PHYS4038/MLiS and AS1/MPAGS

Scientific Programming in python™

mpags-python.github.io

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An introduction to scientific programming with

python™

Session 5:
Scientific Python

Scientific Python (SciPy)

- Suite of numerical and scientific tools for Python
- http://scipy.org/
- http://docs.scipy.org/

Scipy subpackages

- cluster Clustering algorithms
- constants Physical and mathematical constants
- fftpack Fast Fourier Transform routines
- integrate Integration and ordinary differential equation solvers
- interpolate Interpolation and smoothing splines
- io Input and Output
- linalg Linear algebra
- ndimage N-dimensional image processing
- odr Orthogonal distance regression
- optimize Optimization and root-finding
- signal Signal processing
- sparse Sparse matrices and associated routine
- spatial Spatial data structures and algorithms
- special Special functions
- stats Statistical distributions and functions

```
# scipy submodules
# must be explicitly
# imported, e.g.,
import scipy.fftpack
# or
from scipy import stats
```

SciPy

Some simple examples:

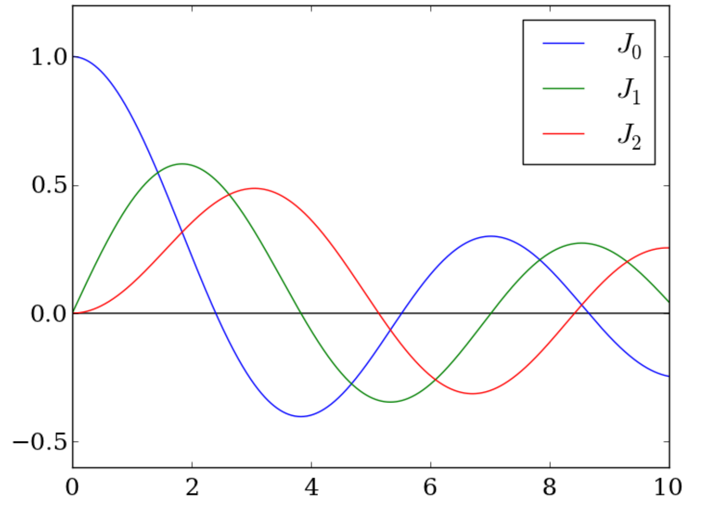
- Special functions (special)
- Root finding (optimize)
- Integration (integrate)
- Statistics (stats)
- Image processing (ndimage)
- Interpolation (interpolate)
- Optimisation (optimize)

Scipy – special functions

- Huge number of functions, including…
  - Bessel functions
  - Gamma functions
  - Fresnel integrals
  - Hypergeometric functions
  - Orthogonal polynomials

```
e.g., Bessel functions of order 1, 2, 3
>>> from scipy import special
>>> x = np.arange(0, 10.001, 0.01)
>>> for alpha in range(3):
...     y = special.jv(alpha, x)
...     plt.plot(x, y,
                 label=r'$J_%i$'%alpha)
>>> plt.hlines(0, 0, 10)
>>> plt.legend()
```

$$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} + (x^2 - \alpha^2)y = 0$$



Scipy – root finding

- Accurate automatic root-finding using MINPACK

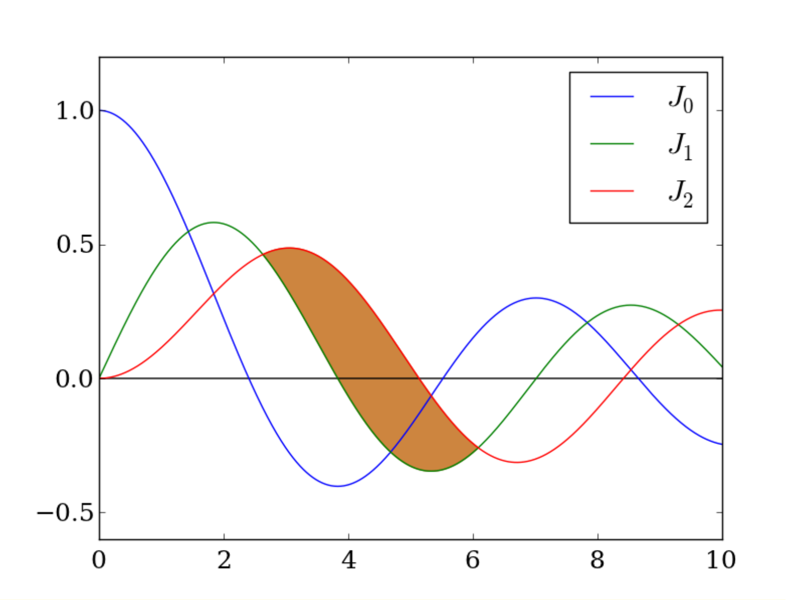
```
>>> from scipy.optimize import fsolve   # n-dimensional root finder
>>> from scipy.special import jv
```

Define a function to solve
First argument is variable (or array of variables) of interest

```
>>> def f(z, a1, a2):
...     return jv(a1, z) - jv(a2, z)
...

>>> fsolve(f, 2.5, args=(1, 2))
array([ 2.62987411])

>>> fsolve(f, 6, args=(1, 2))
array([ 6.08635978])
```




```
>>> plt.fill_between(x, special.jv(1, x), special.jv(2, x),
        where=((x > 2.630) & (x < 6.086)), color="peru")
```

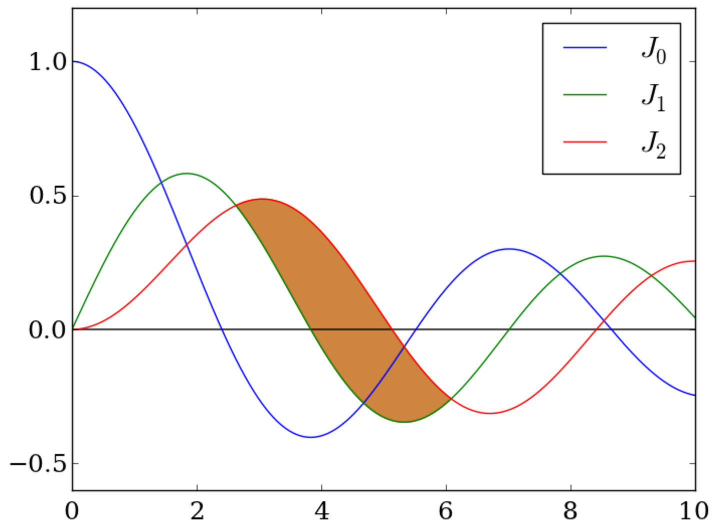
Scipy – integration

- Accurate automatic integration using QUADPACK
  - including uncertainty estimate

```
>>> from scipy.integrate import quad   # one-dimensional integration
Using previous function (first argument is variable of interest)
>>> r = fsolve(f, (2.5, 6), args=(1, 2))

>>> print r
[ 2.62987411  6.08635978]

>>> quad(f, r[0], r[1], args=(1, 2))
(-0.98961158607157, 1.09868956829247e-14)
```



- Can specify limits at infinity

  `(-np.inf, np.inf)`

```
>>> quad(exp, -np.inf, 0)
(1.0000000000000002, 5.842606742906004e-11)
```

Scipy – integration

- QUADPACK and MINPACK routines provide warning messages
- Extra details returned if parameter full_output=True

```
>>> quad(tan, 0, pi/2.0-0.0001)
(9.210340373641296, 2.051912874185855e-09)

>>> quad(tan, 0, pi/2.0)
Warning: Extremely bad integrand behavior occurs at some points of the
  integration interval.
(38.58895946215512, 8.443496712555953)

>>> quad(tan, 0, pi/2.0+0.0001)
Warning: The maximum number of subdivisions (50) has been achieved.
  If increasing the limit yields no improvement it is advised to analyze
  the integrand in order to determine the difficulties.  If the position of a
  local difficulty can be determined (singularity, discontinuity) one will
  probably gain from splitting up the interval and calling the integrator
  on the subranges.  Perhaps a special-purpose integrator should be used.
(6.896548923283743, 2.172542103965056)
```

Scipy – statistics

- Probability distributions
  - including: norm, chi2, t, expon, poisson, binom, boltzmann, …
  - methods:
    - rvs – return array of random variates
    - pdf – probability density function
    - cdf – cumulative density function
    - ppf – percent point function
    - … and many more
- Statistical functions
  - including:
    - mean, median, skew, kurtosis, …
    - normaltest, probplot, …
    - pearsonr, spearmanr, wilcoxon, …
    - ttest_1samp, ttest_ind, ttest_rel, …
    - kstest, ks_2samp, …

```
>>> lambda = 10
>>> p = stats.poisson(lambda)

# P(n > 20)
>>> 1 - p.cdf(20)
0.0015882606618580573

# N: P(n < N) = 0.05, 0.95
>>> p.ppf((0.05, 0.95))
array([  5.,   15.])

# true 95% CI bounds on lambda
>>> stats.gamma.ppf((0.025, 0.975),
                    lambda+0.5, 1)
array([  6.14144889,   18.73943795])
```

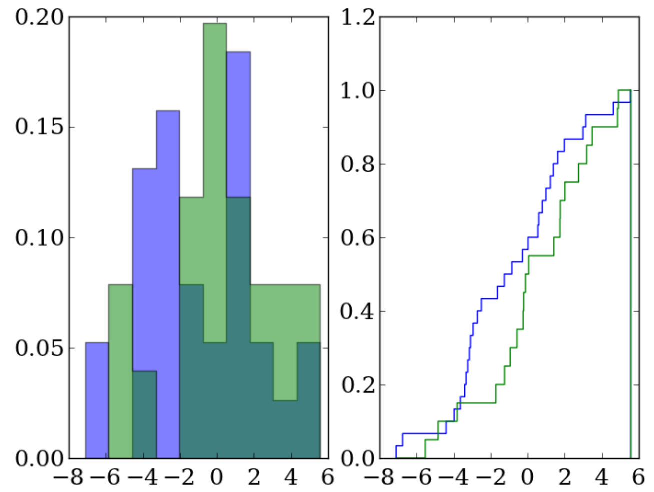
Scipy – statistics

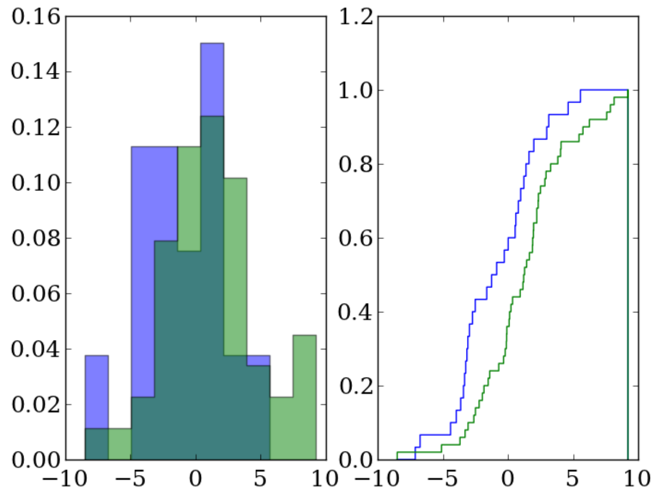
```
>>> x = stats.norm.rvs(-1, 3, size=30)  # specify pdf parameters
>>> n = stats.norm(1, 3)  # create 'frozen' pdf
>>> y = n.rvs(20)
>>> z = n.rvs(50)
>>> p = plt.subplot(121)
>>> h = plt.hist((x, y), normed=True,
        histtype='stepfilled', alpha=0.5)
>>> p = plt.subplot(122)
>>> h = plt.hist((x, y), histtype='step',
        cumulative=True, normed=True, bins=1000)

>>> stats.ks_2samp(x, y)
(0.29999999999999999, 0.18992875018013033)
>>> stats.ttest_ind(x, y)
(-1.4888787966012809, 0.14306062943339182)

>>> stats.ks_2samp(x, z)
(0.31333333333333335, 0.039166429989206733)
>>> stats.ttest_ind(x, z)
(-2.7969511393118509, 0.0064942129302196124)

>>> stats.kstest(x, stats.norm(1, 3).cdf)
(0.313889035681928, 0.0039905619713858087)
```

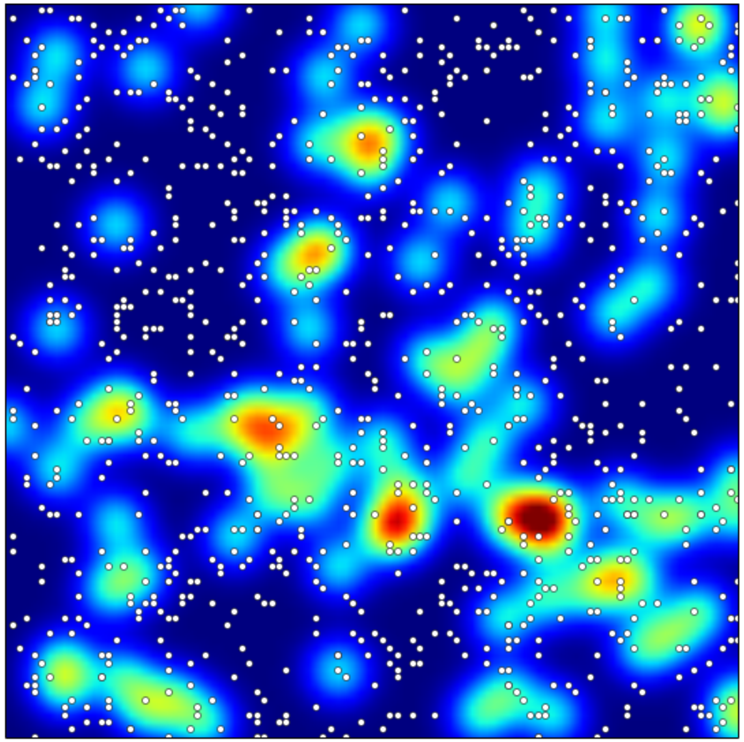


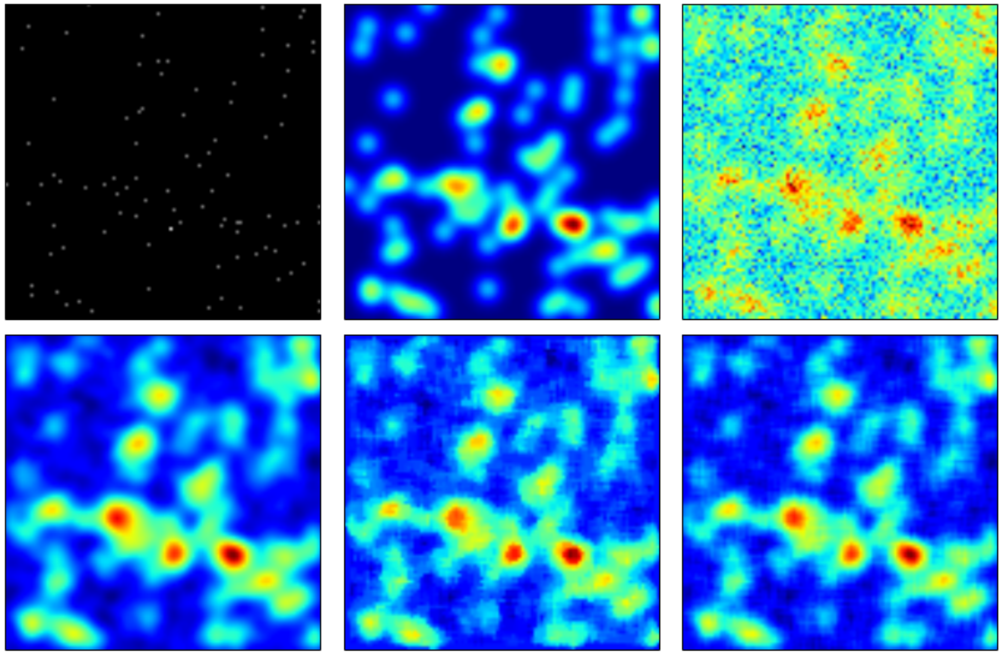


Scipy – filtering and interpolation

Notebook filtering and interpolation example

[link to online notebook]





Scipy – optimisation

- Local optimisation
  - `minimize` function
    - lots of options, different optimizers, constraints

- Least squares fitting
  - `curve_fit`
    - uses Levenberg-Marquardt algorithm

Details at http://docs.scipy.org/doc/scipy/reference/tutorial/optimize.html

Notebook fitting example

[link to online notebook]

Other / more options…

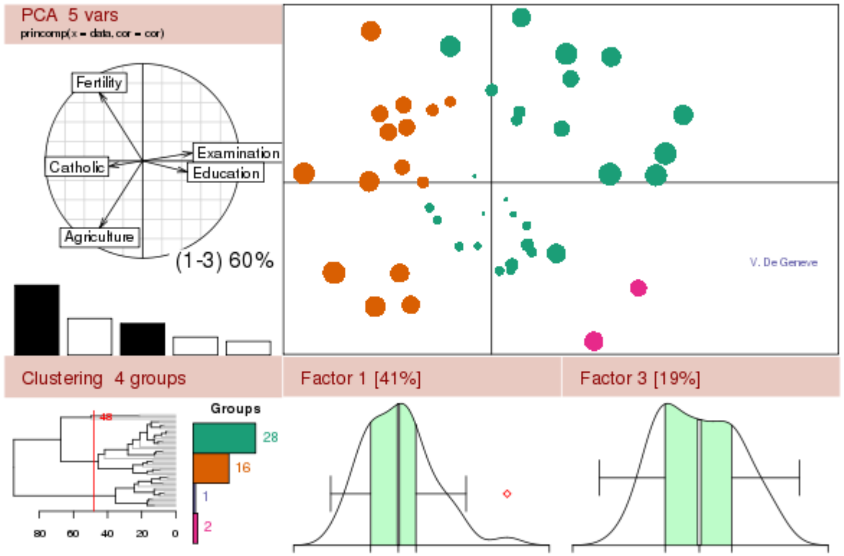
astropy

astropy
A Community Python Library for Astronomy

- Astronomical constants, units, times and dates
- Astronomical coordinate systems
- Cosmology calculations
- Virtual Observatory integration
- Astronomy specific additions to numpy/scipy tools:
    - n-dimensional datasets, tables
    - model fitting, convolution, filtering, statistics
- Open source, on GitHub

RPy

- http://rpy.sourceforge.net/
- Wraps R – a statistics analysis language
  - very powerful
  - used by statisticians
  - many advanced stats capabilities
  - quite specialised
- http://www.r-project.org



PyGSL

- Python wrappers of GNU Scientific Library functions
- [PyGSL: http://pygsl.sourceforge.net/](http://pygsl.sourceforge.net/)
- [GSL: http://www.gnu.org/software/gsl/](http://www.gnu.org/software/gsl/)

- Incomplete documentation for Python functions, but almost all of GSL is wrapped, so refer to GSL documentation.

- Most functionality implemented in SciPy
  - or other, more Pythonic, tools
  - comprehensive and sometimes more tested

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