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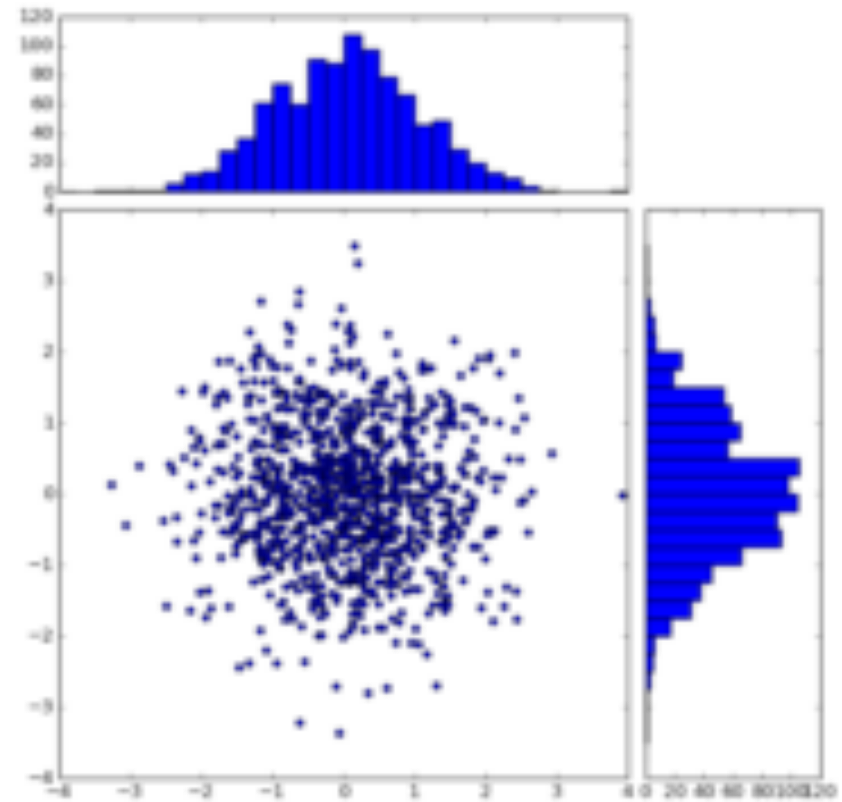
NumPy, SciPy and Matplotlib



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- NumPy and SciPy are open-source add-on modules to Python that provide common mathematical and numerical routines in pre- compiled, fast functions.
- The NumPy (Numeric Python) package provides basic routines for manipulating large arrays and matrices of numeric data.
- The SciPy (Scientific Python) package extends the functionality of NumPy with a substantial collection of useful algorithms, like minimization, Fourier transformation, regression, and other applied mathematical techniques.

They are listed on PyPI, so can be installed with

```
pip install numpy scipy
```

`http://www.scipy.org/install.html` has other alternatives

Import the modules into your program like most Python packages:

```
import numpy

import numpy as np
```

```
import scipy

import scipy as sp
```

- The array is the basic, essential unit of NumPy

– Designed to be accessed just like Python lists

– All elements are of the same type

– Ideally suited for storing and manipulating large numbers of elements

```
>>> a = np.array([1, 4, 5, 8], float32)

>>> a
array([1., 4., 5., 8.])

>>> type(a)
<type 'numpy.ndarray'>
>>> a[:2]
Array([1., 4.])

>>> a[3]
8.0
```

Just like lists, an array can have multiple dimensions (obviously useful for matrices)

```
>>> a = np.array([[1, 2, 3], [4, 5, 6]], 'float32')

>>> a
array([[1., 2., 3.],
       [4., 5., 6]])

>>> a[0,0]
1.0

>>> a[0,1]
2.0

>> a.shape
(2,3)
```

Arrays can be reshaped:

```
>>> a = np.array(range(10), dtype='uint8')
>>> a
array([ 0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

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

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

>>> b.shape
(5, 2)
```

b points at same data in memory, new "view"

Plain assignment creates a view, copies need to be explicit:

```
>>> a = np.array([1, 2, 3], dtype='float')
>>> b = a           # same array, same data (py)
>>> c = a.view()    # new array,  same data (np)
>>> d = a.copy()    # new array,  new data (np)

>>> a[0] = 99

>>> a
array([99., 2., 3.])

>>> b
array([99., 2., 3.])

>>> c
array([99., 2., 3.])

>>> d
array([1., 2., 3.])
```

- One can fill an array with a single value
- Arrays can be transposed easily

```
>>> a = np.array([1, 2, 3],dtype='float')

>>> a
array([1.0, 2.0, 3.0])

>>> a.fill(0)
array([0.0, 0.0, 0.0])

>>> a = np.array(range(6), 'float').reshape((2, 3))
>>> a
array([[ 0., 1., 2.],
       [ 3., 4., 5.]])

>>> a.transpose()
array([[ 0., 3.],
       [ 1., 4.],
       [ 2., 5.]])
```

Combining arrays can be done through concatenation. Careful, the data is copied!

```
>>> a = np.array([1,2], ‘float’)
>>> b = np.array([3,4,5,6], ‘float’)
>>> c = np.array([7,8,9], ‘float’)

>>> np.concatenate((a, b, c))
array([1., 2., 3., 4., 5., 6., 7., 8., 9.])
```

Multi-dimensional arrays can be concatenated along a specific axis:

```
>>> a = np.array([[1, 2], [3, 4]], ‘float’)
>>> b = np.array([[5, 6], [7, 8]], ‘float’)

>>> np.concatenate((a,b),axis=0)
array([[ 1., 2.],
       [ 3., 4.],
       [ 5., 6.],
       [ 7., 8.]])

>>> np.concatenate((a,b),axis=1)
array([[ 1., 2., 5., 6.],
       [ 3., 4., 7., 8.]]
```

```
>>> np.arange(5, dtype='float')
array([ 0., 1., 2., 3., 4.])

>>> np.linspace(30,40,5)
array([ 30. ,  32.5,  35. ,  37.5,  40. ])

>>> np.ones((2,3), dtype='float')
array([[ 1., 1., 1.],
       [ 1., 1., 1.]])

>>> np.zeros(7, dtype='int')
array([0, 0, 0, 0, 0, 0, 0])

>>> a = np.array([[1, 2, 3], [4, 5, 6]], 'float')
>>> np.zeros_like(a)
array([[ 0., 0., 0.],
       [ 0., 0., 0.]])
>>> np.ones_like(a)
array([[ 1., 1., 1.],
       [ 1., 1., 1.]])
```

Element-by-element processing is defined trivially:

```
>>> a = np.array([1,2,3], ‘float')
>>> b = np.array([5,2,6], ‘float’)
>>> a + b
array([6., 4., 9.])
>>> a - b
array([-4., 0., -3.])
>>> a * b # is _not_ a dot-product!
array([5., 4., 18.])
>>> b / a
array([5., 1., 2.])
>>> a % b
array([1., 0., 3.])
>>> b**a
array([5., 4., 216.])
```

Watch out for automatic shape extension ("broadcasting"):

```
>>> a = np.array([[1, 2], [3, 4], [5, 6]], 'float')
>>> b = np.array([-1, 3], 'float')
>>> a
array([[ 1., 2.],
       [ 3., 4.],
       [ 5., 6.]])
>>> b
array([-1., 3.])

>>> a + b
array([[ 0., 5.],
       [ 2., 7.],
       [ 4., 9.]])
```

b was extended to match shape (3,2):

```
array([[ -1., 3.],
       [ -1., 3.],
       [ -1., 3.]])
```

Control shape extension with **newaxis**:

```
>>> a = np.zeros((2,2), float)
array([[ 0., 0.],
       [ 0., 0.]])
>>> b = np.array([-1., 3.], float)
array([-1., 3.])

>>> a + b
array([[-1., 3.],
       [-1., 3.]])

>>> a + b[np.newaxis,:]
array([[-1., 3.],
       [-1., 3.]])

>>> a + b[:,np.newaxis]
array([[-1., -1.],
       [ 3., 3.]])
```

NumPy offers a large library of common mathematical functions that can be applied elementwise to arrays

– Among these are: `abs`, `sign`, `sqrt`, `log`, `log10`, `exp`, `sin`, `cos`, `tan`, `arcsin`, `arccos`, `arctan`, `sinh`, `cosh`, `tanh`, `arcsinh`, `arccosh`, and `arctanh`

```
>>> a = np.linspace(0.3, 0.6, 4)
array([ 0.3,  0.4,  0.5,  0.6])

>>> np.sin(a)
>>> array([ 0.29552021,  0.38941834,  0.47942554,  0.56464247])
```

```
>>> a = np.array([2, 4, 3], float)
>>> a.sum()
9.0
>>> a.prod()
24.0

>>> np.sum(a)
9.0
>>> np.prod(a)
24.0

>>> a = np.array([2, 1, 9], float)
>>> a.mean()
4.0
>>> a.var()
12.666666666666666
>>> a.std()
3.5590260840104371
```

Axis can be selected for marginal statistic:

```
>>> a = np.array([[0, 2], [3, -1], [3, 5]], float)
>>> a.mean(axis=0)
array([ 2., 2.])
>>> a.mean(axis=1)
array([ 1., 1., 4.])
>>> a.min(axis=1)
array([ 0., -1., 3.])
>>> a.max(axis=0)
array([ 3., 5.])
```

Array comparisons with <,==,> result in boolean arrays that can also be used as filters:

```
>>> a = np.array([[6, 4], [5, 9]], float)

>>> a >= 6
array([[ True, False],
       [False, True]], dtype=bool)

>>> a[a >= 6]
array([ 6., 9.])
```

Perhaps the most powerful feature of NumPy is the vector and matrix operations

Provide compiled code performance similar to machine specific BLAS, uses BLAS internally

Performing a vector-vector, vector-matrix or matrix-matrix multiplication using **dot**

Also supports **inner**, **outer**, **cross**

```
>>> a = np.array([[0, 1], [2, 3]], float)
>>> b = np.array([2, 3], float)
>>> c = np.array([[1, 1], [4, 0]], float)
>>> a
array([[ 0., 1.],
       [ 2., 3.]])

>>> np.dot(b, a)
array([ 6., 11.])

>>> np.dot(a, b)
array([ 3., 13.])

>>> np.dot(a, c)
array([[ 4., 0.],
       [ 14., 2.]])

>>> np.dot(c, a)
array([[ 2., 4.],
       [ 0., 4.]])
```

A number of built-in routines for linear algebra are in the `linalg` submodule:

```
>>> a = np.array([[4, 2, 0], [9, 3, 7], [1, 2, 1]], float)
array([[ 4., 2., 0.],
       [ 9., 3., 7.],
       [ 1., 2., 1.]])

>>> np.linalg.det(a)
-53.999999999999993

>>> vals, vecs = np.linalg.eig(a)
>>> vals
array([ 9. , 2.44948974, -2.44948974])
>>> vecs
array([[-0.3538921 , -0.56786837, 0.27843404],
       [-0.88473024, 0.44024287, -0.89787873],
       [-0.30333608, 0.69549388, 0.34101066]])
```

```
>>> b = np.linalg.inv(a)
>>> b
array([[ 0.14814815, 0.07407407, -0.25925926],
       [ 0.2037037 , -0.14814815, 0.51851852],
       [-0.27777778, 0.11111111, 0.11111111]])
>>> np.dot(a, b)
array([[ 1.00000000e+00, 5.55111512e-17, 2.22044605e-16],
       [ 0.00000000e+00, 1.00000000e+00, 5.55111512e-16],
       [ 1.11022302e-16, 0.00000000e+00, 1.00000000e+00]])

>>> a = np.array([[1, 3, 4], [5, 2, 3]], float)
>>> U, s, Vh = np.linalg.svd(a)
>>> U
array([[-0.6113829 , -0.79133492],
       [-0.79133492, 0.6113829 ]])
>>> s
array([ 7.46791327, 2.86884495])
>>> Vh
array([[-0.61169129, -0.45753324, -0.64536587],
       [ 0.78971838, -0.40129005, -0.464......
```

- Polynomial Mathematics
- Statistical computations
- Full suite of pseudo-random number generators and operations
- Discrete Fourier transforms,
- more complex linear algebra operations
- size / shape / type testing of arrays,
- splitting and joining arrays, histograms
- creating arrays of numbers spaced in various ways
- creating and evaluating functions on grid arrays
- treating arrays with special (NaN, Inf) values
- set operations
- creating various kinds of special matrices
- evaluating special mathematical functions (e.g. Bessel functions)

- To learn more, consult the NumPy documentation at
  `http://docs.scipy.org/doc/`

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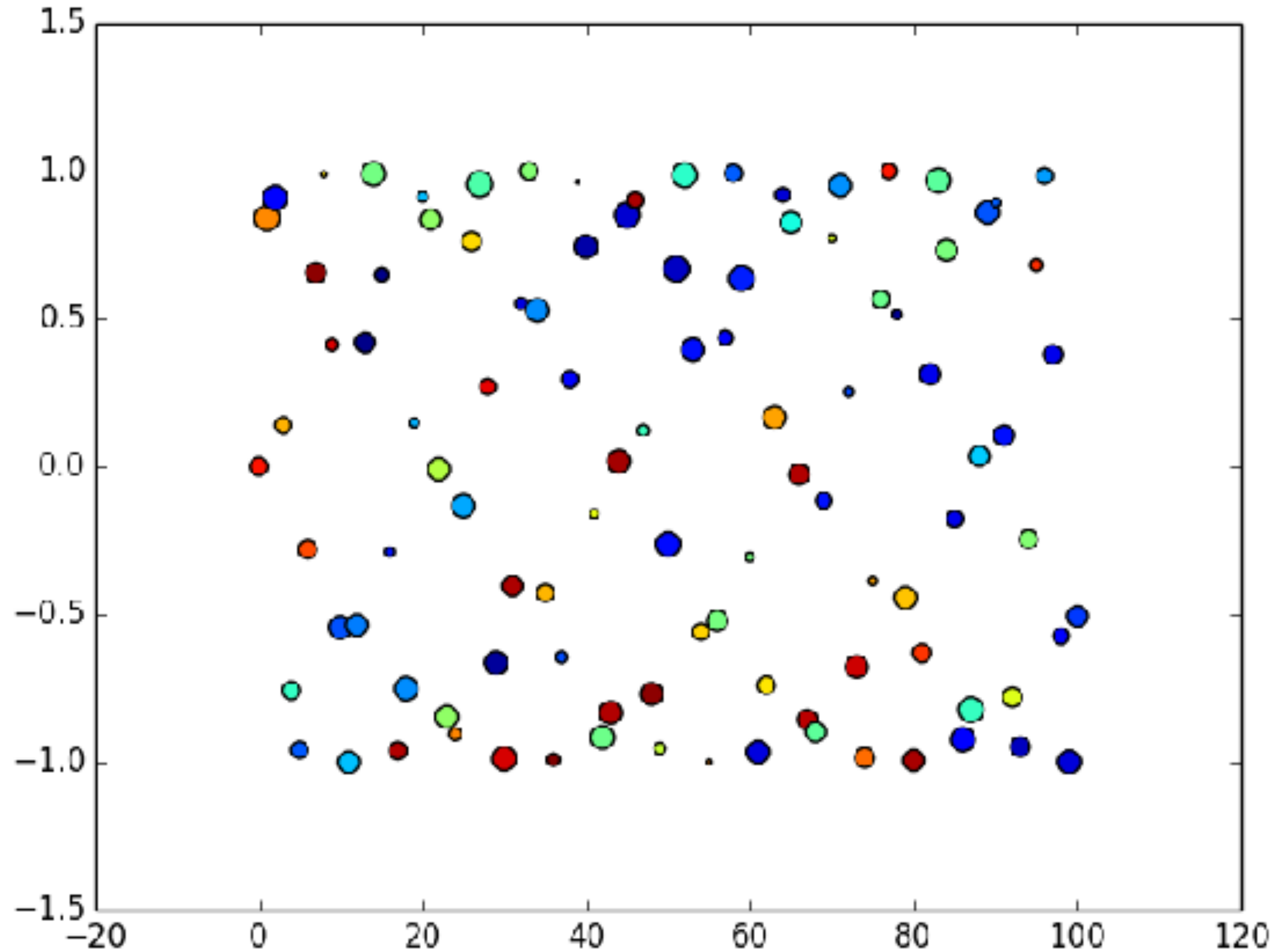
SciPy is built on top of numpy and has specialist scientific routines like:

```
cluster                          --- Vector Quantization / Kmeans
fftpack                          --- Discrete Fourier Transform algorithms
integrate                        --- Integration routines
interpolate                      --- Interpolation Tools
io                               --- Data input and output
lib                              --- Python wrappers to external libraries
lib.lapack                       --- Wrappers to LAPACK library
linalg                           --- Linear algebra routines
misc                             --- Various utilities that don't have
                                     another home.
ndimage                          --- n-dimensional image package
odr                              --- Orthogonal Distance Regression
optimize                         --- Optimization Tools
signal                           --- Signal Processing Tools
sparse                           --- Sparse Matrices
sparse.linalg                    --- Sparse Linear Algebra
sparse.linalg.dsolve             --- Linear Solvers
sparse.linalg.dsolve.umfpack --- :Interface to the UMFPACK library:
                                     Conjugate Gradient Method (LOBPCG)
sparse.linalg.eigen.lobpcg   --- Locally Optimal Block Preconditioned
                                     Conjugate Gradient Method (LOBPCG) [*]
special                          --- Airy Functions [*]
lib.blas                         --- Wrappers to BLAS library [*]
sparse.linalg.eigen              --- Sparse Eigenvalue Solvers [*]
stats                            --- Statistical Functions [*]
spatial                          --- Spatial data structures and algorithms
```

Matplotlib

Powerful library for 2D data plotting, some 3D capability

Very well designed: common tasks easy, complex tasks possible.



Matplotlib

```
>>> import pylab as pl
>>> xs = pl.linspace(0,100,101)
>>> ys = pl.sin(xs)
>>> cols = pl.random(101)
>>> sizes = 100.0 * pl.random(101)

>>> pl.scatter(xs,ys,c=cols,s=sizes)

>>> pl.savefig('test.svg')
```

Typical workflow in the beginning:
Go to gallery, pick something close to desired plot, and modify

```
http://docs.scipy.org/doc
```

```
http://matplotlib.org/gallery/index.html
```

Exercise: particle animation

Exercise: large data memmap

```
https://users.hepforge.org/
      ~dgrell/ictp16/landcover.html
```