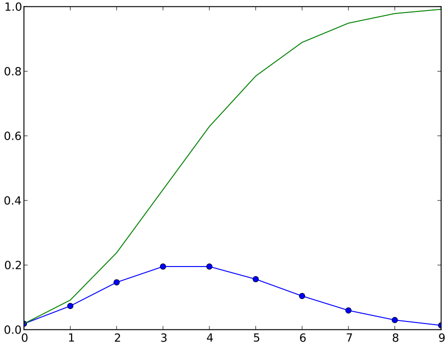
```
In [80]: from scipy.stats import
  poisson

In [81]: x = arange(10)

In [82]: plot(x, poisson.pmf(x, 4),
  'o-')

In [83]:
```



Note that discrete distributions have Probability Mass Functions (PMF) instead of Probability Distribution Functions (PDF).

Statistics, a discrete example

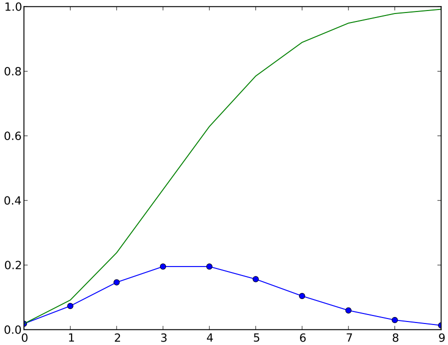
```
In [80]: from scipy.stats import
  poisson

In [81]: x = arange(10)

In [82]: plot(x, poisson.pmf(x, 4),
  'o-')

In [83]: plot(x, poisson.cdf(x, 4)

In [84]:
```



Note that discrete distributions have Probability Mass Functions (PMF) instead of Probability Distribution Functions (PDF).

Statistics, a discrete example

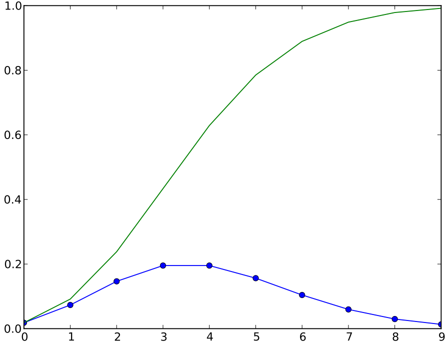
```
In [80]: from scipy.stats import
  poisson

In [81]: x = arange(10)

In [82]: plot(x, poisson.pmf(x, 4),
  'o-')

In [83]: plot(x, poisson.cdf(x, 4)

In [84]: poisson.mean(4)
Out[84]: 4.0

In [85]:
```



Note that discrete distributions have Probability Mass Functions (PMF) instead of Probability Distribution Functions (PDF).

Statistics, a discrete example

```
In [80]: from scipy.stats import
  poisson

In [81]: x = arange(10)

In [82]: plot(x, poisson.pmf(x, 4),
  'o-')

In [83]: plot(x, poisson.cdf(x, 4)

In [84]: poisson.mean(4)
Out[84]: 4.0

In [85]: poisson.var(4)
Out[85]: 4.0
```



Note that discrete distributions have Probability Mass Functions (PMF) instead of Probability Distribution Functions (PDF).

poly1d, a strange module

numpy.poly1d allows manipulation of polynomials in symbolic form.

- Very powerful in certain contexts (linear stability analyses).

```
In [86]: from numpy import poly1d

In [87]: p = poly1d([2,2,3])

In [88]: p
Out[88]: poly1d([2, 2, 3])

In [89]: print p
____2
2 x + 2 x + 3
```

That last print statement is supposed to be $2x^2 + 2x + 3$.

```
In [90]: p(1.2)
Out[90]: 8.2800000000000011

In [91]: p.c
Out[91]: array([2, 2, 3])

In [92]: q = poly1d([3, 4, 5, 6])

In [93]: (p * q).order
Out[93]: 5

In [94]: print p * q
```

Out[94]: $6x^5 + 14x^4 + 27x^3 + 34x^2 + 27x + 18$

```
In [95]:  q.roots
Out[95]:
array([-1.26532809+0.j,
-0.03400262+1.2567663j,
-0.03400262-1.2567663j])
```

Polynomial fitting

```
In [96]:
```

Polynomial fitting

```
In [96]: from numpy import arange, zeros
  polyfit, polyval
In [97]:
```

Polynomial fitting

```
In [96]: from numpy import arange, zeros
  polyfit, polyval
In [97]: import random

In [98]:
```

Polynomial fitting

```
In [96]: from numpy import arange, zeros
  polyfit, polyval
In [97]: import random

In [98]: x = arange(50.)

In [99]:
```

Polynomial fitting

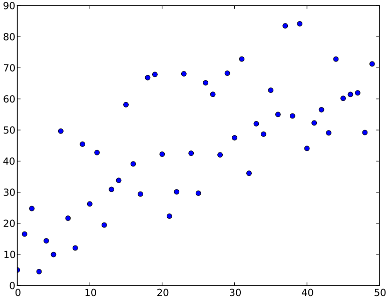
```
In [96]: from numpy import arange, zeros
  polyfit, polyval
In [97]: import random

In [98]: x = arange(50.)

In [99]: y = zeros(50.)

In [100]:
```

Polynomial fitting

```
In [96]: from numpy import arange, zeros
  polyfit, polyval
In [97]: import random

In [98]: x = arange(50.)

In [99]: y = zeros(50.)

In [100]: for i in arange(50.):
  y[i] = x[i] + 50.0 * random.random()

In [101]:
```

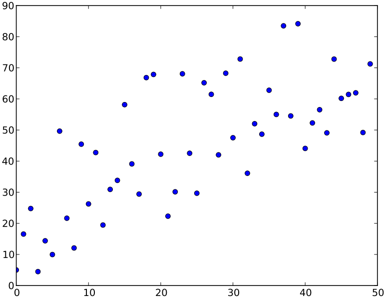
Polynomial fitting

```
In [96]: from numpy import arange, zeros
  polyfit, polyval
In [97]: import random

In [98]: x = arange(50.)

In [99]: y = zeros(50.)

In [100]: for i in arange(50.):
  y[i] = x[i] + 50.0 * random.random()

In [101]: plot(x, y, 'o')

In [102]:
```



Polynomial fitting

```
In [96]: from numpy import arange, zeros
 polyfit, polyval
In [97]: import random

In [98]: x = arange(50.)

In [99]: y = zeros(50.)

In [100]: for i in arange(50.):
 y[i] = x[i] + 50.0 * random.random()

In [101]: plot(x, y, 'o')

In [102]: fit = polyfit(x, y, 1)

In [103]:
```



Polynomial fitting

```
In [96]: from numpy import arange, zeros
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In [97]: import random

In [98]: x = arange(50.)

In [99]: y = zeros(50.)

In [100]: for i in arange(50.):
  y[i] = x[i] + 50.0 * random.random()

In [101]: plot(x, y, 'o')

In [102]: fit = polyfit(x, y, 1)

In [103]: fit
Out[103]: array([ 1.0073584,
20.64695036])

In [104]:
```
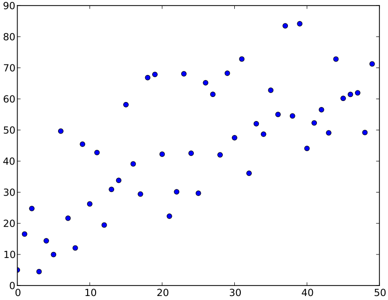
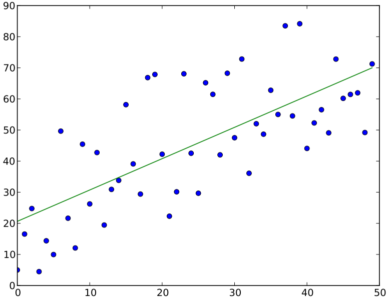



Polynomial fitting

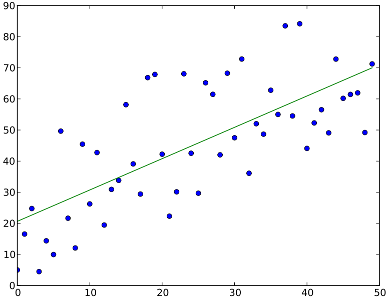
```
In [96]: from numpy import arange, zeros
  polyfit, polyval
In [97]: import random

In [98]: x = arange(50.)

In [99]: y = zeros(50.)

In [100]: for i in arange(50.):
  y[i] = x[i] + 50.0 * random.random()

In [101]: plot(x, y, 'o')

In [102]: fit = polyfit(x, y, 1)

In [103]: fit
Out[103]: array([ 1.0073584,
20.64695036])

In [104]: plot(x, polyval(fit, x))
```




```
In [105]:
```

Polynomial fitting

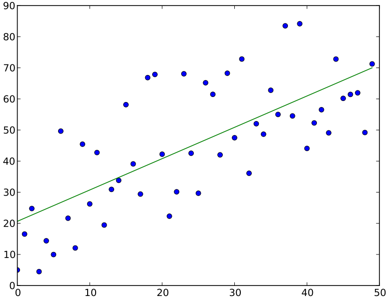
```
In [96]: from numpy import arange, zeros
  polyfit, polyval
In [97]: import random

In [98]: x = arange(50.)

In [99]: y = zeros(50.)

In [100]: for i in arange(50.):
  y[i] = x[i] + 50.0 * random.random()

In [101]: plot(x, y, 'o')

In [102]: fit = polyfit(x, y, 1)

In [103]: fit
Out[103]: array([ 1.0073584,
20.64695036])

In [104]: plot(x, polyval(fit, x))
```




```
In [105]: fit = polyfit(x, y, 2)

In [106]:
```

Polynomial fitting

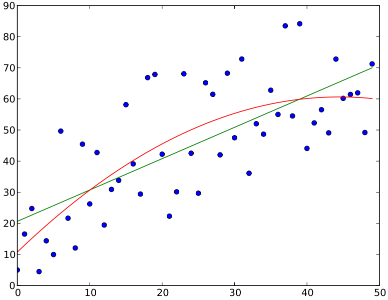
```
In [96]: from numpy import arange, zeros
  polyfit, polyval
In [97]: import random

In [98]: x = arange(50.)

In [99]: y = zeros(50.)

In [100]: for i in arange(50.):
  y[i] = x[i] + 50.0 * random.random()

In [101]: plot(x, y, 'o')

In [102]: fit = polyfit(x, y, 1)

In [103]: fit
Out[103]: array([ 1.0073584,
20.64695036])

In [104]: plot(x, polyval(fit, x))
```




```
In [105]: fit = polyfit(x, y, 2)

In [106]: fit
Out[106]: array([ -0.02520835,
  2.24256777, 10.76527546])

In [107]:
```

Polynomial fitting

```
In [96]: from numpy import arange, zeros
 polyfit, polyval
In [97]: import random

In [98]: x = arange(50.)

In [99]: y = zeros(50.)

In [100]: for i in arange(50.):
 y[i] = x[i] + 50.0 * random.random()

In [101]: plot(x, y, 'o')

In [102]: fit = polyfit(x, y, 1)

In [103]: fit
Out[103]: array([ 1.0073584,
20.64695036])

In [104]: plot(x, polyval(fit, x))
```




```
In [105]: fit = polyfit(x, y, 2)

In [106]: fit
Out[106]: array([ -0.02520835,
 2.24256777, 10.76527546])

In [107]: plot(x, polyval(fit, x))
```

Useful websites

If there is some functionality that you hope exists, it probably does.

- NumPy: `http://wiki.scipy.org/Tentative_NumPy_Tutorial`
- SciPy: `http://docs.scipy.org/doc/scipy/reference/tutorial`

Summary

- When manipulating numbers in blocks, use the array type, not lists.
- Use the copy() function to copy array variables.
- Array types do element-by-element multiplication, addition, etc.
- If you want to do standard array arithmetic, use the built-in scipy.linalg functions: dot, inv, det, eig, *etc.*
- SciPy comes with fairly complete set of statistical distributions, tests, and functions. If you need it it's probably there.
- numpy.poly1d can really simplify your life in certain circumstances.

Homework 2

1. In the following two questions, use version control on your answers. Submit the output of 'hg log' for each question. We expect to see several commits.

2. Consider a product of two variables which are drawn from known distributions: $\boldsymbol{X} = \boldsymbol{a} \times \boldsymbol{b}$. $\boldsymbol{a}$ is from a normal distribution, centered on -2, with a standard deviation of 1.5. $\boldsymbol{b}$ is from a generalized logistic distribution (type I, sometimes called the skew-logistic distribution), with c = 5.

   Write a Python program which plots a histogram of $\boldsymbol{X}$, for 10000 samples of $\boldsymbol{a}$ and $\boldsymbol{b}$. Save the output figure using the 'savefig' command. By interpreting the histogram, print an estimate of the most probable value of $\boldsymbol{X}$.

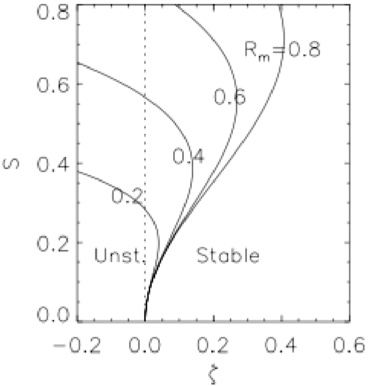
   This is an example of a Monte Carlo simulation, a class of simulations which involve calculating quantities from variables that come from probability distributions, rather than variables that have exact values.

Homework 2, continued

3. Write a Python program which calculates the roots of the equation

$$S^4 + S^2(\zeta - 2) + \zeta = 0$$

and plots the result as a function of ζ. Only consider $0.0 \leq S \leq 0.8$ and $0.0 \leq \zeta \leq 0.6$. Plot the curve, and submit it with your program.



The above equation is a special case of this equation:

$$\zeta \geq \frac{2S^2}{S^2 - 1} - \frac{S^4(1 + \epsilon^2)}{2R_m^2(S^2 + 1)}$$

which is equation 3 in MNRAS **325**, L1-L5 (2001), with $\epsilon = 1$ and $R_m = 1$. The figure above shows the solutions for various other values of R_m.