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Essential Data Skills for Business Analytics

Lecture 12 (04/17, 04/19): Optimization and Statistics: SciPy

Decision, Operations & Information Technologies
Robert H. Smith School of Business
Spring, 2017

Scientific Applications

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- There are a few third-party packages available for scientific computing that extend Python's basic math module:
  - NumPy/SciPy – numerical and scientific function libraries.
  - Numba – Python compiler that support JIT compilation.
  - ALGLIB – numerical analysis library.
  - PyGSL – Python interface for GNU Scientific Library.
  - ScientificPython – collection of scientific computing modules.

SciPy

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- By far, the most commonly used packages are those in the SciPy stack. These packages include:
  - NumPy – fundamental package for scientific computing.
  - SciPy – efficient numerical routines.
  - Matplotlib – plotting library.
  - IPython – interactive computing.
  - SymPy – symbolic computation library.
  - Pandas – data analysis library.
  - …

Install SciPy Stack

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- https://www.scipy.org/install.html
- Mac and Linux users can install pre-built binary packages for the SciPy stack using pip.
- Pip can install pre-built binary packages in the wheel package format.
- Pip does not work well for Windows because the standard pip package index site, PyPI, does not yet have Windows wheels for some packages, such as SciPy.

Install SciPy Stack

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- To install via pip on Mac or Linux, first upgrade pip to the latest version:

  python -m pip install --upgrade pip

- Then install the SciPy stack packages with pip by using the --user flag. This installs packages for your local user, and does not need extra permissions to write to the system directories:

  pip install --user numpy scipy matplotlib ipython sympy pandas

NumPy

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- The fundamental package for scientific computing with Python. It contains:
  - A powerful N-dimensional array (ndarray) object.
  - Sophisticated (broadcasting/universal) functions.
  - Tools for integrating C/C++ and Fortran code.
  - Useful linear algebra, Fourier transform, and random number capabilities.
- Besides its obvious scientific uses, NumPy can also be used as an efficient multi-dimensional container of generic data.

NumPy & Class ndarray

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```
>>> import numpy
>>> import numpy as np
>>> from numpy import *
```

docs.scipy.org/doc/numpy/reference/generated/numpy.ndarray.html

```
>>> dir(numpy)
>>> dir(numpy.ndarray)
>>> help(dtype)
>>> help(ndarray)
>>> help(ndarray.dtype)
```

NumPy Data Types

- NumPy supports a much greater variety of numerical types than Python does:
  - bool_
  - int_, intc, intp, u/int8, u/int16, u/int32, u/int64
  - float_, float16, float32, float64
  - complex_, complex64, complex128
- NumPy numerical types are instances of dtype (data-type) objects:
  - numpy.dtype(object, align, copy)

NumPy Data Types

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```
>>> x = np.float32(1.0)
>>> x
1.0
>>> y = np.int_([1,2,4])
>>> y
array([1, 2, 4])
>>> z = np.arange(3, dtype=np.uint8)
array([0, 1, 2], dtype=uint8)
>>> z.dtype
dtype('uint8')
```

NymPy Arrays

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- The main feature of NumPy is an array object:
  - Arrays can be N-dimensional.
  - Array elements have to be the same type.
  - Array elements can be accessed, sliced, and manipulated in the same way as the lists.
  - The number of elements in the array is fixed.
  - Shape of the array can be changed.
- Built-in NumPy array creation:
  - array(), arange(), ones(), zeros(), …

NumPy Arrays

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```
>>> np.array([2,3,1,0])
array([2, 3, 1, 0])
>>> np.array([[1,2.0],[0,0],(1+1j,3.)])
array([[ 1.+0.j, 2.+0.j],
       [ 0.+0.j, 0.+0.j],
       [ 1.+1.j, 3.+0.j]])

>>> np.zeros((2,3))
array([[ 0., 0., 0.],
       [ 0., 0., 0.]])
```

NumPy Arrays

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```
>>> np.arange(10)
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> np.arange(2,10,dtype=np.float)
array([ 2., 3., 4., 5., 6., 7., 8.,
9.])
>>> np.arange(2,3,0.1)
array([ 2. , 2.1, 2.2, 2.3, 2.4, 2.5,
2.6, 2.7, 2.8, 2.9])
```

NumPy Arrays

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```
>>> a = np.arange(3)
>>> print(a)
[0, 1, 2]
>>> a
array([0, 1, 2])
>>> np.arange(9).reshape(3,3)
array([[0, 1, 2],
       [3, 4, 5],
       [6, 7, 8]]
>>> np.arange(8).reshape(2,2,2)
array([[[0, 1],
        [2, 3]],

       [[4, 5],
        [6, 7]]])
```

NumPy Arrays

- linspace(start, stop[, num, endpoint, retstep, dtype]) – creates arrays with a specified number of elements, and spaced equally between the specified beginning and end values.

- random.random([size]) – creates arrays with random floats over the interval [0.,1.).
- random.randint(low[, high, size, dtype]) – creates arrays with random integers from low (inclusive) to high (exclusive).

NumPy Arrays

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```
>>> np.linspace(1.,4.,6)
array([ 1. , 1.6, 2.2, 2.8, 3.4, 4. ])


>>> np.random.random((2,3))
array([[ 0.96826, 0.30919, 0.58381],
       [ 0.56865, 0.33730, 0.41241]])
>>> np.random.randint(1,7,(2,3))
array([[2, 4, 5, 2, 3, 6],
       [6, 3, 1, 4, 1, 5]]
```

NumPy Linear Algebra

- All linear algebra routines expect an object that can be converted into a 2-dimensional array.
- The output is also a two-dimensional array.
  - dot(a, b[, out]) – dot product of two arrays.
  - trace(a[, offset, axis1, axis2, dtype, out]) – returns the sum along diagonals of the array.
  - inv(a) – computes the inverse of a matrix.
  - eig(a) – eigenvalues and right eigenvectors of a square array.
  - solve(a, b) – solves a linear matrix equation, or system of linear scalar equations.

NumPy LinAlg

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```
>>> from numpy import *
>>> from numpy.linalg import *
>>> a = array([[1.0,2.0],[3.0,4.0]])
>>> print(a)
array([[ 1., 2.],
       [ 3., 4.]])
>>> a.transpose()
array([[ 1., 3.],
       [ 2., 4.]])
>>> inv(a) # inverse
array([[-2. , 1. ],
       [ 1.5, -0.5]])
```

NumPy LinAlg

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```
>>> u = eye(2) # unit 2x2 matrix; "eye" ~ "I"
>>> u
array([[ 1., 0.],
       [ 0., 1.]])
>>> trace(u)
2.0
>>> j = array([[0.0,-1.0],[1.0,0.0]])
>>> dot(j, j) # matrix product
array([[-1., 0.],
       [ 0., -1.]])
>>> eig(j) # get eigenvalues & eigenvectors
(array([ 0.+1.j, 0.-1.j]),
 array([[ 0.70710+0.j,      0.70710+0.j],
        [ 0.00000-0.70710j, 0.00000+0.70710j]]))
```

NumPy LinAlg

- There are two alcohol solutions: 50% & 90%.
- How many gallons of each solution to be mixed to get 10 gallons of 74% alcohol solution?

$x_1+x_2=10$, $0.5x_1+0.9x_2=0.74*10=7.4 \rightarrow AX=Y$

```
>>> A = array([[1.0,1.0],[0.5,0.9]])
>>> Y = array([[10.0],[7.4]])
>>> solve(A, Y) # solve linear equations
array([[ 4.],
       [ 6.]])
```

NumPy LinAlg

- A drone flying with the wind could cover 60 miles in 2 hours.
- The return trip against the wind took 2.5 hours.
- How fast was the drone?
- What was the air speed?

Trip	Rate	Time	Distance
With wind	d + w	2	60
Against wind	d - w	2.5	60

```
>>> A = array([[2.0,2.0],[2.5,-2.5]])
>>> Y = array([[60.0],[60.0]])
>>> solve(A, Y) # solve linear equations
array([[ 27.],
       [  3.]])
```

NymPy Matrix Versus Array

- NumPy matrices are strictly 2-dimensional, while NumPy arrays (ndarrays) are N-dimensional.
- Matrix objects are a subclass of ndarray, so they inherit all the attributes and methods of ndarrays.
- The main advantage of NumPy matrices is that they provide a convenient notation for matrix multiplication:
  - e.g. If A and B are matrices, then A*B is their matrix product.

NymPy Matrices

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```
>>> A = matrix('1.0 2.0; 3.0 4.0')
>>> A
matrix([[ 1., 2.],
        [ 3., 4.]])
>>> type(A)
<class 'numpy.matrixlib.defmatrix.matrix'>
>>> Y = matrix('5.0; 7.0')
>>> print(A.I) # inverse
[[-2.   1. ]
 [ 1.5 -0.5]]
>>> print(A.I*Y) # multiplication
[[-3.],
 [ 4.]])
>>> solve(A, Y) # solving linear equations
matrix([[-3.],
        [ 4.]])
```

SciPy

- A collection of mathematical algorithms and convenience functions built on the NumPy extension of Python.
- An interactive Python session for manipulating and visualizing data.
- A data-processing and system-prototyping environment rivaling systems such as MATLAB, IDL, Octave, R-Lab, and SciLab.

```
>>> from numpy import *
>>> from matplotlib import *
>>> from matplotlib.pyplot import *
```

SciPy Sub-Modules

- **cluster** – clustering algorithms
- **integrate** – integration and ordinary differential equation solvers
- **interpolate** – interpolation and smoothing splines
- **io** – input and output
- **linalg** – linear algebra
- **optimize** – optimization and root-finding routines
- **stats** – statistical distributions and functions

```
>>> from scipy import linalg, optimize
>>> from scipy import *
```

SciPy Clustering

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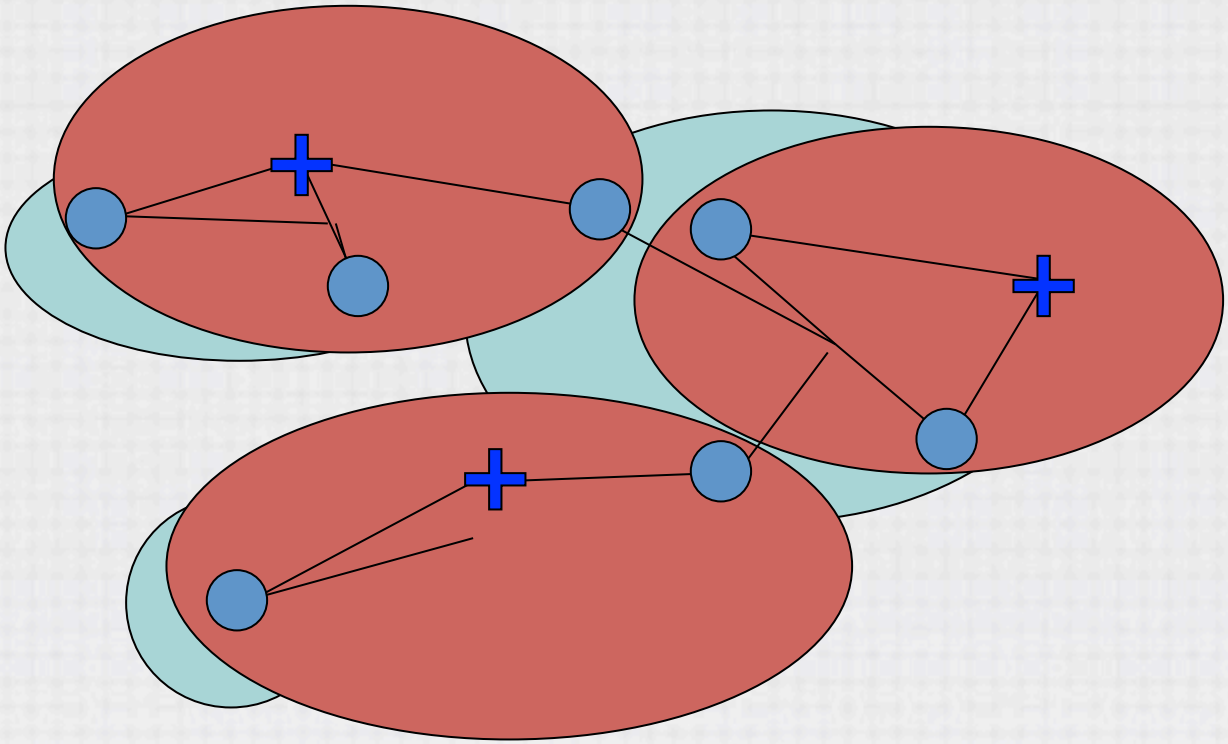
```
>>> from scipy.cluster.vq import *
```

- Clustering – finds clusters and cluster centers in a set of unlabeled data.
- Intuitively, a cluster comprises a group of data points whose inter-point distances are small compared to the distances to points outside of the cluster.

SciPy *k*-means Clustering

- scipy.cluster.vq
  - **kmeans(obs, k_or_guess[, iter, thresh, ...])** – perform k-means on a set of observation vectors forming k clusters
  - **kmeans2(data, k[, iter, thresh, minit, ...])** – classify a set of observations into k clusters using the k-means algorithm
- Given an initial set of *k* centers, the *k*-means algorithm alternates the two steps:
  - For each center, we identify the subset of training points (its cluster) that is closer to it than any other center.
  - The means of each feature for the data points in each cluster are computed, and this mean vector becomes the new center for that cluster.

k-means Clustering (*k*=3)



SciPy 2-means Clustering

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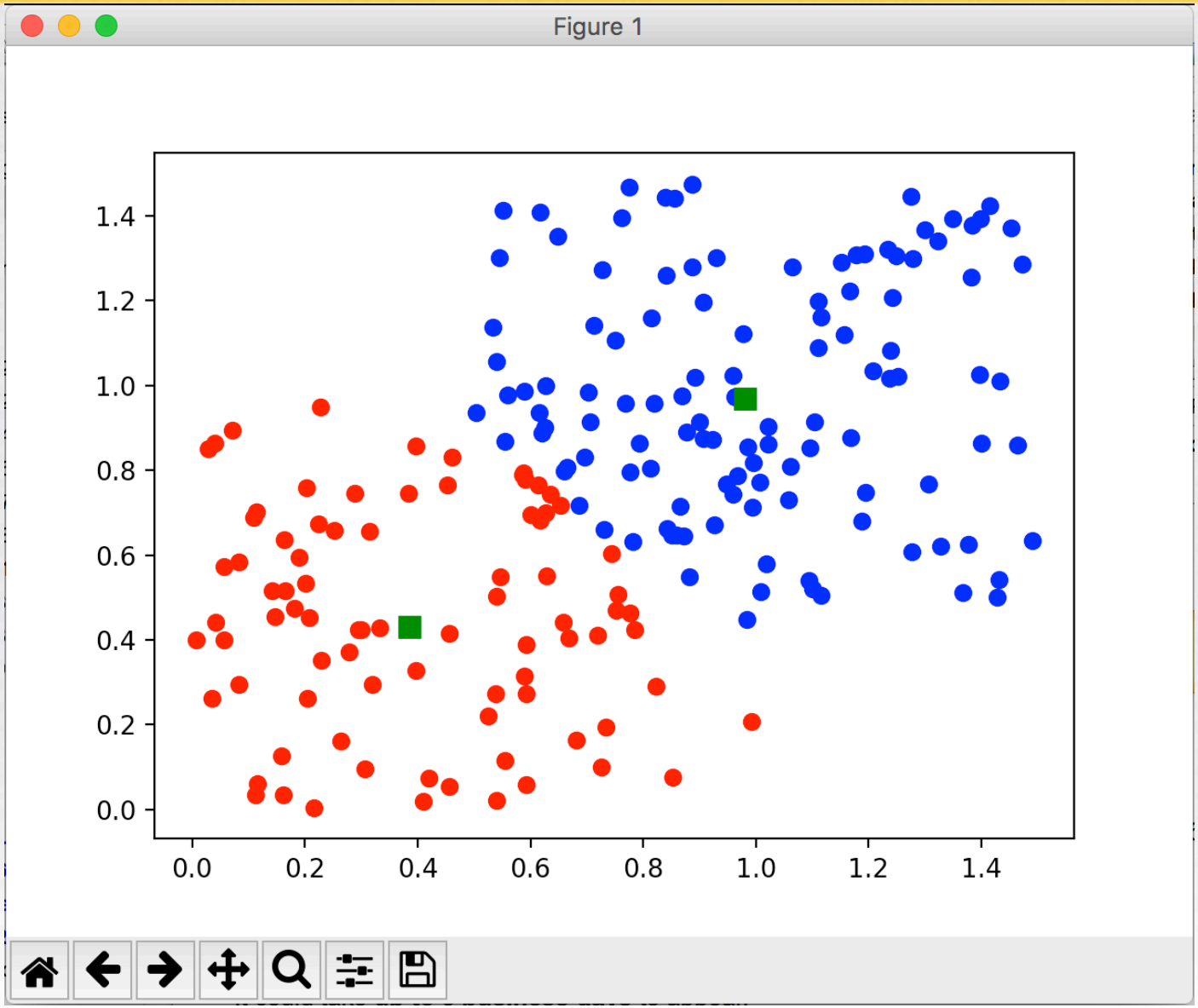
```
from pylab import *
from numpy import *
from numpy.random import *
from scipy.cluster.vq import *

# data generation
data = vstack((rand(100,2)+array([.5,.5]),rand(100,2)))
# computing k-means with k = 2 (2 clusters)
centroids,_ = kmeans(data,2)
# assign each sample to a cluster
index,_ = vq(data,centroids)
# some plotting using numpy's logical indexing
plot(data[index==0,0],data[index==0,1],'or',
     data[index==1,0],data[index==1,1],'ob')
plot(centroids[:,0],centroids[:,1],'sg',markersize=8)
show()
```

SciPy 2-means Clustering



SciPy *3*-means Clustering

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```
...
# data generation
data = vstack((rand(100,2)+array([.5,.5]),rand(100,2)))
# computing k-means with k = 3 (3 clusters)
centroids,_ = kmeans(data,3)
# assign each sample to a cluster
index,_ = vq(data,centroids)
# some plotting using numpy's logical indexing
plot(data[index==0,0],data[index==0,1],'or',
     data[index==1,0],data[index==1,1],'ob',
     data[index==2,0],data[index==2,1],'om')
plot(centroids[:,0],centroids[:,1],'sg',markersize=8)
show()
```

SciPy *3*-means Clustering

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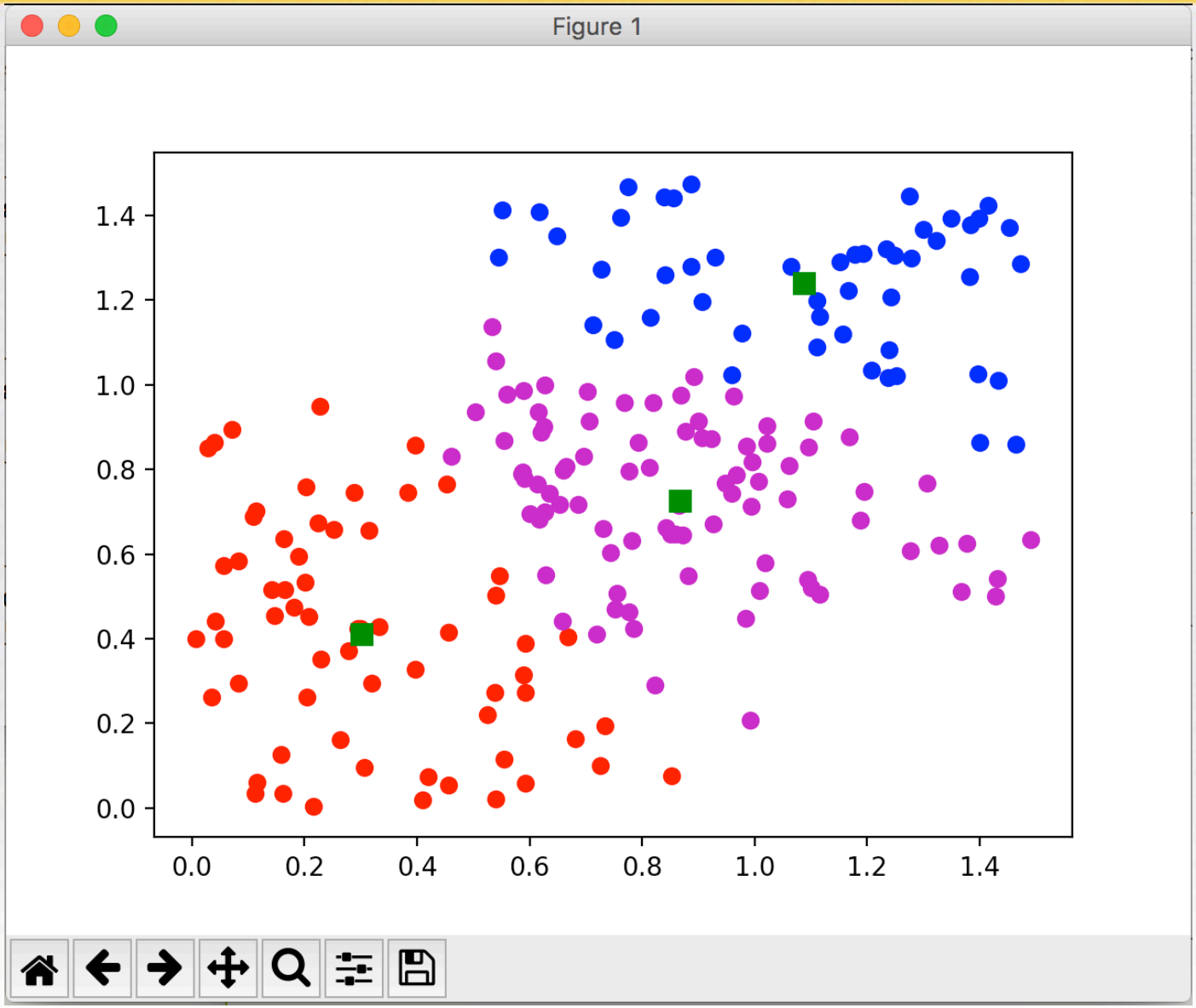

SciPy Integration

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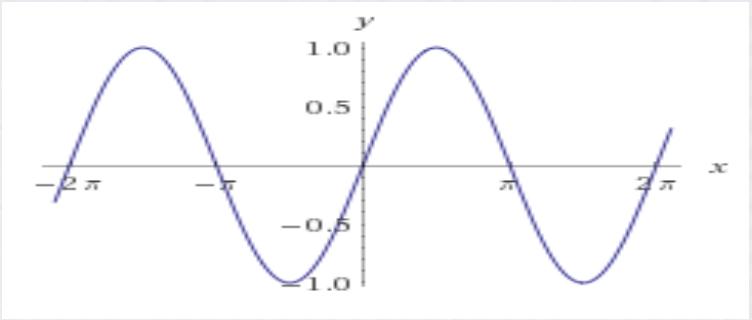
- Methods for Integrating Functions given a function object:
  - **quad** – general purpose integration
  - **dblquad** – general purpose double integration
  - **tplquad** – general purpose triple integration
  - **fixed_quad** – integrate f(x) using Gaussian quadrature
  - **quadrature** – Integrate with tolerance using Gaussian quadrature
  - **romberg** – integrate f(x) using Romberg integration
- Methods for I.F. given a fixed set of samples:
  - **trapz** – use trapezoidal rule to compute integral
  - **cumtrapz** – use trapezoidal rule to cumulatively compute integral
  - **simps** – use Simpson's rule to compute integral
  - **romb** – use Romberg Integration to compute integral

SciPy Integration

- **np.sin** defines the sine function
- Integral *x=0* to *x=π* using **quad**



$$\int \sin(x)\, dx$$

```
>>> result = scipy.integrate.quad(np.sin,
0,np.pi)
>>> print(result)
(2.0, 2.2204460492503130e-14)
# 2 with a very small error margin!
>>> result = scipy.integrate.quad(np.sin,-
np.inf,+np.inf)
>>> print(result)
(0.0, 0.0) # Integral does not converge
```

SciPy Optimization

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```
>>> from scipy.optimize import *
>>> help(scipy.optimize)
```

- Provides several commonly used optimization algorithms:
  - Unconstrained and constrained minimization of multivariate scalar functions (minimize) using BFGS, Nelder-Mead Simplex, Newton Conjugate Gradient, COBYLA, SLSQP, …
  - Global (brute-force) optimization routines (e.g. basinhopping, differential_evolution)
  - Least-squares minimization (least_squares) and curve fitting (curve_fit) algorithms
  - Scalar univariate functions minimizers (minimize_scalar) and root finders (newton)
  - Multivariate equation system solvers (root) using hybrid Powell, Levenberg-Marquardt, large-scale Newton-Krylov, …

SciPy Curve Fitting

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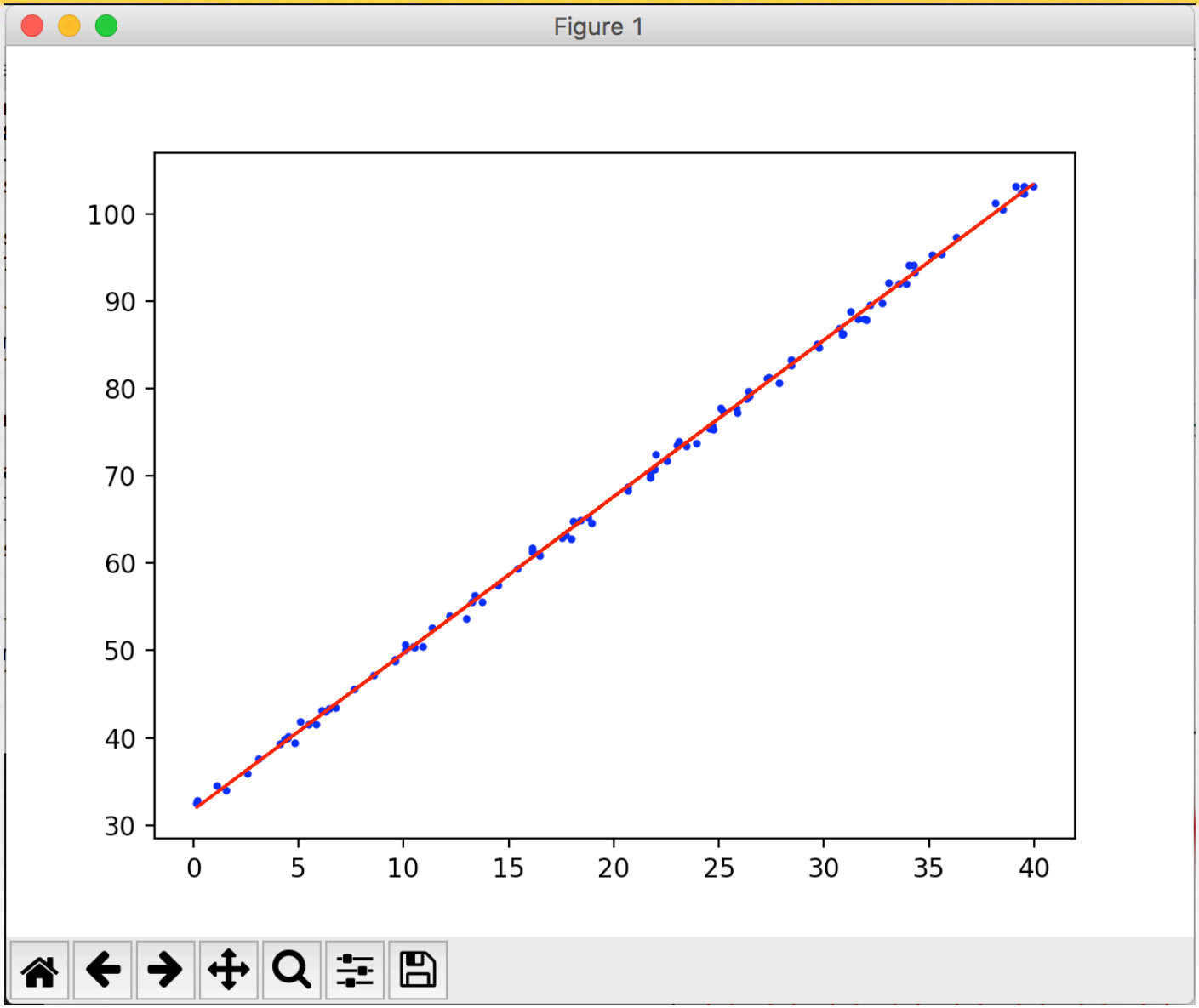
```
from pylab import *
from numpy import *
from numpy.random import *
from scipy.optimize import *
# lenear regression
def linreg(x,a,b):
    return a*x+b
# data generation
input = randint(0,40,100)
x = input+rand(100)
y = (input*1.8+32)+rand(100)
# curve fitting
attributes,variances = curve_fit(linreg,x,y)
# estimated y
y_modeled = x*attributes[0]+attributes[1]
# plot true and modeled results
plot(x,y,'ob',markersize=2)
plot(x,y_modeled,'-r',linewidth=1)
show()
```

SciPy Curve Fitting



SciPy Linear Regression

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```
from pylab import *
from numpy import *
from numpy.random import *
from scipy.stats import *
# data generation
input = randint(0,40,100)
x = input+rand(100)
y = (input*1.8+32)+rand(100)
# linear regression
slope,intercept,r_value,p_value,slope_std_error = stats.linregress(x,y)
# estimated y
y_modeled = x*slope+intercept
# plot true and modeled results
plot(x,y,'ob',markersize=2)
plot(x,y_modeled,'-r',linewidth=1)
show()
```

SciPy Linear Regression