intro_Scipy

June 1, 2016

```
In [1]: # Just to know last time this was run:
        import time
        print time.ctime()
```

```
Wed Jun  1 17:03:05 2016
```

1 E Introduction to Scipy

This is part of the Python lecture given by Christophe Morisset at IA-UNAM. More informations at: http://python-astro.blogspot.mx/

Scipy is a library with a lot of foncionalities, we will not cover everything here, but rather point to some of them with examples. Some useful links about scipy:

- https://scipy-lectures.github.io/intro/scipy.html
- http://docs.scipy.org/doc/scipy/reference/tutorial/

```
In [2]: %matplotlib inline
        import numpy as np
        import matplotlib.pyplot as plt
```

```
/Users/christophemorisset/anaconda/lib/python2.7/site-packages/matplotlib/font_mana
  warnings.warn('Matplotlib is building the font cache using fc-list. This may take
```

```
In [3]: import scipy # This imports a lot of numpy stuff, but not the important mod
```

1.0.1 Some usefull methods

```
In [4]: from scipy.stats import nanmean
```

```
In [5]: a = np.array([-2, -1, 1., 2, 3])
        b = np.log10(a)
        mask = np.isfinite(b)
        print a
        print b
        print mask
        print a.mean()
        print b.mean()
        print b[mask].mean()
        print nanmean(b)
```

```
[-2. -1.  1.  2.  3.]
[        nan         nan  0.          0.30103     0.47712125]
[False False  True  True  True]
0.6
nan
0.259383750128
0.259383750128
```

```
/Users/christophemorisset/anaconda/lib/python2.7/site-packages/ipykernel/__main__.p
  from ipykernel import kernelapp as app
```

```
In [6]: from scipy.special import gamma
        print gamma(10.3)
```

```
716430.689062
```

```
In [7]: from scipy import constants as cst
        print cst.astronomical_unit # A lot of constants
        from scipy.constants import codata # a lot more, with units. From NIST
        print codata.value('proton mass'), codata.unit('proton mass')
```

```
1.49597870691e+11
1.672621898e-27 kg
```

1.0.2 Integrations

```
In [8]: from scipy.integrate import trapz, cumtrapz, simps
        #help(scipy.integrate) # a big one...
        print '-----------------------------------------------------------------------
        help(trapz)
        print '-----------------------------------------------------------------------
        help(cumtrapz)
        print '-----------------------------------------------------------------------
        help(simps)
```

```
---------------------------------------------------------------------------------
Help on function trapz in module numpy.lib.function_base:

trapz(y, x=None, dx=1.0, axis=-1)
    Integrate along the given axis using the composite trapezoidal rule.
    Integrate `y` (`x`) along given axis.

    Parameters
    ----------
    y : array_like
        Input array to integrate.
    x : array_like, optional
        The sample points corresponding to the `y` values. If `x` is None,
        the sample points are assumed to be evenly spaced `dx` apart. The
        default is None.
    dx : scalar, optional
        The spacing between sample points when `x` is None. The default is 1.
    axis : int, optional
        The axis along which to integrate.

    Returns
    -------
    trapz : float
        Definite integral as approximated by trapezoidal rule.

    See Also
    --------
    sum, cumsum

    Notes
    -----
    Image [2]_ illustrates trapezoidal rule -- y-axis locations of points
    will be taken from `y` array, by default x-axis distances between
    points will be 1.0, alternatively they can be provided with `x` array
    or with `dx` scalar.  Return value will be equal to combined area under
    the red lines.


    References
    ----------
    .. [1] Wikipedia page: http://en.wikipedia.org/wiki/Trapezoidal_rule

    .. [2] Illustration image:
           http://en.wikipedia.org/wiki/File:Composite_trapezoidal_rule_illustratio

    Examples
    --------
    >>> np.trapz([1,2,3])
    4.0
    >>> np.trapz([1,2,3], x=[4,6,8])
    8.0
    >>> np.trapz([1,2,3], dx=2)
    8.0
```

```
    >>> a = np.arange(6).reshape(2, 3)
    >>> a
    array([[0, 1, 2],
           [3, 4, 5]])
    >>> np.trapz(a, axis=0)
    array([ 1.5,  2.5,  3.5])
    >>> np.trapz(a, axis=1)
    array([ 2.,  8.])

--------------------------------------------------------------------------------
Help on function cumtrapz in module scipy.integrate.quadrature:

cumtrapz(y, x=None, dx=1.0, axis=-1, initial=None)
    Cumulatively integrate y(x) using the composite trapezoidal rule.

    Parameters
    ----------
    y : array_like
        Values to integrate.
    x : array_like, optional
        The coordinate to integrate along.  If None (default), use spacing `dx`
        between consecutive elements in `y`.
    dx : int, optional
        Spacing between elements of `y`.  Only used if `x` is None.
    axis : int, optional
        Specifies the axis to cumulate.  Default is -1 (last axis).
    initial : scalar, optional
        If given, uses this value as the first value in the returned result.
        Typically this value should be 0.  Default is None, which means no
        value at ``x[0]`` is returned and `res` has one element less than `y`
        along the axis of integration.

    Returns
    -------
    res : ndarray
        The result of cumulative integration of `y` along `axis`.
        If `initial` is None, the shape is such that the axis of integration
        has one less value than `y`.  If `initial` is given, the shape is equal
        to that of `y`.

    See Also
    --------
    numpy.cumsum, numpy.cumprod
    quad: adaptive quadrature using QUADPACK
    romberg: adaptive Romberg quadrature
    quadrature: adaptive Gaussian quadrature
    fixed_quad: fixed-order Gaussian quadrature
    dblquad: double integrals
    tplquad: triple integrals
    romb: integrators for sampled data
    ode: ODE integrators
    odeint: ODE integrators

    Examples
    --------
    >>> from scipy import integrate
    >>> import matplotlib.pyplot as plt

    >>> x = np.linspace(-2, 2, num=20)
    >>> y = x
    >>> y_int = integrate.cumtrapz(y, x, initial=0)
    >>> plt.plot(x, y_int, 'ro', x, y[0] + 0.5 * x**2, 'b-')
    >>> plt.show()

-----------------------------------------------------------------------------------
Help on function simps in module scipy.integrate.quadrature:

simps(y, x=None, dx=1, axis=-1, even='avg')
    Integrate y(x) using samples along the given axis and the composite
    Simpson's rule.  If x is None, spacing of dx is assumed.

    If there are an even number of samples, N, then there are an odd
    number of intervals (N-1), but Simpson's rule requires an even number
    of intervals.  The parameter 'even' controls how this is handled.

    Parameters
    ----------
    y : array_like
        Array to be integrated.
    x : array_like, optional
        If given, the points at which `y` is sampled.
    dx : int, optional
        Spacing of integration points along axis of `y`. Only used when
        `x` is None. Default is 1.
    axis : int, optional
        Axis along which to integrate. Default is the last axis.
    even : {'avg', 'first', 'str'}, optional
        'avg' : Average two results:1) use the first N-2 intervals with
                  a trapezoidal rule on the last interval and 2) use the last
                  N-2 intervals with a trapezoidal rule on the first interval.

        'first' : Use Simpson's rule for the first N-2 intervals with
                a trapezoidal rule on the last interval.

        'last' : Use Simpson's rule for the last N-2 intervals with a
               trapezoidal rule on the first interval.
    See Also
    --------
    quad: adaptive quadrature using QUADPACK
    romberg: adaptive Romberg quadrature
    quadrature: adaptive Gaussian quadrature
    fixed_quad: fixed-order Gaussian quadrature
    dblquad: double integrals
    tplquad: triple integrals
    romb: integrators for sampled data
    cumtrapz: cumulative integration for sampled data
    ode: ODE integrators
    odeint: ODE integrators

    Notes
    -----
    For an odd number of samples that are equally spaced the result is
    exact if the function is a polynomial of order 3 or less.  If
    the samples are not equally spaced, then the result is exact only
    if the function is a polynomial of order 2 or less.
```

```
In [9]: dir(scipy.integrate)

Out[9]: ['IntegrationWarning',
         'Tester',
         '__all__',
         '__builtins__',
         '__doc__',
         '__file__',
         '__name__',
         '__package__',
         '__path__',
         '_dop',
         '_ode',
         '_odepack',
         '_quadpack',
         'absolute_import',
         'complex_ode',
         'cumtrapz',
         'dblquad',
         'division',
         'fixed_quad',
         'lsoda',
         'newton_cotes',
         'nquad',
         'ode',
         'odeint',
         'odepack',
         'print_function',
         'quad',
         'quad_explain',
         'quadpack',
         'quadrature',
         'romb',
         'romberg',
         's',
         'simps',
         'test',
         'tplquad',
         'trapz',
         'vode']
```

```
In [10]: # Defining x and y
         x = np.linspace(0, 10, 100)
         y = np.sin(x)
         # Compare the integrales using two methods
         print trapz(y, x)
         print simps(y, x)
```

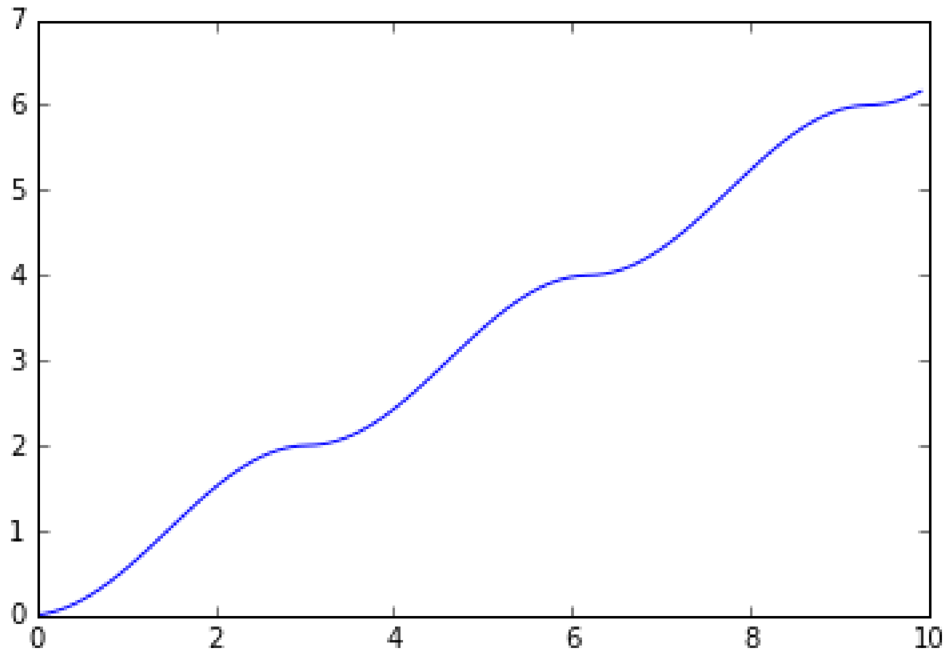
```
1.83750758633
1.83909194697
```

```
In [11]: # Cumulative integrale
         print cumtrapz(np.abs(y), x)
```

```
[  5.09284951e-03   2.03194796e-02   4.55246645e-02   8.04514533e-02
   1.24743789e-01   1.77950140e-01   2.39528101e-01   3.08849923e-01
   3.85208914e-01   4.67826642e-01   5.55860873e-01   6.48414152e-01
   7.44542958e-01   8.43267317e-01   9.43580798e-01   1.04446077e+00
   1.14487882e+00   1.24381125e+00   1.34024951e+00   1.43321048e+00
   1.52174647e+00   1.60495491e+00   1.68198755e+00   1.75205909e+00
   1.81445519e+00   1.86853977e+00   1.91376146e+00   1.94965927e+00
   1.97586722e+00   1.99211816e+00   1.99824642e+00   2.00334164e+00
   2.01754235e+00   2.04174210e+00   2.07569419e+00   2.11905248e+00
   2.17137499e+00   2.23212830e+00   2.30069308e+00   2.37637035e+00
   2.45838864e+00   2.54591181e+00   2.63804762e+00   2.73385681e+00
   2.83236266e+00   2.93256097e+00   3.03343028e+00   3.13394229e+00
   3.23307235e+00   3.32980988e+00   3.42316870e+00   3.51219709e+00
   3.59598746e+00   3.67368561e+00   3.74449946e+00   3.80770711e+00
   3.86266420e+00   3.90881048e+00   3.94567550e+00   3.97288346e+00
   3.99015699e+00   3.99732000e+00   4.00241706e+00   4.01559036e+00
   4.03878211e+00   4.07175590e+00   4.11417558e+00   4.16560871e+00
   4.22553095e+00   4.29333144e+00   4.36831900e+00   4.44972917e+00
   4.53673204e+00   4.62844065e+00   4.72392010e+00   4.82219704e+00
   4.92226959e+00   5.02311758e+00   5.12371293e+00   5.22303013e+00
   5.32005670e+00   5.41380353e+00   5.50331491e+00   5.58767835e+00
   5.66603380e+00   5.73758248e+00   5.80159500e+00   5.85741879e+00
   5.90448477e+00   5.94231312e+00   5.97051821e+00   5.98881251e+00
   5.99700951e+00   6.00210788e+00   6.01425236e+00   6.03643367e+00
   6.06842568e+00   6.10990226e+00   6.16044057e+00]
```

```
In [12]: # Cumulative integral
         print len(x), len(cumtrapz(np.abs(y), x))
         f, ax = plt.subplots()
         ax.plot(x[0:-1], cumtrapz(np.abs(y), x));
```

```
100 99
```



```
In [13]: from scipy.integrate import quad # To compute a definite integral
         from scipy.special import jv # Bessel function
         #help(quad)
         print quad(lambda x: jv(2.5, x), 0, 10) # Integrate the Bessel function o
```

```
(0.8209075326034347, 1.1793289815399173e-08)
```

We now want to evaluate:

$$\int_0^1 1 + 2x + 3x^2 dx$$

```
In [15]: # We want here integrate a user-defined function (here polynome) between (
         def f(x, a, b, c):
             """ Returning a 2nd order polynome """
             return a + b * x + c * x**2
         %timeit I = quad(f, 0, 1, args=(1,2,3)) # args will send 1, 2, 3 to f
         I = quad(f, 0, 1, args=(1,2,3)) # args will send 1, 2, 3 to f
         print I
         Integ = I[0]
         print Integ
```

```
100000 loops, best of 3: 11.5 µs per loop
(3.0, 3.3306690738754696e-14)
3.0
```

1.0.3 Interpolations

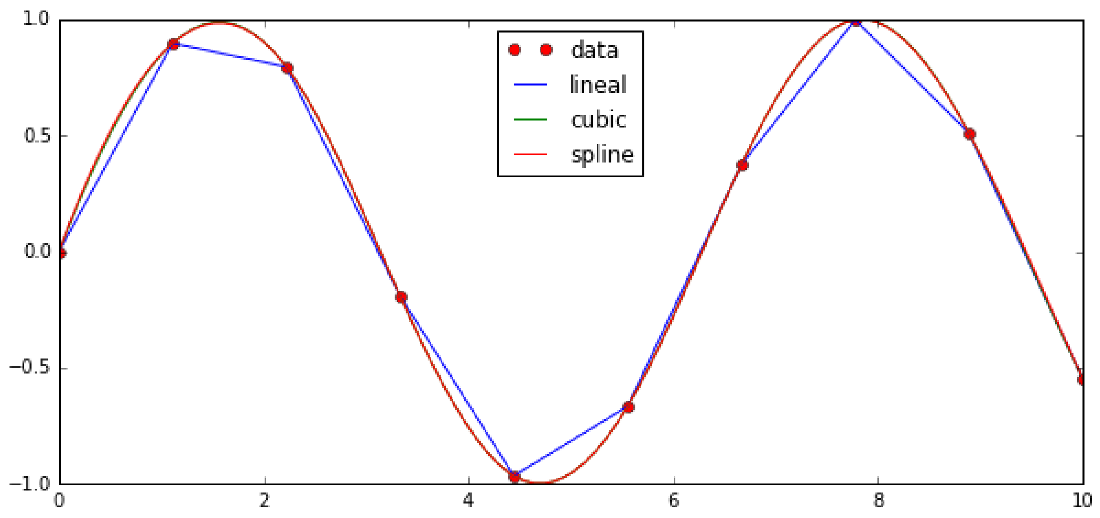
```
In [16]: from scipy.interpolate import interp1d, interp2d, splrep, splev, griddata
```

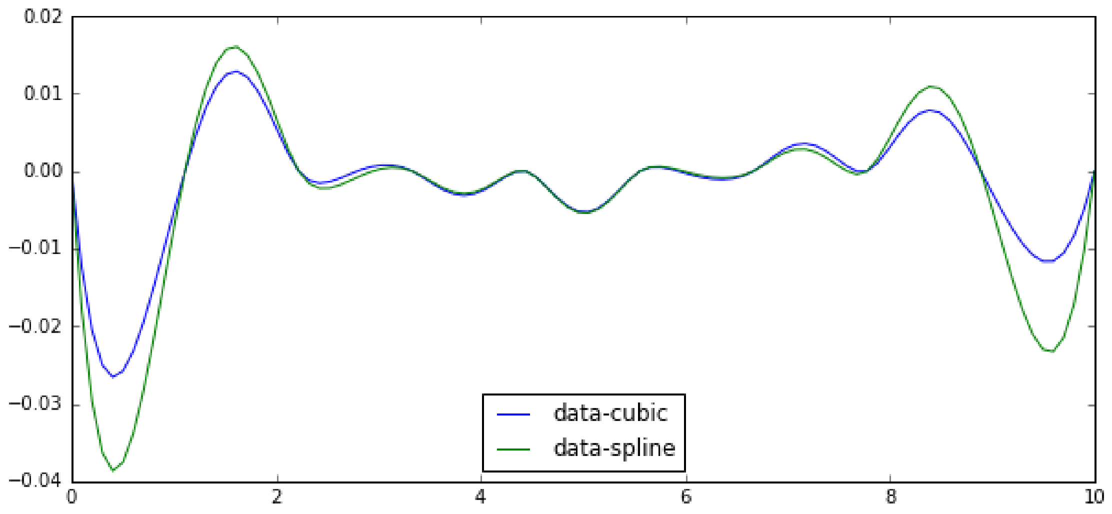
```
In [17]: #help(scipy.interpolate) # a huge one...
         help(interp1d)
```

```
Help on class interp1d in module scipy.interpolate.interpolate:

class interp1d(scipy.interpolate.polyint._Interpolator1D)
 |  Interpolate a 1-D function.
 |
 |  `x` and `y` are arrays of values used to approximate some function f:
 |  ``y = f(x)``.  This class returns a function whose call method uses
 |  interpolation to find the value of new points.
 |
 |  Parameters
 |  ----------
 |  x : (N,) array_like
 |      A 1-D array of real values.
 |  y : (...,N,...) array_like
 |      A N-D array of real values. The length of `y` along the interpolation
 |      axis must be equal to the length of `x`.
 |  kind : str or int, optional
 |      Specifies the kind of interpolation as a string
 |      ('linear', 'nearest', 'zero', 'slinear', 'quadratic, 'cubic'
 |      where 'slinear', 'quadratic' and 'cubic' refer to a spline
 |      interpolation of first, second or third order) or as an integer
 |      specifying the order of the spline interpolator to use.
 |      Default is 'linear'.
 |  axis : int, optional
 |      Specifies the axis of `y` along which to interpolate.
 |      Interpolation defaults to the last axis of `y`.
 |  copy : bool, optional
 |       If True, the class makes internal copies of x and y.
 |       If False, references to `x` and `y` are used. The default is to copy.
 |   bounds_error : bool, optional
 |       If True, a ValueError is raised any time interpolation is attempted on
 |       a value outside of the range of x (where extrapolation is
 |       necessary). If False, out of bounds values are assigned `fill_value`.
 |       By default, an error is raised unless `fill_value="extrapolate"`.
 |   fill_value : array-like or (array-like, array_like) or "extrapolate", optional
 |       - if a ndarray (or float), this value will be used to fill in for
 |         requested points outside of the data range. If not provided, then
 |         the default is NaN. The array-like must broadcast properly to the
 |         dimensions of the non-interpolation axes.
 |       - If a two-element tuple, then the first element is used as a
 |         fill value for ``x_new < x[0]`` and the second element is used for
 |         ``x_new > x[-1]``. Anything that is not a 2-element tuple (e.g.,
 |         list or ndarray, regardless of shape) is taken to be a single
 |         array-like argument meant to be used for both bounds as
 |         ``below, above = fill_value, fill_value``.
 |
 |         .. versionadded:: 0.17.0
 |       - If "extrapolate", then points outside the data range will be
 |         extrapolated. ("nearest" and "linear" kinds only.)
 |
 |         .. versionadded:: 0.17.0
 |   assume_sorted : bool, optional
 |       If False, values of `x` can be in any order and they are sorted first.
 |       If True, `x` has to be an array of monotonically increasing values.
 |
 |   Methods
 |   -------
 |   __call__
 |
 |   See Also
 |   --------
 |   splrep, splev
 |       Spline interpolation/smoothing based on FITPACK.
 |   UnivariateSpline : An object-oriented wrapper of the FITPACK routines.
 |   interp2d : 2-D interpolation
 |
 |   Examples
 |   --------
 |   >>> import matplotlib.pyplot as plt
 |   >>> from scipy import interpolate
 |   >>> x = np.arange(0, 10)
 |   >>> y = np.exp(-x/3.0)
 |   >>> f = interpolate.interp1d(x, y)
 |
 |   >>> xnew = np.arange(0, 9, 0.1)
 |  >>> ynew = f(xnew)   # use interpolation function returned by `interp1d`
 |  >>> plt.plot(x, y, 'o', xnew, ynew, '-')
 |  >>> plt.show()
 |
 |  Method resolution order:
 |      interp1d
 |      scipy.interpolate.polyint._Interpolator1D
 |      __builtin__.object
 |
 |  Methods defined here:
 |
 |  __init__(self, x, y, kind='linear', axis=-1, copy=True, bounds_error=None, fill
 |      Initialize a 1D linear interpolation class.
 |
 |  ----------------------------------------------------------------------
 |  Data descriptors defined here:
 |
 |  __dict__
 |      dictionary for instance variables (if defined)
 |
 |  __weakref__
 |      list of weak references to the object (if defined)
 |
 |  fill_value
 |
 |  ----------------------------------------------------------------------
 |  Methods inherited from scipy.interpolate.polyint._Interpolator1D:
 |
 |  __call__(self, x)
 |      Evaluate the interpolant
 |
 |      Parameters
 |      ----------
 |      x : array_like
 |          Points to evaluate the interpolant at.
 |
 |      Returns
 |      -------
 |      y : array_like
 |          Interpolated values. Shape is determined by replacing
 |          the interpolation axis in the original array with the shape of x.
 |
 |  ----------------------------------------------------------------------
 |  Data descriptors inherited from scipy.interpolate.polyint._Interpolator1D:
 |
 |  dtype
```

```
In [18]: x = np.linspace(0, 10, 10)
         y = np.sin(x)
         f = interp1d(x, y) # this creates a function that can be call at any inter
         f2 = interp1d(x, y, kind='cubic') # The same but using cubic interpolatio
         tck = splrep(x, y, s=0) # This initiate the spline interpolating function,
         # tck is a sequence of length 3 returned by `splrep` or `splprep` contain
         f3 = lambda x: splev(x, tck) # Evaluate the B-spline or its derivatives.
```

```
In [19]: # Defining the high resolution mesh
         xfine = np.linspace(0, 10, 100)
         yfine = np.sin(xfine)
         # Plot to compare the results
         fig, (ax1, ax2) = plt.subplots(2, figsize=(10,10))

         ax1.plot(x, y, 'or', label='data')
         ax1.plot(xfine, f(xfine), label='lineal')
         ax1.plot(xfine, f2(xfine), label='cubic')
         ax1.plot(xfine, f3(xfine), label='spline')
         ax1.legend(loc=9)

         ax2.plot(xfine, (yfine-f2(xfine)), label='data-cubic')
         ax2.plot(xfine, (yfine-f3(xfine)), label='data-spline')
         ax2.legend(loc=8);
```





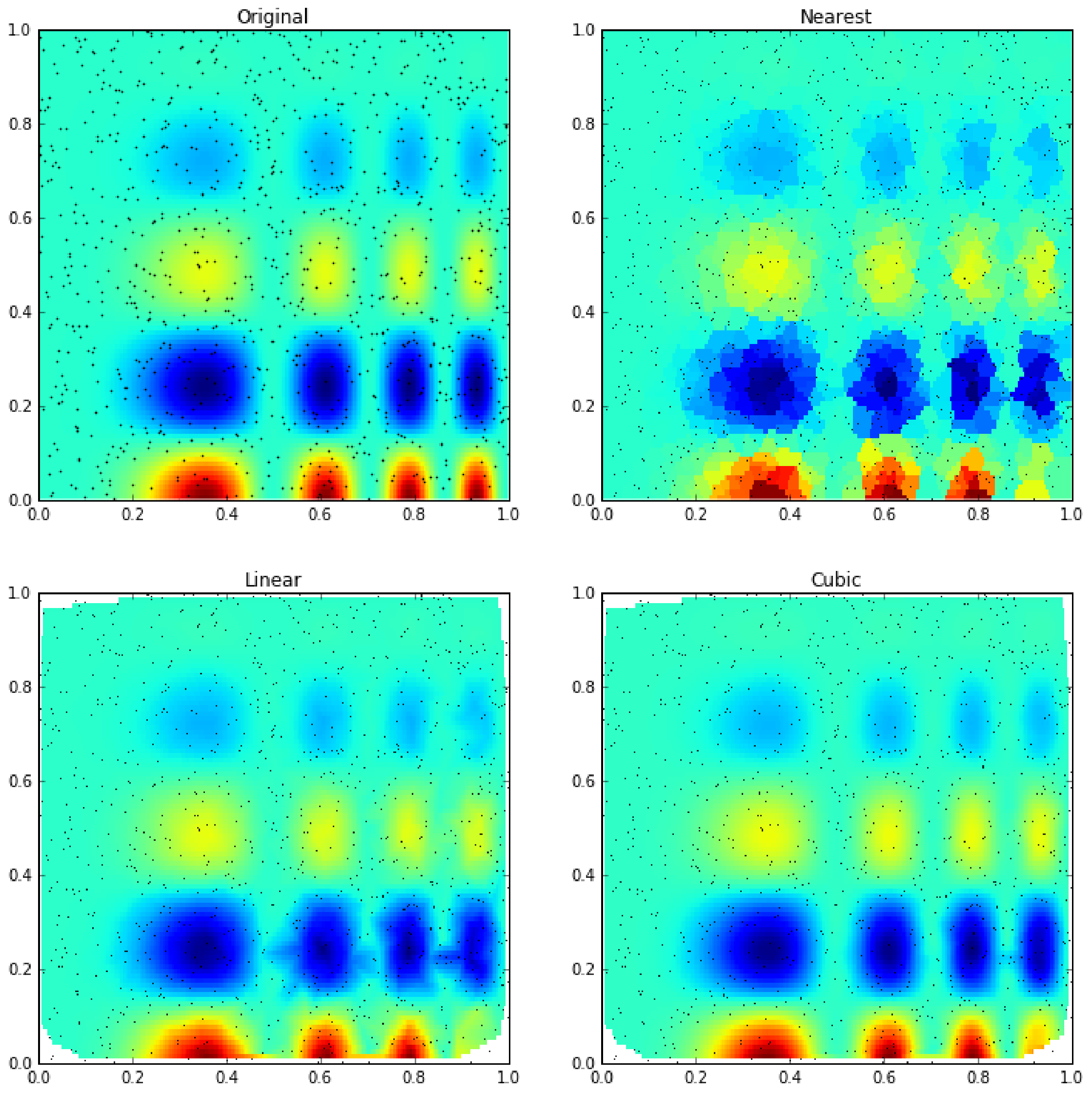
```
In [20]: x0 = 3.5
         print np.sin(x0), f(x0), f2(x0), f3(x0)

-0.35078322769 -0.306630335983 -0.349437256954 -0.349597252402
```

2D interpolation

```
In [21]: # Defining a 2D-function
         def func(x, y):
             return x * (1+x) * np.cos(4*np.pi*x) * np.sin(4*np.pi*y**2)**2

In [22]: # Initializing a 2D coordinate grid. Note the use of j to specify that the
         grid_x, grid_y = np.mgrid[0:1:100j, 0:1:200j]
```

```
In [23]: print grid_x
         print grid_y

[[ 0.          0.          0.         ...,  0.          0.          0.        ]
 [ 0.01010101  0.01010101  0.01010101 ...,  0.01010101  0.01010101
   0.01010101]
 [ 0.02020202  0.02020202  0.02020202 ...,  0.02020202  0.02020202
   0.02020202]
 ...,
 [ 0.97979798  0.97979798  0.97979798 ...,  0.97979798  0.97979798
   0.97979798]
 [ 0.98989899  0.98989899  0.98989899 ...,  0.98989899  0.98989899
   0.98989899]
 [ 1.          1.          1.         ...,  1.          1.          1.        ]]
[[ 0.          0.00502513  0.01005025 ...,  0.98994975  0.99497487  1.        ]
 [ 0.          0.00502513  0.01005025 ...,  0.98994975  0.99497487  1.        ]
 [ 0.          0.00502513  0.01005025 ...,  0.98994975  0.99497487  1.        ]
 ...,
 [ 0.          0.00502513  0.01005025 ...,  0.98994975  0.99497487  1.        ]
 [ 0.          0.00502513  0.01005025 ...,  0.98994975  0.99497487  1.        ]
 [ 0.          0.00502513  0.01005025 ...,  0.98994975  0.99497487  1.        ]]


In [24]: # Generating 1000 x 2 points randomly
         points = np.random.rand(1000, 2)
         values = func(points[:,0], points[:,1])

In [25]: # griddata is the 2D-interpolating method. We want to obtain values on (gr
         # using "points" and "values".
         %timeit grid_z0 = griddata(points, values, (grid_x, grid_y), method='neare
         %timeit grid_z1 = griddata(points, values, (grid_x, grid_y), method='linea
         %timeit grid_z2 = griddata(points, values, (grid_x, grid_y), method='cubic

100 loops, best of 3: 14.3 ms per loop
100 loops, best of 3: 9.96 ms per loop
100 loops, best of 3: 16.4 ms per loop


In [27]: # 4 subplots
         grid_z0 = griddata(points, values, (grid_x, grid_y), method='nearest')
         grid_z1 = griddata(points, values, (grid_x, grid_y), method='linear')
         grid_z2 = griddata(points, values, (grid_x, grid_y), method='cubic')
         fig, ((ax1, ax2), (ax3, ax4)) = plt.subplots(2, 2, figsize=(12, 12))

         ax1.imshow(func(grid_x, grid_y), extent=(0,1,0,1), interpolation='none',
                    origin='upper')
         ax1.plot(points[:,0], points[:,1], 'ko', ms=1)
         ax1.set_title('Original')
```

```
ax2.imshow(grid_z0, extent=(0,1,0,1), interpolation='none',
           origin='upper')
ax2.plot(points[:,0], points[:,1], 'k.', ms=1)
ax2.set_title('Nearest')

ax3.imshow(grid_z1, extent=(0,1,0,1), interpolation='none',
           origin='upper')
ax3.plot(points[:,0], points[:,1], 'k.', ms=1)
ax3.set_title('Linear')

ax4.imshow(grid_z2, extent=(0,1,0,1), interpolation='none',
           origin='upper')
ax4.plot(points[:,0], points[:,1], 'k.', ms=1)
ax4.set_title('Cubic');
```



1.0.4 Linear algebra

Scipy is able to deal with matrices, solving linear equations, solving linear least-squares problems and pseudo-inverses, finding eigenvalues and eigenvectors, and more, see here: http://docs.scipy.org/doc/scipy/reference/tutorial/linalg.html

1.0.5 Data fit

```
In [28]: from scipy.optimize import curve_fit # this is used to adjust a set of dat
```

```
In [29]: help(curve_fit)
```

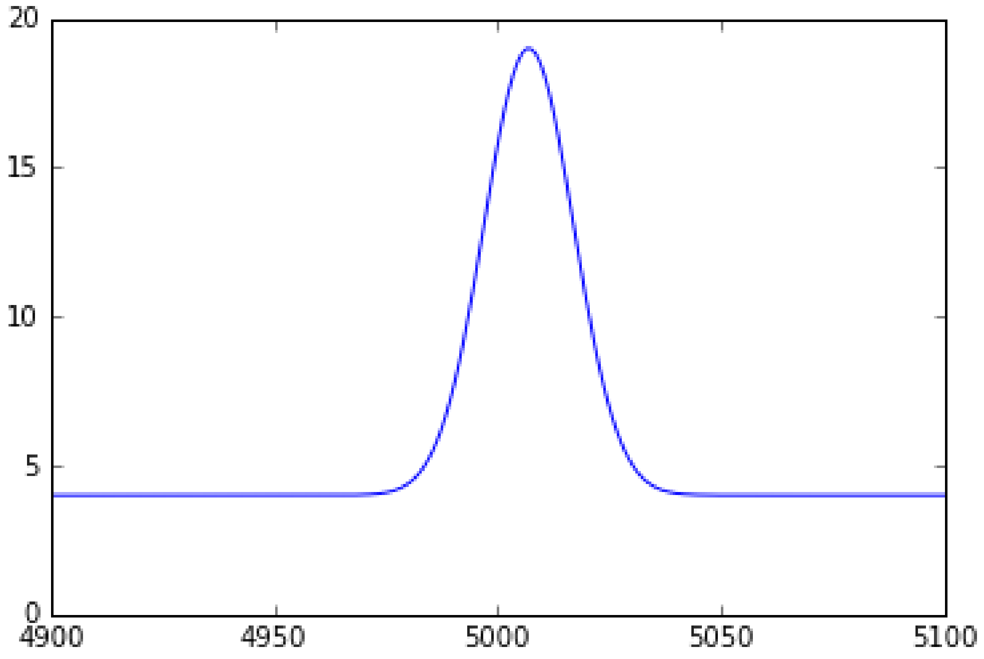
```
Help on function curve_fit in module scipy.optimize.minpack:

curve_fit(f, xdata, ydata, p0=None, sigma=None, absolute_sigma=False, check_finite=
    Use non-linear least squares to fit a function, f, to data.

    Assumes ``ydata = f(xdata, *params) + eps``

    Parameters
    ----------
    f : callable
        The model function, f(x, ...).  It must take the independent
        variable as the first argument and the parameters to fit as
        separate remaining arguments.
    xdata : An M-length sequence or an (k,M)-shaped array
        for functions with k predictors.
        The independent variable where the data is measured.
    ydata : M-length sequence
        The dependent data --- nominally f(xdata, ...)
    p0 : None, scalar, or N-length sequence, optional
        Initial guess for the parameters.  If None, then the initial
        values will all be 1 (if the number of parameters for the function
        can be determined using introspection, otherwise a ValueError
        is raised).
    sigma : None or M-length sequence, optional
        If not None, the uncertainties in the ydata array. These are used as
        weights in the least-squares problem
        i.e. minimising ``np.sum( ((f(xdata, *popt) - ydata) / sigma)**2 )``
        If None, the uncertainties are assumed to be 1.
    absolute_sigma : bool, optional
        If False, `sigma` denotes relative weights of the data points.
        The returned covariance matrix `pcov` is based on *estimated*
        errors in the data, and is not affected by the overall
        magnitude of the values in `sigma`. Only the relative
        magnitudes of the `sigma` values matter.
        If True, `sigma` describes one standard deviation errors of
        the input data points. The estimated covariance in `pcov` is
        based on these values.
    check_finite : bool, optional
        If True, check that the input arrays do not contain nans of infs,
        and raise a ValueError if they do. Setting this parameter to
        False may silently produce nonsensical results if the input arrays
        do contain nans. Default is True.
    bounds : 2-tuple of array_like, optional
        Lower and upper bounds on independent variables. Defaults to no bounds.
        Each element of the tuple must be either an array with the length equal
        to the number of parameters, or a scalar (in which case the bound is
        taken to be the same for all parameters.) Use ``np.inf`` with an
        appropriate sign to disable bounds on all or some parameters.

        .. versionadded:: 0.17
    method : {'lm', 'trf', 'dogbox'}, optional
        Method to use for optimization.  See `least_squares` for more details.
        Default is 'lm' for unconstrained problems and 'trf' if `bounds` are
        provided. The method 'lm' won't work when the number of observations
        is less than the number of variables, use 'trf' or 'dogbox' in this
        case.

        .. versionadded:: 0.17
    kwargs
        Keyword arguments passed to `leastsq` for ``method='lm'`` or
        `least_squares` otherwise.

    Returns
    -------
    popt : array
        Optimal values for the parameters so that the sum of the squared error
        of ``f(xdata, *popt) - ydata`` is minimized
    pcov : 2d array
        The estimated covariance of popt. The diagonals provide the variance
        of the parameter estimate. To compute one standard deviation errors
        on the parameters use ``perr = np.sqrt(np.diag(pcov))``.

        How the `sigma` parameter affects the estimated covariance
        depends on `absolute_sigma` argument, as described above.

        If the Jacobian matrix at the solution doesn't have a full rank, then
        'lm' method returns a matrix filled with ``np.inf``, on the other hand
        'trf'  and 'dogbox' methods use Moore-Penrose pseudoinverse to compute
        the covariance matrix.

    Raises
    ------
```

```
    OptimizeWarning
        if covariance of the parameters can not be estimated.

    ValueError
        if either `ydata` or `xdata` contain NaNs.

    See Also
    --------
    least_squares : Minimize the sum of squares of nonlinear functions.
    stats.linregress : Calculate a linear least squares regression for two sets
                       of measurements.

    Notes
    -----
    With ``method='lm'``, the algorithm uses the Levenberg-Marquardt algorithm
    through `leastsq`. Note that this algorithm can only deal with
    unconstrained problems.

    Box constraints can be handled by methods 'trf' and 'dogbox'. Refer to
    the docstring of `least_squares` for more information.

    Examples
    --------
    >>> import numpy as np
    >>> from scipy.optimize import curve_fit
    >>> def func(x, a, b, c):
    ...     return a * np.exp(-b * x) + c

    >>> xdata = np.linspace(0, 4, 50)
    >>> y = func(xdata, 2.5, 1.3, 0.5)
    >>> ydata = y + 0.2 * np.random.normal(size=len(xdata))

    >>> popt, pcov = curve_fit(func, xdata, ydata)

    Constrain the optimization to the region of ``0 < a < 3``, ``0 < b < 2``
    and ``0 < c < 1``:

    >>> popt, pcov = curve_fit(func, xdata, ydata, bounds=(0, [3., 2., 1.]))
```

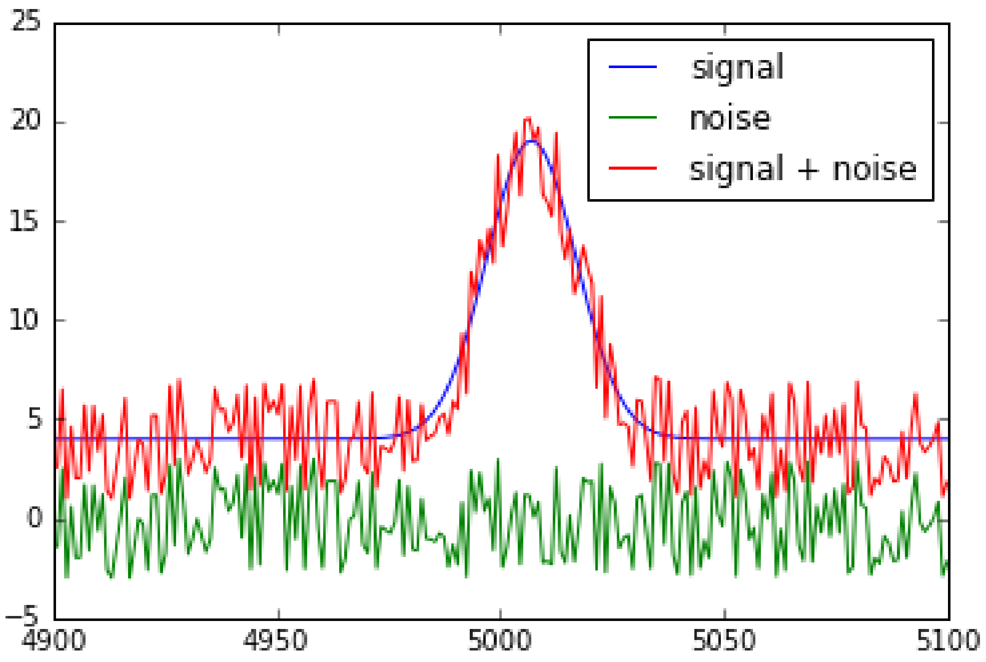
```
In [30]: def gauss(x, A, B, C, S):
             # This is a gaussian function.
             return A + B*np.exp(-1 * (x - C)**2 / (2 * S**2))
```

```
In [31]: # We define the parameters used to generate the signal (gaussian at lambda
         N_lam = 200
         A = 4.
```

```
B = 15.
Lam0 = 5007.
Sigma = 10.
# We define a wavelength range
lam = np.linspace(4900, 5100, N_lam)
# Computing the signal
fl = gauss(lam, A, B, Lam0, Sigma)
f, ax =plt.subplots()
ax.plot(lam, fl)
ax.set_ylim(0,20);
```

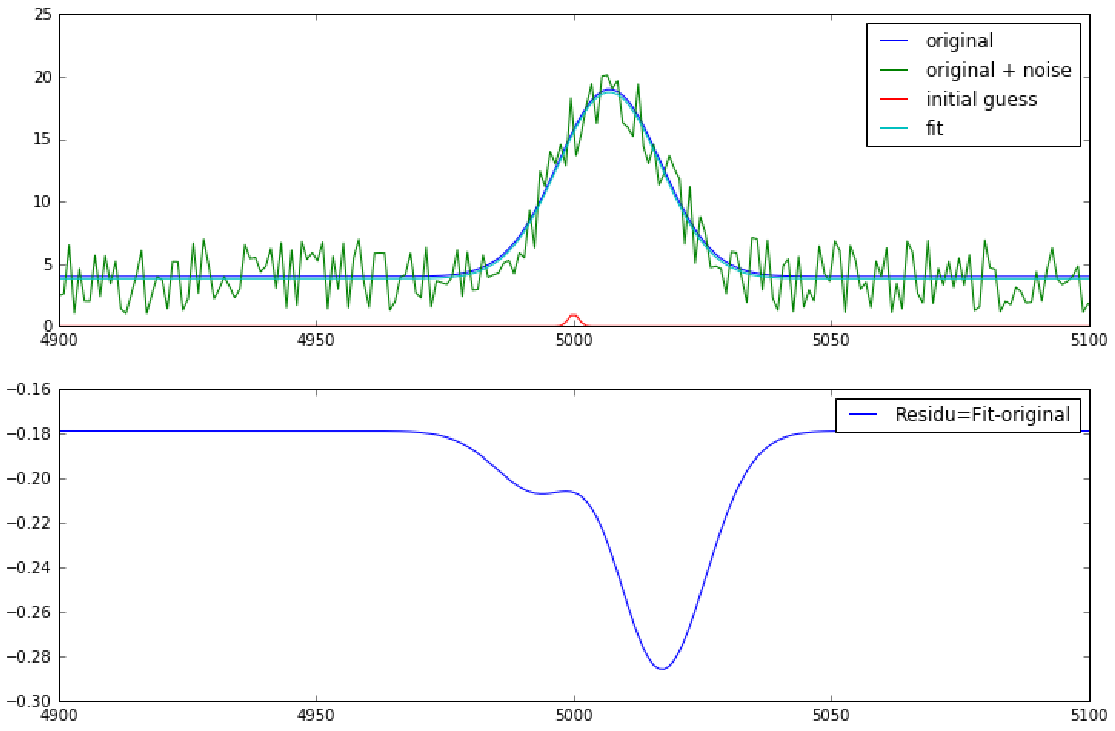


```
In [32]: SN = 5. # Signal/Noise
         noise = B / SN * (np.random.rand(N_lam)*2 - 1)
         fl2 = fl + noise
         f, ax =plt.subplots()
         ax.plot(lam, fl, label='signal')
         ax.plot(lam, noise, label='noise')
         ax.plot(lam, fl2, label='signal + noise')
         ax.legend(loc='best');
```



```
In [33]: # Initial guess:
         A_i = 0.
         B_i = 1.
         Lam0_i = 5000.
         Sigma_i = 1.
         fl_init = gauss(lam, A_i, B_i, Lam0_i, Sigma_i)
         error = np.ones_like(lam) * np.mean(np.abs(noise)) # We define the error

In [34]: # fitting the noisy data with the gaussian function, using the initial gue
         fit, covar = curve_fit(gauss, lam, fl2, [A_i, B_i, Lam0_i, Sigma_i], error
         print('   A      B     Lam0      S')
         print('{0:.2f} {1:5.2f} {2:.2f} {3:5.2f}'.format(A, B, Lam0, Sigma))
         print('{0:.2f} {1:5.2f} {2:.2f} {3:5.2f}'.format(A_i, B_i, Lam0_i, Sigma_i
         print('{0[0]:.2f} {0[1]:5.2f} {0[2]:5.2f} {0[3]:.2f}'.format(fit))

   A      B     Lam0      S
4.00 15.00 5007.00 10.00
0.00  1.00 5000.00  1.00
3.82 14.95 5006.96 9.96


In [35]: # Computing the fit on the lambdas
         fl_fit = gauss(lam, fit[0], fit[1], fit[2], fit[3])

In [36]: fig, (ax1, ax2) = plt.subplots(2, 1, figsize=(12, 8))
```

```
        ax1.plot(lam, fl, label='original')
        ax1.plot(lam, fl2, label='original + noise')
        ax1.plot(lam, fl_init, label='initial guess')
        ax1.plot(lam, fl_fit, label='fit')
        ax1.legend()

        ax2.plot(lam, fl_fit - fl, label='Residu=Fit-original')
        ax2.legend();
```



```
In [37]: # Integrating using the Simpson method the gaussian (without the continuum
         print simps(fl - A, lam)
         print simps(fl2 - fit[0], lam)
         print simps(fl_fit - fit[0], lam)
```

```
375.994241195
374.861103061
373.225105596
```

```
In [38]: khi_sq = (((fl2-fl_fit) / error)**2).sum() # The problem here is to deter
         khi_sq_red = khi_sq / (len(lam) - 4 - 1) # reduced khi_sq = khi_sq / (N -
         print khi_sq, khi_sq_red
```

```
252.019224164 1.29240627777
```

1.0.6 Multivariate estimation

```
In [39]: from scipy import stats
```

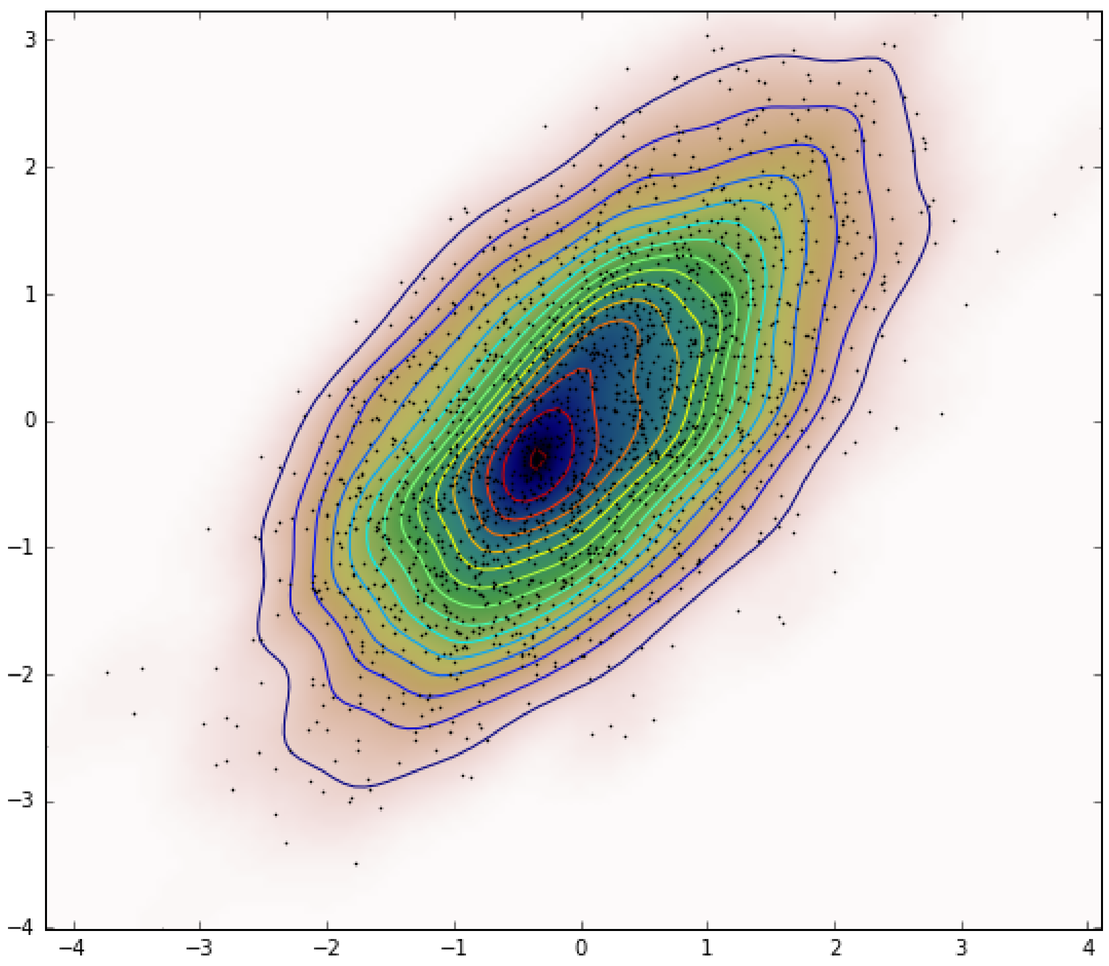
```
In [40]: def measure(n):
             """Measurement model, return two coupled measurements."""
             m1 = np.random.normal(size=n)
             m2 = np.random.normal(scale=0.5, size=n)
             return m1+m2, m1-m2
```

```
In [41]: # Define the
         m1, m2 = measure(2000)
         xmin = m1.min()
         xmax = m1.max()
         ymin = m2.min()
         ymax = m2.max()
         print xmin, xmax, ymin, ymax
```

```
-4.22246586473 4.11472562257 -4.00698468532 3.22607780801
```

```
In [42]: X, Y = np.mgrid[xmin:xmax:100j, ymin:ymax:100j]
         positions = np.vstack([X.ravel(), Y.ravel()])
         values = np.vstack([m1, m2])
         kernel = stats.gaussian_kde(values)
         Z = np.reshape(kernel.evaluate(positions).T, X.shape)
```

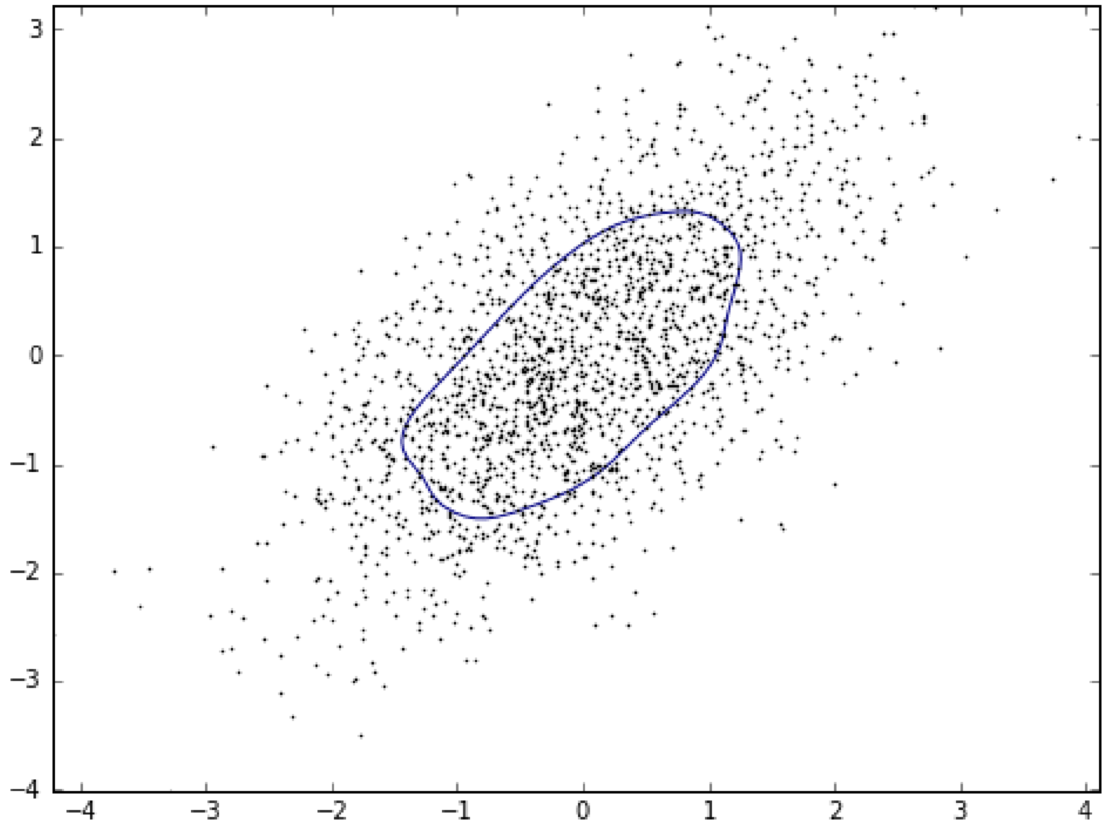
```
In [44]: fig, ax = plt.subplots(figsize=(12, 8))
         ax.imshow(np.rot90(Z), cmap=plt.cm.gist_earth_r, extent=[xmin, xmax, ymin,
         ax.plot(m1, m2, 'k.', markersize=2)
         ax.set_xlim([xmin, xmax])
         ax.set_ylim([ymin, ymax])
         levels = [0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09, 0.10, 0.11
         cs = ax.contour(X, Y, Z, levels=levels); # I dont't know what those levels
```



```
In [45]: # We save the contour paths in a list
         paths = []
         for collec in cs.collections:
             try:
                 paths.append(collec.get_paths()[0])
             except:
                 pass

In [46]: # Looking for the number of points inside each contour
         print len(m1)
         for level, path in zip(levels, paths):
             print('level {0:4.2f} contains {1:2.0f}% of the data'.format(level,
                                                                           path.contai
```

```
2000
level 0.01 contains 96% of the data
level 0.02 contains 90% of the data
level 0.03 contains 83% of the data
level 0.04 contains 76% of the data
level 0.05 contains 70% of the data
level 0.06 contains 63% of the data
level 0.07 contains 56% of the data
level 0.08 contains 50% of the data
level 0.09 contains 42% of the data
level 0.10 contains 36% of the data
level 0.11 contains 29% of the data
level 0.12 contains 19% of the data
level 0.13 contains 10% of the data
level 0.14 contains  5% of the data
level 0.15 contains  0% of the data
```

```
In [47]: fig, ax = plt.subplots(figsize=(8, 6))
         ax.plot(m1, m2, 'k.', markersize=2)
         ax.set_xlim([xmin, xmax])
         ax.set_ylim([ymin, ymax])
         cs = ax.contour(X, Y, Z, levels=[0.078]); #  seems to correspond to 50% of
```

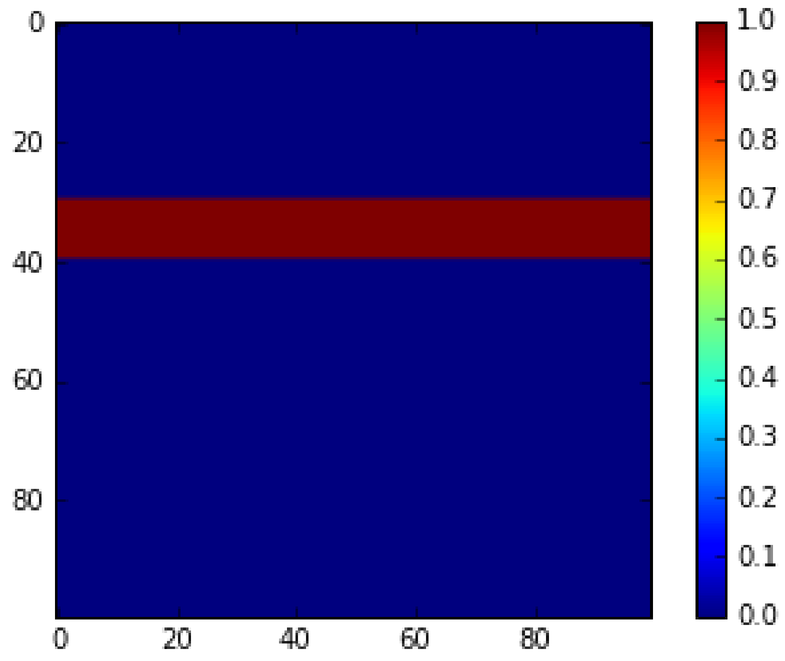


1.0.7 Convolution

More information there: http://docs.scipy.org/doc/scipy/reference/tutorial/ndimage.html

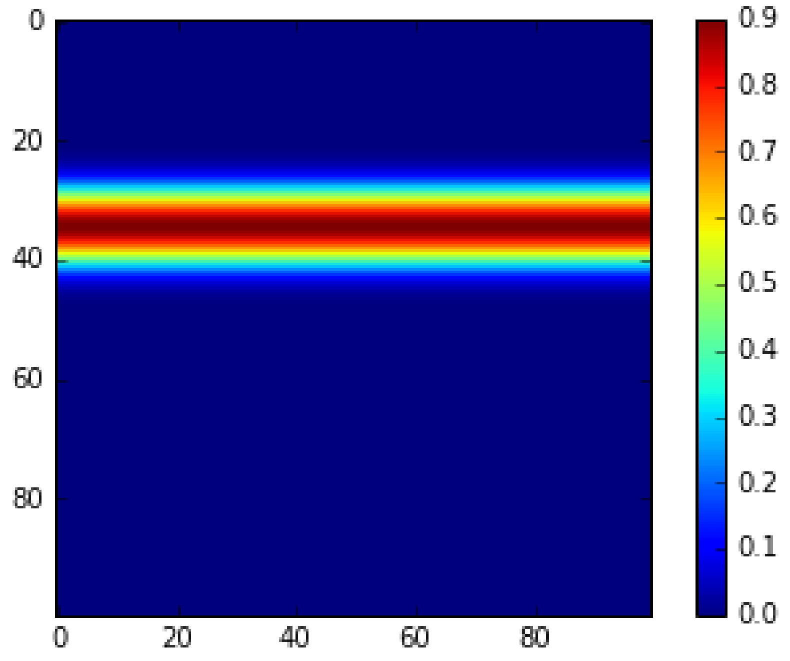
```
In [48]: # Let's define an image representing a long slit of width 10 pixels
         slit = np.zeros((100, 100))
         slit[30:40, :] = 1
```

```
In [49]: plt.imshow(slit)
         plt.colorbar();
```

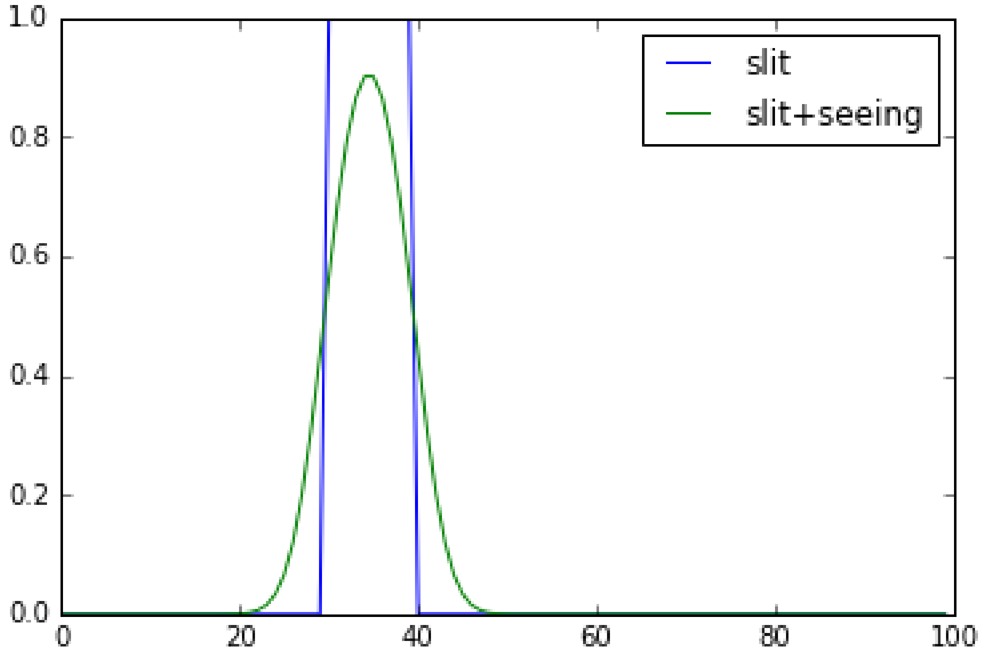


```
In [50]: # This is the routine to apply a gaussian convolution
         from scipy.ndimage.filters import gaussian_filter
```

```
In [51]: slit_seeing = gaussian_filter(slit, 3) # Convolve with a gaussian, 3 is th
         plt.imshow(slit_seeing)
         plt.colorbar();
```



```
In [52]: f, ax =plt.subplots()
         ax.plot(slit[:,50], label='slit') # original slit
         ax.plot(slit_seeing[:,50], label='slit+seeing') # slit with seeing
         ax.legend(loc='best');
```



```
In [53]: # Check that the slit transmission is conserved:
         print simps(slit[:,50]), simps(slit_seeing[:,50])

10.0 10.0
```

1.0.8 Quantiles

```
In [54]: from scipy.stats.mstats import mquantiles

In [55]: #help(mquantiles)

In [56]: data = np.random.randn(1000)

In [57]: mquantiles(data, [0.16, 0.84]) # should return something close to -1, 1 (t

Out[57]: array([-1.0245078 ,  1.04750432])

In [58]: data = np.array([[   6.,    7.,    1.],
                          [  47.,   15.,    2.],
                          [  49.,   36.,    3.],
                          [  15.,   39.,    4.],
                          [  42.,   40., -999.],
                          [  41.,   41., -999.],
                          [   7., -999., -999.],
                          [  39., -999., -999.],
                          [  43., -999., -999.],
                          [  40., -999., -999.],
                          [  36., -999., -999.]])

In [59]: mq = mquantiles(data, axis=0, limit=(0, 50))
         print mq
         print type(mq)
         mq?
         print mq.mask

[[ 19.2   14.6    1.45]
 [ 40.    37.5    2.5 ]
 [ 42.8   40.05   3.55]]
<class 'numpy.ma.core.MaskedArray'>
False
```

1.0.9 Input/Output

Scipy has many modules, classes, and functions available to read data from and write data to a variety of file formats.

Including MATLAB and IDL files. See http://docs.scipy.org/doc/scipy/reference/io.html