

```
>>> import scipy
```

SciPy - a brief introduction



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Scientific Tools for Python

- SciPy is the scientific toolbox for Python, aimed at mathematics, science and engineering applications.
- It is built on NumPy, i.e., NumPy arrays are the most practical data type; they are generic, efficient and straight-forward to handle.
- SciPy is open-source software, compiled on top of NumPy
- SciPy is also a conference for scientific Python discussion: next meeting is July 16 - 21, in Austin, TX; <http://conference.scipy.org/scipy2012/>

SciPy resources

- <http://scipy-lectures.github.com/>
SciPy lecture notes, fairly complete and usefully formatted
- http://www.tau.ac.il/~kineret/amit/scipy_tutorial/
Older lecture notes (2004) by Travis Oliphant (Enthought/Continuum); incomplete but very detailed and informative.
- <http://scipy-central.org/>
Collection of code snippets and modules, cookbooks, miscellany
- <http://docs.scipy.org/doc/scipy/reference/>
SciPy reference guide, tutorial
- [http://www.scipy.org/NumPy for Matlab Users](http://www.scipy.org/NumPy_for_Matlab_Users)

Getting data in and out of SciPy

- See Josh Bloom's lecture tomorrow morning;
also <http://www.scipy.org/Cookbook/InputOutput>
- Python provides powerful read/write routines for ascii files and some binary types (C/Fortran)
- Arbitrary input and output
`np.loadtxt()/savetxt()`, `np.genfromtxt()/recfromcsv()`,
`np.save()/load()`

Certain proprietary (but common) binary formats:

`scipy.io.matlab`, `scipy.io.idl`

Special binaries (Matlab, IDL, HDF5): `scipy.io`

- Support for Matlab, IDL, HDF5 (through the PyTables module), as well as Matrix Market and NetCDF.
- Includes support for advanced data structures in these languages
- E.g., Matlab data:

```
>>> from scipy import io
>>> struct = io.loadmat('file.mat', struct_as_record=True)
>>> io.savemat('file.mat', struct)
```

Building and referencing your own arrays quickly

- (Row) vector of numbers: `np/sp.r_` and `np/sp.linspace`

```
>>> np.r_[1.:11.] # N.b. (1,2,...,10)
```

```
>>> np.linspace(a,b,n)
```

- n-d grid of coordinates: `np/sp.mgrid`

```
>>> x,y = np.mgrid(1:5,1:5) # A 4x4 array
```

```
>>> r = np.sqrt(x**2 + y**2)
```

- n-d array: `np/sp.c_` and `np.tile`

```
>>> x = np.linspace(0,10,11);
```

```
>>> np.c_[x,x]
```

SciPy packages

- See Sunday lecture on Scientific Programming for fuller discussion of these

SciPy: numerical algorithms galore

- **linalg** : Linear algebra routines (including BLAS/LAPACK)
- **sparse** : Sparse Matrices (including UMFPACK, ARPACK,...)
- **fftpack** : Discrete Fourier Transform algorithms
- **cluster** : Vector Quantization / Kmeans
- **odr** : Orthogonal Distance Regression
- **special** : Special Functions (Airy, Bessel, etc).
- **stats** : Statistical Functions
- **optimize** : Optimization Tools
- **maxentropy** : Routines for fitting maximum entropy models
- **integrate** : Numerical Integration routines
- **ndimage** : n-dimensional image package
- **interpolate** : Interpolation Tools
- **signal** : Signal Processing Tools
- **io** : Data input and output

Symbolic mathematics with Python

- <http://sympy.org/>
SymPy home page
- <http://docs.sympy.org>
Reference, tutorial
- Think of SymPy as Mathematica for Python, including integration, geometry, linear algebra, statistics, ODE solving and tensor algebra

```
>>> import sympy
```


Interfacing with other languages

- E.g., <http://www.scipy.org/PerformancePython>
An interesting and useful comparison of possibilities
- Cython (<- Pyrex)
The most comprehensive option; requires a lecture of its own
- f2py
Interface with Fortran, great for number-crunching
- PyPy (<- Psyco)
Truly amazing, but does not support NumPy :(
- scipy.weave
Very cool to use, perhaps becoming less common(?)

Blending languages: f2py

- You will need: Python, a Fortran compiler (e.g. g95, gfortran) and f2py
- This can be a breakout exercise

Blending languages: weave

- See also: <http://www.scipy.org/Cookbook/Weave>
- You will need: a C/C++ compiler
- This can also be a breakout exercise