

intro_Scipy

September 17, 2023

```
[ ]: # The following is to know when this notebook has been run and with which ↵  
      ↪python version.  
import time, sys  
print(time.ctime())  
print(sys.version.split('|')[0])
```

Sun Sep 17 09:40:19 2023
3.9.16 (main, Jan 11 2023, 10:02:19)
[Clang 14.0.6]

1 E Introduction to Scipy

This is part of the Python lecture given by Christophe Morisset at IA-UNAM.

Scipy is a library with a lot of functionalities, 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>
- <https://docs.scipy.org/doc/scipy/tutorial/index.html>

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

```
[ ]: import scipy # This imports a lot of scipy stuff, but not the "important" ↵  
      ↪modules
```

1.0.1 Some usefull methods

```
[ ]: from scipy.special import gamma  
%timeit g1 = gamma(10.3)  
%timeit g1 = gamma(10)  
%timeit g2 = 9*8*7*6*5*4*3*2  
%timeit g3 = 10*9*8*7*6*5*4*3*2  
g1 = gamma(10.3)  
g2 = 9*8*7*6*5*4*3*2  
g3 = 10*9*8*7*6*5*4*3*2  
print(g1, g2, g3)
```

917 ns \pm 49.2 ns per loop (mean \pm std. dev. of 7 runs, 1,000,000 loops each)
 1.41 μ s \pm 135 ns per loop (mean \pm std. dev. of 7 runs, 1,000,000 loops each)
 16.4 ns \pm 0.608 ns per loop (mean \pm std. dev. of 7 runs, 100,000,000 loops each)
 16.8 ns \pm 0.772 ns per loop (mean \pm std. dev. of 7 runs, 100,000,000 loops each)
 716430.6890623764 362880 3628800

```
[ ]: from scipy import constants as cst
print(cst.astronomical_unit) # A lot of constants
print('{} {}'.format(cst.value('proton mass'), cst.unit('proton mass')))
```

149597870700.0

1.67262192369e-27 kg

List there: <http://docs.scipy.org/doc/scipy/reference/constants.html#constants-database>

1.0.2 Integrations

```
[ ]: 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 scipy.integrate._quadrature:

trapz(y, x=None, dx=1.0, axis=-1)
    An alias of `trapezoid`.

    `trapz` is kept for backwards compatibility. For new code, prefer
    `trapezoid` instead.

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

cumtrapz(y, x=None, dx=1.0, axis=-1, initial=None)
    An alias of `cumulative_trapezoid`.

    `cumtrapz` is kept for backwards compatibility. For new code, prefer
    `cumulative_trapezoid` instead.

-----
--
```

Help on function `simps` in module `scipy.integrate._quadrature`:

```
simps(y, x=None, dx=1.0, axis=-1, even='avg')
```

An alias of ``simpson``.

``simps`` is kept for backwards compatibility. For new code, prefer ``simpson`` instead.

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

```
[ ]: ['AccuracyWarning',
      'BDF',
      'DOP853',
      'DenseOutput',
      'IntegrationWarning',
      'LSODA',
      'OdeSolution',
      'OdeSolver',
      'RK23',
      'RK45',
      'Radau',
      '__all__',
      '__builtins__',
      '__cached__',
      '__doc__',
      '__file__',
      '__loader__',
      '__name__',
      '__package__',
      '__path__',
      '__spec__',
      '_bvp',
      '_dop',
      '_ivp',
      '_ode',
      '_odepack',
      '_quad_vec',
      '_quadpack',
      '_quadrature',
      'complex_ode',
      'cumtrapz',
      'cumulative_trapezoid',
      'dblquad',
      'fixed_quad',
      'lsoda',
      'newton_cotes',
```

```

'nquad',
'ode',
'odeint',
'odepack',
'quad',
'quad_explain',
'quad_vec',
'quadpack',
'quadrature',
'romb',
'romberg',
'simps',
'simpson',
'solve_bvp',
'solve_ivp',
'test',
'tplquad',
'trapezoid',
'trapz',
'vode']

```

```

[ ]: # Defining x and y
x = np.linspace(0, np.pi, 100)
%timeit y = np.sin(x)
y = np.sin(x)
# Compare the integrals using two methods
%timeit i1 = trapz(y, x)
%timeit i2 = simps(y, x)

print(trapz(y, x))
print(simps(y, x))

x = np.linspace(0, np.pi, 10)
y = np.sin(x)
%timeit i1 = trapz(y, x)
%timeit i2 = simps(y, x)
print(trapz(y, x))
print(simps(y, x))

```

```

1.76 µs ± 133 ns per loop (mean ± std. dev. of 7 runs, 100,000 loops each)
17.2 µs ± 872 ns per loop (mean ± std. dev. of 7 runs, 100,000 loops each)
183 µs ± 23.1 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
1.9998321638939929
1.9999999690165366
16.4 µs ± 1.12 µs per loop (mean ± std. dev. of 7 runs, 100,000 loops each)
180 µs ± 24 µs per loop (mean ± std. dev. of 7 runs, 10,000 loops each)
1.9796508112164835

```

1.9995487365804028

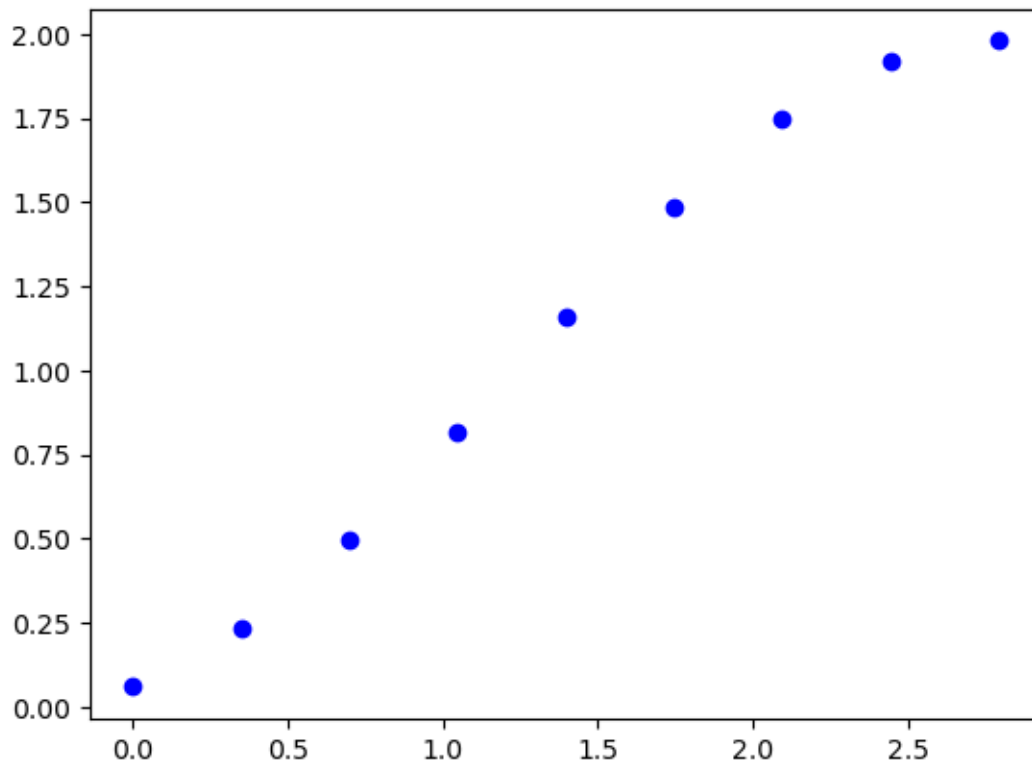
```
[ ]: # Cumulative integrale
cum = cumtrapz(np.abs(y), x)
print(len(x), type(cum), len(cum), cum)
```

```
10 <class 'numpy.ndarray'> 9 [0.05969378 0.23157515 0.4949127  0.81794403
1.16170678 1.48473811
1.74807566 1.91995704 1.97965081]
```

```
[ ]: # Cumulative integral

print('{} {}'.format(len(x), len(cumtrapz(np.abs(y), x))))
f, ax = plt.subplots()
ax.plot(x[0:-1], cumtrapz(np.abs(y), x), 'bo');
```

10 9



```
[ ]: from scipy.integrate import quad # To compute a definite integral
help(quad)
```

Help on function quad in module scipy.integrate._quadpack_py:

```
quad(func, a, b, args=(), full_output=0, epsabs=1.49e-08, epsrel=1.49e-08,
limit=50, points=None, weight=None, wvar=None, wopts=None, maxp1=50, limlst=50)
    Compute a definite integral.
```

Integrate `func` from ``a`` to ``b`` (possibly infinite interval) using a technique from the Fortran library QUADPACK.

Parameters

`func` : {function, `scipy.LowLevelCallable`}

A Python function or method to integrate. If ``func`` takes many arguments, it is integrated along the axis corresponding to the first argument.

If the user desires improved integration performance, then ``f`` may be a ``scipy.LowLevelCallable`` with one of the signatures::

```
double func(double x)
double func(double x, void *user_data)
double func(int n, double *xx)
double func(int n, double *xx, void *user_data)
```

The ``user_data`` is the data contained in the ``scipy.LowLevelCallable``. In the call forms with ``xx``, ``n`` is the length of the ``xx`` array which contains ``xx[0] == x`` and the rest of the items are numbers contained in the ``args`` argument of `quad`.

In addition, certain ctypes call signatures are supported for backward compatibility, but those should not be used in new code.

`a` : float

Lower limit of integration (use `-numpy.inf` for `-infinity`).

`b` : float

Upper limit of integration (use `numpy.inf` for `+infinity`).

`args` : tuple, optional

Extra arguments to pass to ``func``.

`full_output` : int, optional

Non-zero to return a dictionary of integration information.

If non-zero, warning messages are also suppressed and the message is appended to the output tuple.

Returns

`y` : float

The integral of `func` from ``a`` to ``b``.

`abserr` : float

An estimate of the absolute error in the result.

`infodict` : dict

A dictionary containing additional information.

message

A convergence message.

explain

Appended only with 'cos' or 'sin' weighting and infinite integration limits, it contains an explanation of the codes in `infodict['ierlst']`

Other Parameters

`epsabs` : float or int, optional

Absolute error tolerance. Default is 1.49e-8. ``quad`` tries to obtain an accuracy of `abs(i-result) <= max(epsabs, epsrel*abs(i))` where ```i``` = integral of ``func`` from ``a`` to ``b``, and ```result``` is the numerical approximation. See ``epsrel`` below.

`epsrel` : float or int, optional

Relative error tolerance. Default is 1.49e-8.
If ```epsabs <= 0```, ``epsrel`` must be greater than both 5e-29 and ```50 * (machine epsilon)```. See ``epsabs`` above.

`limit` : float or int, optional

An upper bound on the number of subintervals used in the adaptive algorithm.

`points` : (sequence of floats,ints), optional

A sequence of break points in the bounded integration interval where local difficulties of the integrand may occur (e.g., singularities, discontinuities). The sequence does not have to be sorted. Note that this option cannot be used in conjunction with ```weight```.

`weight` : float or int, optional

String indicating weighting function. Full explanation for this and the remaining arguments can be found below.

`wvar` : optional

Variables for use with weighting functions.

`wopts` : optional

Optional input for reusing Chebyshev moments.

`maxpl` : float or int, optional

An upper bound on the number of Chebyshev moments.

`limlst` : int, optional

Upper bound on the number of cycles (≥ 3) for use with a sinusoidal weighting and an infinite end-point.

See Also

`dblquad` : double integral

`tplquad` : triple integral

`nquad` : n-dimensional integrals (uses ``quad`` recursively)

`fixed_quad` : fixed-order Gaussian quadrature

`quadrature` : adaptive Gaussian quadrature

`odeint` : ODE integrator

```
ode : ODE integrator
simpson : integrator for sampled data
romb : integrator for sampled data
scipy.special : for coefficients and roots of orthogonal polynomials
```

Notes

****Extra information for quad() inputs and outputs****

If full_output is non-zero, then the third output argument (infodict) is a dictionary with entries as tabulated below. For infinite limits, the range is transformed to (0,1) and the optional outputs are given with respect to this transformed range. Let M be the input argument limit and let K be infodict['last']. The entries are:

'neval'

The number of function evaluations.

'last'

The number, K, of subintervals produced in the subdivision process.

'alist'

A rank-1 array of length M, the first K elements of which are the left end points of the subintervals in the partition of the integration range.

'blist'

A rank-1 array of length M, the first K elements of which are the right end points of the subintervals.

'rlist'

A rank-1 array of length M, the first K elements of which are the integral approximations on the subintervals.

'elist'

A rank-1 array of length M, the first K elements of which are the moduli of the absolute error estimates on the subintervals.

'iord'

A rank-1 integer array of length M, the first L elements of which are pointers to the error estimates over the subintervals with $L=K$ if $K \leq M/2+2$ or $L=M+1-K$ otherwise. Let I be the sequence `infodict['iord']` and let E be the sequence `infodict['elist']`. Then `E[I[1]], ..., E[I[L]]` forms a decreasing sequence.

If the input argument points is provided (i.e., it is not None), the following additional outputs are placed in the output dictionary. Assume the points sequence is of length P.

'pts'

A rank-1 array of length P+2 containing the integration limits

and the break points of the intervals in ascending order.
This is an array giving the subintervals over which integration
will occur.

'level'

A rank-1 integer array of length M (=limit), containing the
subdivision levels of the subintervals, i.e., if (aa,bb) is a
subinterval of ``(pts[1], pts[2])`` where ``pts[0]`` and ``pts[2]``
are adjacent elements of ``infodict['pts']``, then (aa,bb) has level 1
if ``|bb-aa| = |pts[2]-pts[1]| * 2**(-1)``.

'ndin'

A rank-1 integer array of length P+2. After the first integration
over the intervals (pts[1], pts[2]), the error estimates over some
of the intervals may have been increased artificially in order to
put their subdivision forward. This array has ones in slots
corresponding to the subintervals for which this happens.

****Weighting the integrand****

The input variables, *weight* and *wvar*, are used to weight the
integrand by a select list of functions. Different integration
methods are used to compute the integral with these weighting
functions, and these do not support specifying break points. The
possible values of weight and the corresponding weighting functions are.

``weight``	Weight function used	``wvar``
'cos'	cos(w*x)	wvar = w
'sin'	sin(w*x)	wvar = w
'alg'	$g(x) = ((x-a)**\alpha)*((b-x)**\beta)$	wvar = (alpha, beta)
'alg-loga'	$g(x)*\log(x-a)$	wvar = (alpha, beta)
'alg-logb'	$g(x)*\log(b-x)$	wvar = (alpha, beta)
'alg-log'	$g(x)*\log(x-a)*\log(b-x)$	wvar = (alpha, beta)
'cauchy'	$1/(x-c)$	wvar = c

wvar holds the parameter w, (alpha, beta), or c depending on the weight
selected. In these expressions, a and b are the integration limits.

For the 'cos' and 'sin' weighting, additional inputs and outputs are
available.

For finite integration limits, the integration is performed using a
Clenshaw-Curtis method which uses Chebyshev moments. For repeated
calculations, these moments are saved in the output dictionary:

'momcom'

The maximum level of Chebyshev moments that have been computed,

i.e., if `M_c` is `infodict['momcom']` then the moments have been computed for intervals of length `|b-a| * 2**(-l)`,
`l=0,1,...,M_c`.

`'nnlog'`

A rank-1 integer array of length `M(=limit)`, containing the subdivision levels of the subintervals, i.e., an element of this array is equal to `l` if the corresponding subinterval is `|b-a| * 2**(-l)`.

`'chebmo'`

A rank-2 array of shape `(25, maxp1)` containing the computed Chebyshev moments. These can be passed on to an integration over the same interval by passing this array as the second element of the sequence `wopts` and passing `infodict['momcom']` as the first element.

If one of the integration limits is infinite, then a Fourier integral is computed (assuming $w \neq 0$). If `full_output` is 1 and a numerical error is encountered, besides the error message attached to the output tuple, a dictionary is also appended to the output tuple which translates the error codes in the array `info['ierlst']` to English messages. The output information dictionary contains the following entries instead of `'last'`, `'alist'`, `'blist'`, `'rlist'`, and `'elist'`:

`'lst'`

The number of subintervals needed for the integration (call it `K_f`).

`'rslst'`

A rank-1 array of length `M_f=limlst`, whose first `K_f` elements contain the integral contribution over the interval `(a+(k-1)c, a+kc)` where `c = (2*floor(|w|) + 1) * pi / |w|` and `k=1,2,...,K_f`.

`'erlst'`

A rank-1 array of length `M_f` containing the error estimate corresponding to the interval in the same position in `infodict['rslist']`.

`'ierlst'`

A rank-1 integer array of length `M_f` containing an error flag corresponding to the interval in the same position in `infodict['rslist']`. See the explanation dictionary (last entry in the output tuple) for the meaning of the codes.

****Details of QUADPACK level routines****

``quad`` calls routines from the FORTRAN library QUADPACK. This section provides details on the conditions for each routine to be called and a short description of each routine. The routine called depends on ``weight``, ``points`` and the integration limits ``a`` and ``b``.

QUADPACK routine	`weight`	`points`	infinite bounds
qagse	None	No	No
qagie	None	No	Yes
qagpe	None	Yes	No
qawoe	'sin', 'cos'	No	No
qawfe	'sin', 'cos'	No	either `a` or `b`
qawse	'alg*'	No	No
qawce	'cauchy'	No	No

The following provides a short description from [1]_ for each routine.

qagse

is an integrator based on globally adaptive interval subdivision in connection with extrapolation, which will eliminate the effects of integrand singularities of several types.

qagie

handles integration over infinite intervals. The infinite range is mapped onto a finite interval and subsequently the same strategy as in ``QAGS`` is applied.

qagpe

serves the same purposes as QAGS, but also allows the user to provide explicit information about the location and type of trouble-spots i.e. the abscissae of internal singularities, discontinuities and other difficulties of the integrand function.

qawoe

is an integrator for the evaluation of

$$\int_a^b \cos(\omega x) f(x) dx$$
 or

$$\int_a^b \sin(\omega x) f(x) dx$$

over a finite interval $[a, b]$, where ω and f are specified by the user. The rule evaluation component is based on the modified Clenshaw-Curtis technique

An adaptive subdivision scheme is used in connection with an extrapolation procedure, which is a modification of that in ``QAGS`` and allows the algorithm to deal with singularities in $f(x)$.

qawfe

calculates the Fourier transform

$$\int_{-\infty}^{\infty} \cos(\omega x) f(x) dx$$
 or

$$\int_{-\infty}^{\infty} \sin(\omega x) f(x) dx$$

for user-provided ω and f . The procedure of ``QAWO`` is applied on successive finite intervals, and convergence

acceleration by means of the ϵ -algorithm is applied to the series of integral approximations.

qawse

approximate $\int_a^b w(x)f(x)dx$, with $a < b$ where $w(x) = (x-a)^\alpha(b-x)^\beta v(x)$ with $\alpha, \beta > -1$, where $v(x)$ may be one of the following functions: 1 , $\log(x-a)$, $\log(b-x)$, $\log(x-a)\log(b-x)$.

The user specifies α , β and the type of the function v . A globally adaptive subdivision strategy is applied, with modified Clenshaw-Curtis integration on those subintervals which contain a or b .

qawce

compute $\int_a^b f(x) / (x-c)dx$ where the integral must be interpreted as a Cauchy principal value integral, for user specified c and f . The strategy is globally adaptive. Modified Clenshaw-Curtis integration is used on those intervals containing the point $x = c$.

References

- .. [1] Piessens, Robert; de Doncker-Kapenga, Elise; Überhuber, Christoph W.; Kahaner, David (1983). QUADPACK: A subroutine package for automatic integration. Springer-Verlag. ISBN 978-3-540-12553-2.

Examples

Calculate $\int_0^4 x^2 dx$ and compare with an analytic result

```
>>> from scipy import integrate
>>> x2 = lambda x: x**2
>>> integrate.quad(x2, 0, 4)
(21.333333333333332, 2.3684757858670003e-13)
>>> print(4**3 / 3.) # analytical result
21.3333333333
```

Calculate $\int_0^\infty e^{-x} dx$

```
>>> invexp = lambda x: np.exp(-x)
>>> integrate.quad(invexp, 0, np.inf)
(1.0, 5.842605999138044e-11)
```

Calculate $\int_1^3 a x \, dx$ for $a = 1, 3$

```
>>> f = lambda x, a: a*x
>>> y, err = integrate.quad(f, 0, 1, args=(1,))
>>> y
0.5
>>> y, err = integrate.quad(f, 0, 1, args=(3,))
>>> y
1.5
```

Calculate $\int_0^1 x^2 + y^2 dx$ with ctypes, holding y parameter as 1::

```
testlib.c =>
    double func(int n, double args[n]){
        return args[0]*args[0] + args[1]*args[1];}
compile to library testlib.*

::

from scipy import integrate
import ctypes
lib = ctypes.CDLL('/home/.../testlib.*') #use absolute path
lib.func.restype = ctypes.c_double
lib.func.argtypes = (ctypes.c_int, ctypes.c_double)
integrate.quad(lib.func, 0, 1, (1))
#(1.3333333333333333, 1.4802973661668752e-14)
print((1.0**3/3.0 + 1.0) - (0.0**3/3.0 + 0.0)) #Analytic result
# 1.3333333333333333
```

Be aware that pulse shapes and other sharp features as compared to the size of the integration interval may not be integrated correctly using this method. A simplified example of this limitation is integrating a y-axis reflected step function with many zero values within the integrals bounds.

```
>>> y = lambda x: 1 if x<=0 else 0
>>> integrate.quad(y, -1, 1)
(1.0, 1.1102230246251565e-14)
>>> integrate.quad(y, -1, 100)
(1.0000000002199108, 1.0189464580163188e-08)
>>> integrate.quad(y, -1, 10000)
(0.0, 0.0)
```

```
[ ]: from scipy.integrate import quad # To compute a definite integral
from scipy.special import jv # Bessel function
%timeit res = quad(np.sin, 0, np.pi)
print(quad(np.sin, 0, np.pi))
```

```
#help(quad)
print(quad(lambda x: jv(2.5, x), 0, 10)) # Integrate the Bessel function of
↳ order 2.5 between 0 and 10
```

21.4 μs \pm 1.7 μs per loop (mean \pm std. dev. of 7 runs, 10,000 loops each)
 (2.0, 2.220446049250313e-14)
 (0.8209075326034347, 1.1793289815399173e-08)

We now want to evaluate:

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

```
[ ]: # We want here integrate a user-defined function (here polynome) between 0 and 1
def f(x, a, b, c):
    """ Returning a 2nd order polynome """
    return a + b * x + c * x**2
def f123(x):
    return 1 + 2 * x + 3 * x**2
def f123b(x, a=1, b=2, c=3):
    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
%timeit I = quad(f123, 0, 1)
%timeit I = quad(f123b, 0, 1)
I = quad(f, 0, 1, args=(1,2,3)) # args will send 1, 2, 3 to f
print(I)
Integ = I[0]
print(Integ)
```

5.28 μs \pm 15.3 ns per loop (mean \pm std. dev. of 7 runs, 100000 loops each)
 4.96 μs \pm 28.7 ns per loop (mean \pm std. dev. of 7 runs, 100000 loops each)
 5.18 μs \pm 19.8 ns per loop (mean \pm std. dev. of 7 runs, 100000 loops each)
 (3.0, 3.3306690738754696e-14)
 3.0

1.0.3 Interpolations

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

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

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

```
class interp1d(scipy.interpolate.polyint._Interpolator1D)
|   interp1d(x, y, kind='linear', axis=-1, copy=True, bounds_error=None,
fill_value=nan, assume_sorted=False)
|
|   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 or as an integer
|     specifying the order of the spline interpolator to use.
|     The string has to be one of 'linear', 'nearest', 'nearest-up', 'zero',
|     'slinear', 'quadratic', 'cubic', 'previous', or 'next'. 'zero',
|     'slinear', 'quadratic' and 'cubic' refer to a spline interpolation of
|     zeroth, first, second or third order; 'previous' and 'next' simply
|     return the previous or next value of the point; 'nearest-up' and
|     'nearest' differ when interpolating half-integers (e.g. 0.5, 1.5)
|     in that 'nearest-up' rounds up and 'nearest' rounds down. 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.
|
|     .. 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.
|
| Attributes
| -----
| fill_value
|
| 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
|
| Notes
| -----
| Calling `interp1d` with NaNs present in input values results in
| undefined behaviour.
|
| Input values `x` and `y` must be convertible to `float` values like
| `int` or `float`.
|
| If the values in `x` are not unique, the resulting behavior is
| undefined and specific to the choice of `kind`, i.e., changing
| `kind` will change the behavior for duplicates.
|
| 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()

```



```

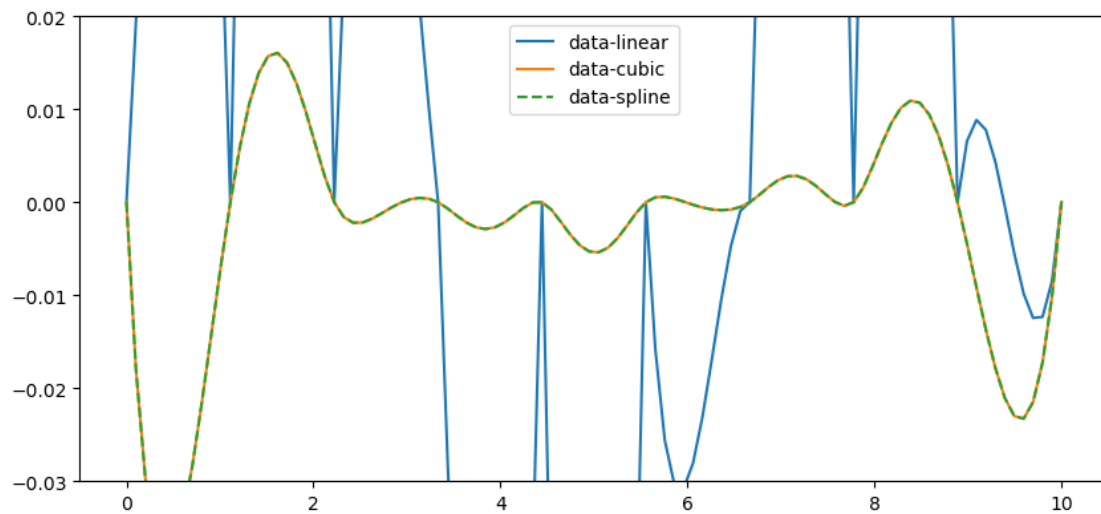
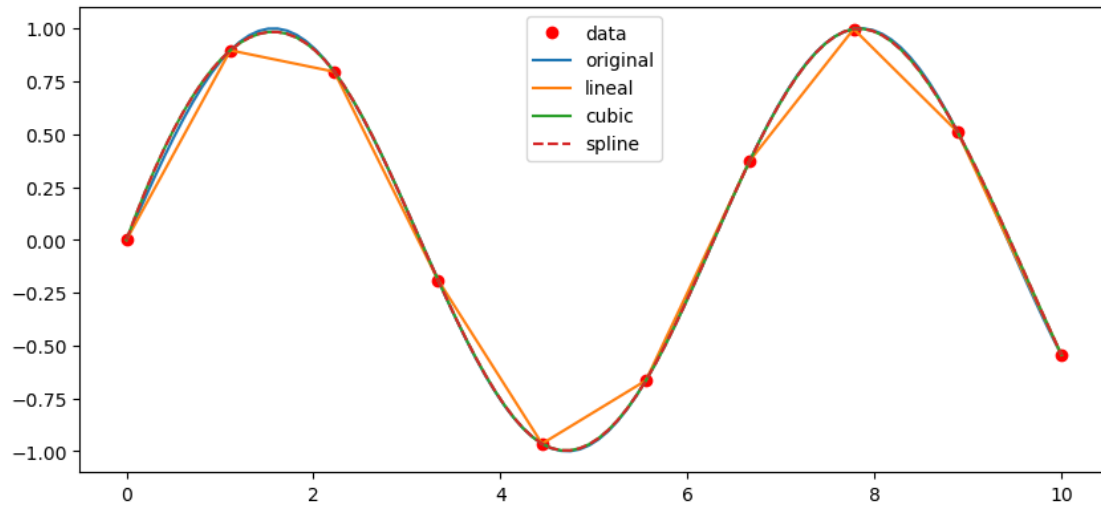
|
| Method resolution order:
|     interp1d
|     scipy.interpolate.polyint._Interpolator1D
|     builtins.object
|
| Methods defined here:
|
|     __init__(self, x, y, kind='linear', axis=-1, copy=True, bounds_error=None,
fill_value=nan, assume_sorted=False)
|         Initialize a 1-D linear interpolation class.
|
| -----
| Data descriptors defined here:
|
|     __dict__
|         dictionary for instance variables (if defined)
|
|     __weakref__
|         list of weak references to the object (if defined)
|
|     fill_value
|         The 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.
|
|         Notes
|         -----
|         Input values `x` must be convertible to `float` values like `int`
|         or `float`.
|
| -----
| Data descriptors inherited from scipy.interpolate.polyint._Interpolator1D:

```

```
|  
| dtype
```

```
[ ]: x = np.linspace(0, 10, 10)  
y = np.sin(x)  
f = interp1d(x, y) # this creates a function that can be call at any  
    ↳ interpolate point  
f2 = interp1d(x, y, kind='cubic') # The same but using cubic interpolation  
tck = splrep(x, y, s=0) # This initiate the spline interpolating function,  
    ↳ finding the B-spline representation of 1-D curve.  
# tck is a sequence of length 3 returned by `splrep` or `splprep` containing  
    ↳ the knots, coefficients, and degree of the spline.  
f3 = lambda x: splev(x, tck) # Evaluate the B-spline or its derivatives.
```

```
[ ]: # 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, yfine, label='original')  
ax1.plot(xfine, f(xfine), label='lineal')  
ax1.plot(xfine, f2(xfine), label='cubic')  
ax1.plot(xfine, f3(xfine), label='spline', ls='--')  
ax1.legend(loc=9)  
  
ax2.plot(xfine, (yfine - f(xfine)), label='data-linear')  
ax2.plot(xfine, (yfine - f2(xfine)), label='data-cubic')  
ax2.plot(xfine, (yfine - f3(xfine)), label='data-spline', ls='--')  
ax2.legend(loc='best')  
ax2.set_ylim((-0.03, 0.02));
```



```
[ ]: x0 = 3.5
print('{} {} {} {}'.format(np.sin(x0), f(x0), f2(x0), f3(x0)))
```

```
-0.35078322768961984 -0.3066303359834792 -0.34959725240218925
-0.3495972524021892
```

2D interpolation

```
[ ]: # 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
```

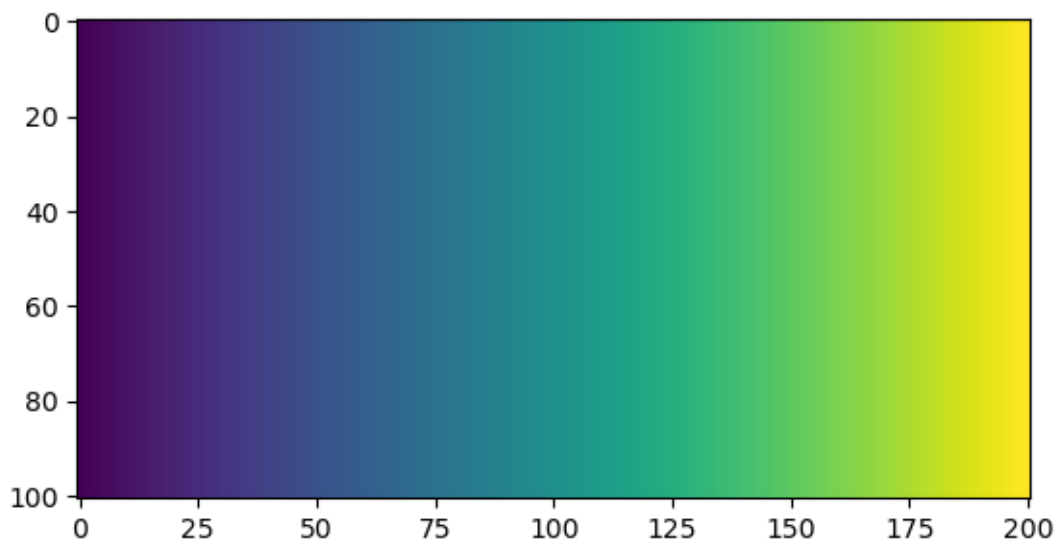
```
[ ]: # Initializing a 2D coordinate grid. Note the use of j to specify that the end
      ↪ point is included.
grid_y, grid_x = np.mgrid[0:1:101j, 0:1:201j]
```

```
[ ]: print(grid_x)
      print(grid_y)
```

```
[[0.    0.005 0.01 ... 0.99  0.995 1.    ]
 [0.    0.005 0.01 ... 0.99  0.995 1.    ]
 [0.    0.005 0.01 ... 0.99  0.995 1.    ]
 ...
 [0.    0.005 0.01 ... 0.99  0.995 1.    ]
 [0.    0.005 0.01 ... 0.99  0.995 1.    ]
 [0.    0.005 0.01 ... 0.99  0.995 1.    ]]
[[0.  0.  0.  ... 0.  0.  0.  ]
 [0.01 0.01 0.01 ... 0.01 0.01 0.01]
 [0.02 0.02 0.02 ... 0.02 0.02 0.02]
 ...
 [0.98 0.98 0.98 ... 0.98 0.98 0.98]
 [0.99 0.99 0.99 ... 0.99 0.99 0.99]
 [1.   1.   1.   ... 1.   1.   1.   ]]
```

```
[ ]: plt.imshow(grid_x)
```

```
[ ]: <matplotlib.image.AxesImage at 0x7fb41fcedac0>
```



```
[ ]: # Generating 1000 x 2 points randomly
      points = np.random.rand(1000, 2)
      print(points)
      values = func(points[:,0], points[:,1])
      print(np.min(points), np.max(points))
```

```
[[0.58285163 0.02017694]
```

```

[0.98469475 0.73882545]
[0.1508262  0.30640621]
...
[0.76712557 0.46335445]
[0.85832259 0.30865531]
[0.54425035 0.38268348]]
0.0004222369284355709 0.999759691718544

```

```

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

```

```

23.5 ms ± 1.56 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
9.94 ms ± 452 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
14.9 ms ± 476 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)

```

```

[ ]: print(np.min(values), np.max(values))

```

```

-1.3216183431172221 1.9716371839860183

```

```

[ ]: # 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))
extent = (0, 1, 0, 1)
origin = 'lower'
ax1.imshow(func(grid_x, grid_y), extent=extent, interpolation='none',
            origin=origin, vmin=-1.4, vmax=2.0)
ax1.plot(points[:,0], points[:,1], 'ko', ms=1)
ax1.set_title('Original')

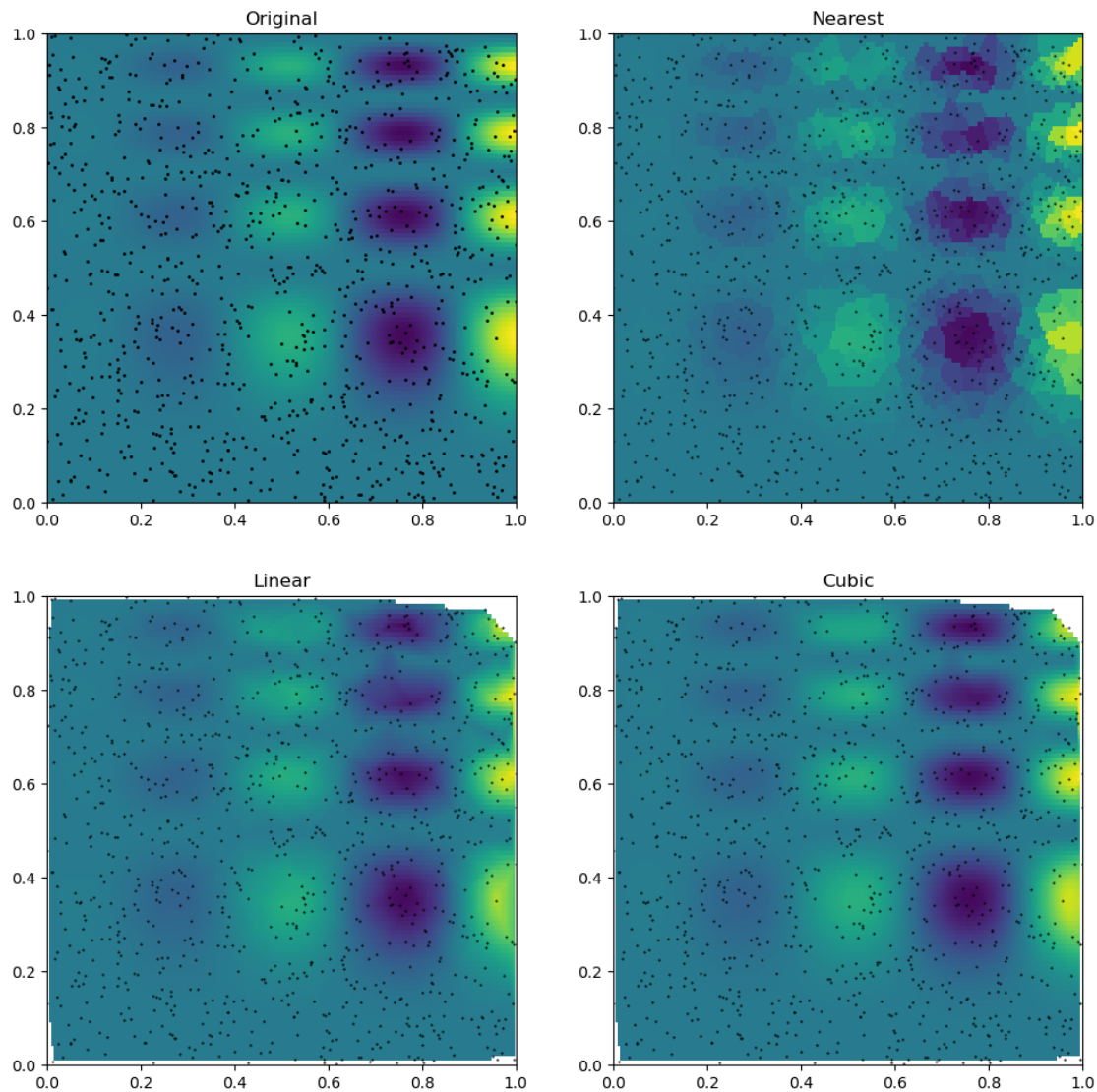
ax2.imshow(grid_z0, extent=extent, interpolation='none',
            origin=origin, vmin=-1.4, vmax=2.0)
ax2.plot(points[:,0], points[:,1], 'k.', ms=1)
ax2.set_title('Nearest')

ax3.imshow(grid_z1, extent=extent, interpolation='none',
            origin=origin, vmin=-1.4, vmax=2.0)
ax3.plot(points[:,0], points[:,1], 'k.', ms=1)
ax3.set_title('Linear')

ax4.imshow(grid_z2, extent=extent, interpolation='none',
            origin=origin, vmin=-1.4, vmax=2.0)
ax4.plot(points[:,0], points[:,1], 'k.', ms=1)

```

```
ax4.set_title('Cubic');
```



```
[ ]: print(grid_z0[10,10], grid_z1[10,10], grid_z2[10,10])
```

```
0.00033012283816004335 0.0006611507622104852 0.0006647105471534465
```

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: <https://docs.scipy.org/doc/scipy/tutorial/linalg.html>

1.0.5 Data fit

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

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

Help on function curve_fit in module scipy.optimize._minpack_py:

```
curve_fit(f, xdata, ydata, p0=None, sigma=None, absolute_sigma=False,
check_finite=True, bounds=(-inf, inf), method=None, jac=None, *,
full_output=False, **kwargs)
```

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 : array_like or object

The independent variable where the data is measured.

Should usually be an M-length sequence or an (k,M)-shaped array for functions with k predictors, but can actually be any object.

ydata : array_like

The dependent data, a length M array - nominally ``f(xdata, ...)``.

p0 : array_like, optional

Initial guess for the parameters (length N). 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 or MxM array, optional

Determines the uncertainty in `ydata`. If we define residuals as ``r = ydata - f(xdata, *popt)`` , then the interpretation of `sigma` depends on its number of dimensions:

- A 1-D `sigma` should contain values of standard deviations of errors in `ydata`. In this case, the optimized function is ``chisq = sum((r / sigma) ** 2)``.

- A 2-D `sigma` should contain the covariance matrix of errors in `ydata`. In this case, the optimized function is ``chisq = r.T @ inv(sigma) @ r``.

.. versionadded:: 0.19

None (default) is equivalent of 1-D `sigma` filled with ones.

`absolute_sigma` : bool, optional
 If True, ``sigma`` is used in an absolute sense and the estimated parameter covariance ``pcov`` reflects these absolute values.

If False (default), only the relative magnitudes of the ``sigma`` values matter.

The returned parameter covariance matrix ``pcov`` is based on scaling ``sigma`` by a constant factor. This constant is set by demanding that the reduced ``chisq`` for the optimal parameters ``popt`` when using the `*scaled*` ``sigma`` equals unity. In other words, ``sigma`` is scaled to match the sample variance of the residuals after the fit. Default is False.

Mathematically,
``pcov(absolute_sigma=False) = pcov(absolute_sigma=True) * chisq(popt)/(M-N)``

`check_finite` : bool, optional
 If True, check that the input arrays do not contain nans or 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 parameters. 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

`jac` : callable, string or None, optional
 Function with signature ``jac(x, ...)`` which computes the Jacobian matrix of the model function with respect to parameters as a dense array_like structure. It will be scaled according to provided ``sigma``. If None (default), the Jacobian will be estimated numerically. String keywords for 'trf' and 'dogbox' methods can be used to select a finite difference scheme, see ``least_squares``.

.. versionadded:: 0.18

`full_output` : boolean, optional
 If True, this function returns additional information: ``infodict``,


```

`mesg`, and `ier`.

.. versionadded:: 1.9
**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
    residuals of ``f(xdata, *popt) - ydata`` is minimized.
pcov : 2-D 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.
infodict : dict (returned only if `full_output` is True)
    a dictionary of optional outputs with the keys:

    ``nfev``
        The number of function calls. Methods 'trf' and 'dogbox' do not
        count function calls for numerical Jacobian approximation,
        as opposed to 'lm' method.
    ``fvec``
        The function values evaluated at the solution.
    ``fjac``
        A permutation of the R matrix of a QR
        factorization of the final approximate
        Jacobian matrix, stored column wise.
        Together with ipvt, the covariance of the
        estimate can be approximated.
        Method 'lm' only provides this information.
    ``ipvt``
        An integer array of length N which defines
        a permutation matrix, p, such that
        fjac*p = q*r, where r is upper triangular
        with diagonal elements of nonincreasing
        magnitude. Column j of p is column ipvt(j)
        of the identity matrix.
        Method 'lm' only provides this information.

```

```

    ``qtf``
        The vector (transpose(q) * fvec).
        Method 'lm' only provides this information.

    .. versionadded:: 1.9
    msg : str (returned only if `full_output` is True)
        A string message giving information about the solution.

    .. versionadded:: 1.9
    ier : int (returned only if `full_output` is True)
        An integer flag. If it is equal to 1, 2, 3 or 4, the solution was
        found. Otherwise, the solution was not found. In either case, the
        optional output variable `msg` gives more information.

    .. versionadded:: 1.9

Raises
-----
ValueError
    if either `ydata` or `xdata` contain NaNs, or if incompatible options
    are used.

RuntimeError
    if the least-squares minimization fails.

OptimizeWarning
    if covariance of the parameters can not be estimated.

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

Notes
-----
Users should ensure that inputs `xdata`, `ydata`, and the output of `f`
are ``float64``, or else the optimization may return incorrect results.

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 matplotlib.pyplot as plt
>>> from scipy.optimize import curve_fit
```

```
>>> def func(x, a, b, c):
...     return a * np.exp(-b * x) + c
```

Define the data to be fit with some noise:

```
>>> xdata = np.linspace(0, 4, 50)
>>> y = func(xdata, 2.5, 1.3, 0.5)
>>> rng = np.random.default_rng()
>>> y_noise = 0.2 * rng.normal(size=xdata.size)
>>> ydata = y + y_noise
>>> plt.plot(xdata, ydata, 'b-', label='data')
```

Fit for the parameters a, b, c of the function `func`:

```
>>> popt, pcov = curve_fit(func, xdata, ydata)
>>> popt
array([2.56274217, 1.37268521, 0.47427475])
>>> plt.plot(xdata, func(xdata, *popt), 'r-',
...          label='fit: a=%5.3f, b=%5.3f, c=%5.3f' % tuple(popt))
```

Constrain the optimization to the region of `0 <= a <= 3`,
`0 <= b <= 1` and `0 <= c <= 0.5`:

```
>>> popt, pcov = curve_fit(func, xdata, ydata, bounds=(0, [3., 1., 0.5]))
>>> popt
array([2.43736712, 1.          , 0.34463856])
>>> plt.plot(xdata, func(xdata, *popt), 'g--',
...          label='fit: a=%5.3f, b=%5.3f, c=%5.3f' % tuple(popt))

>>> plt.xlabel('x')
>>> plt.ylabel('y')
>>> plt.legend()
>>> plt.show()
```

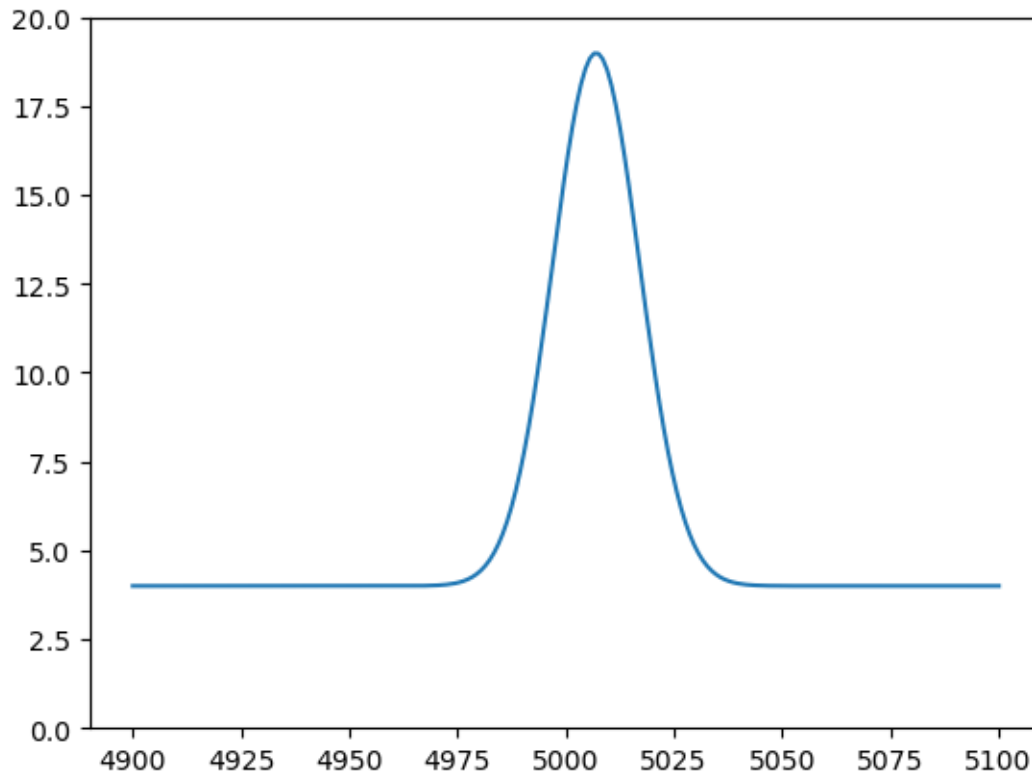
```
[ ]: def gauss(x, A, B, C, S):
      # This is a gaussian function.
      return A + B*np.exp(-1 * (x - C)**2 / (2 * S**2))
```

```
[ ]: # We define the parameters used to generate the signal (gaussian at lambda=5007)
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
f1 = gauss(lam, A, B, Lam0, Sigma)
f, ax = plt.subplots()
ax.plot(lam, f1)
ax.set_ylim(0,20);

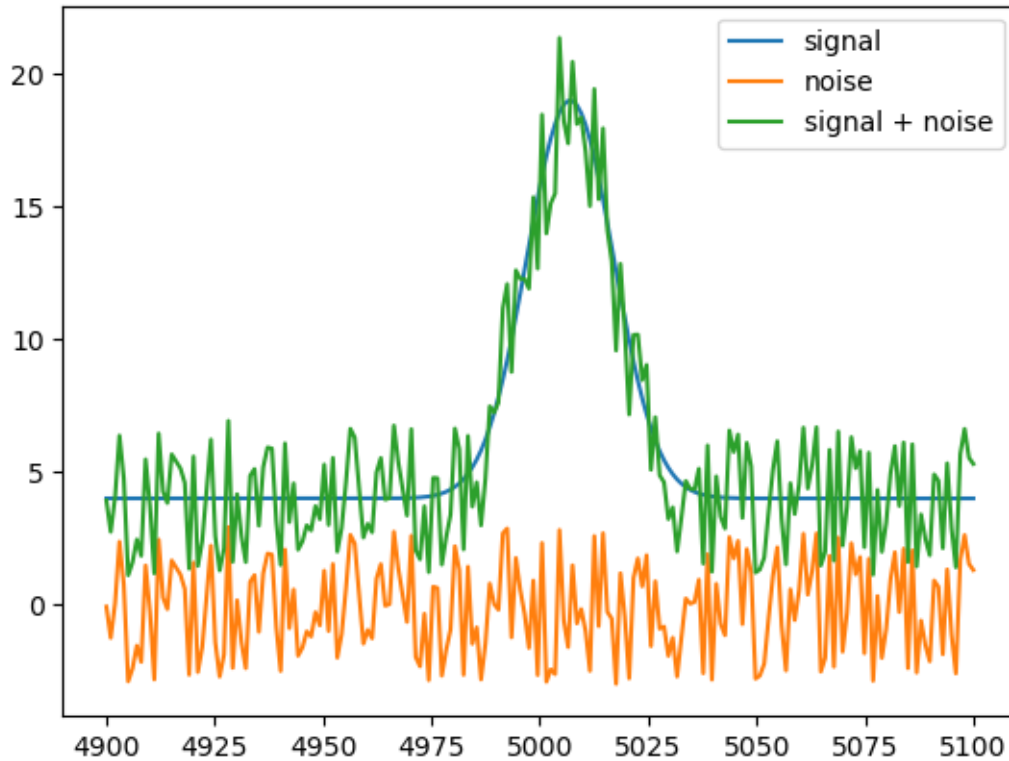
```



```

[ ]: SN = 5. # Signal/Noise
noise = B / SN * (np.random.rand(N_lam)*2 - 1)
f12 = f1 + noise
f, ax = plt.subplots()
ax.plot(lam, f1, label='signal')
ax.plot(lam, noise, label='noise')
ax.plot(lam, f12, label='signal + noise')
ax.legend(loc='best');

```



```
[ ]: # 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 (the
↳ same on each pixel of the spectrum)
```

```
[ ]: # fitting the noisy data with the gaussian function, using the initial guess
↳ and the errors
fit, covar = curve_fit(gauss, lam, fl2, [A_i, B_i, Lam0_i, Sigma_i], error)
print('{0:.2f} {1:5.2f} {2:.2f} {3:5.2f} {4:5.2f}'.format(A_i, B_i, Lam0_i,
↳ Sigma_i, B_i*Sigma_i))
print('{0:.2f} {1:5.2f} {2:.2f} {3:5.2f} {4:5.2f}'.format(A, B, Lam0, Sigma,
↳ B*Sigma))
print('{0[0]:.2f} {0[1]:5.2f} {0[2]:5.2f} {0[3]:.2f} {1:5.2f}'.format(fit,
↳ fit[1]*fit[3]))
```

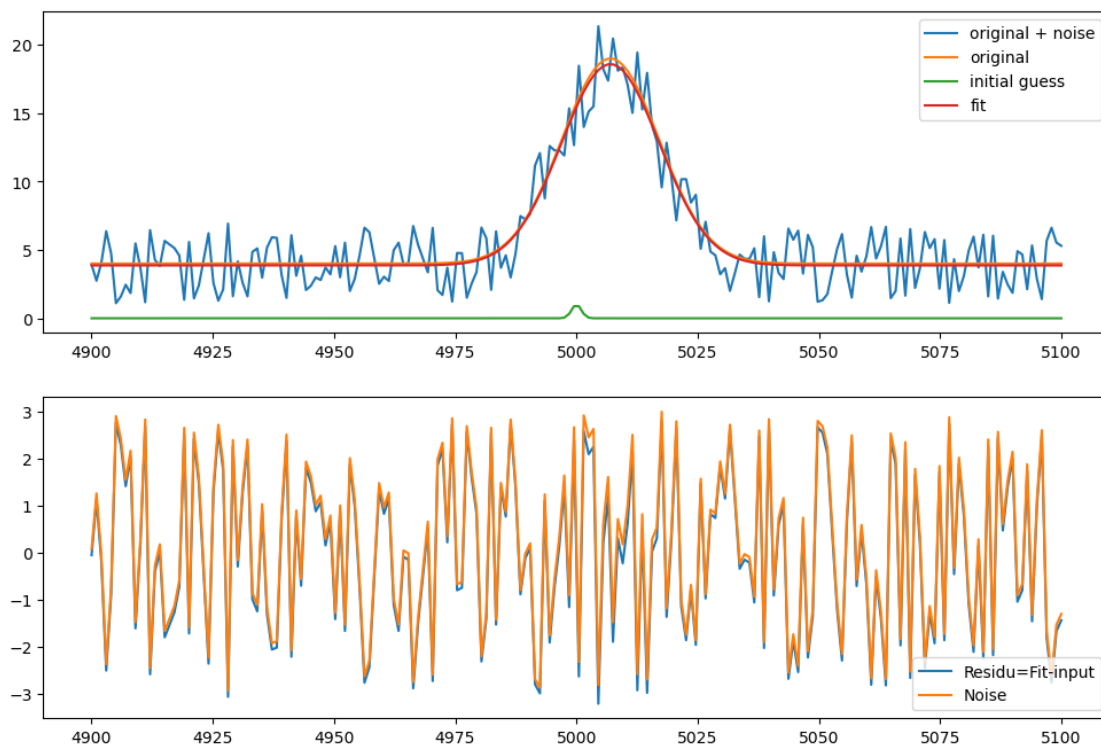
```
0.00 1.00 5000.00 1.00 1.00
4.00 15.00 5007.00 10.00 150.00
3.86 14.72 5007.00 10.10 148.68
```

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

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

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

ax2.plot(lam, fl_fit - fl2, label='Residu=Fit-input')
ax2.plot(lam, -noise, label='Noise')
ax2.legend();
```



```
[ ]: # 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))
```

```
375.99424119465004
371.86873765195986
372.6950491068127
```

```
[ ]: khi_sq = (((fl2-fl_fit) / error)**2).sum() # The problem here is to determine
      ↳ the error...
      khi_sq_red = khi_sq / (len(lam) - 4 - 1) # reduced khi_sq = khi_sq / (N -
      ↳ free_params - 1)
      print('khi^2={}, khi^2_reduced={}'.format(khi_sq, khi_sq_red))
```

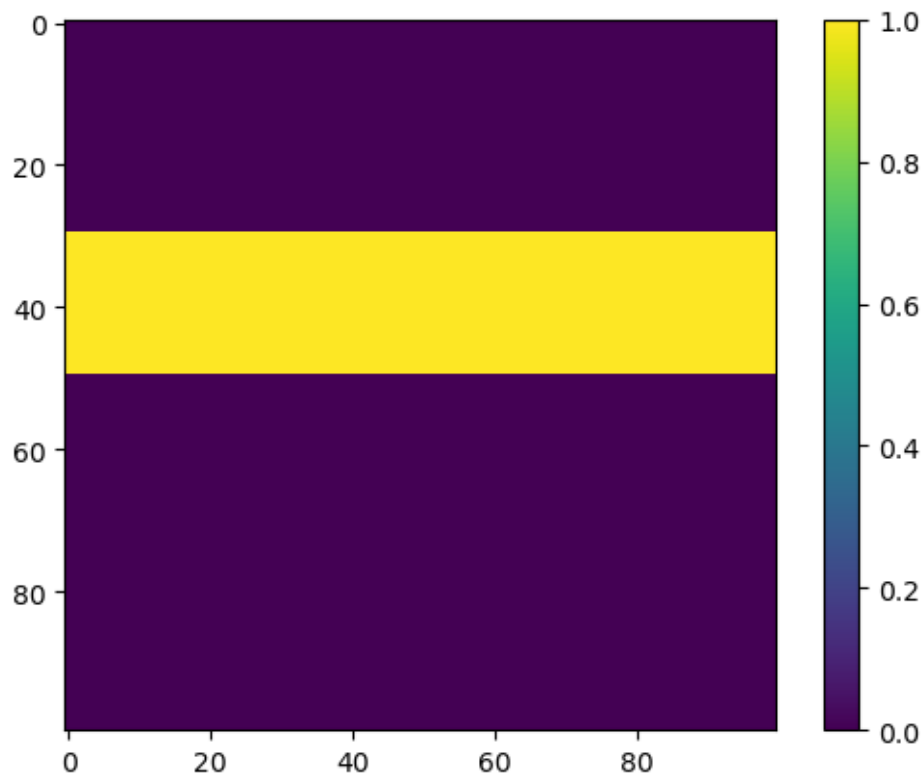
khi^2=260.59689695712905, khi^2_reduced=1.3363943433698926

1.0.6 Convolution

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

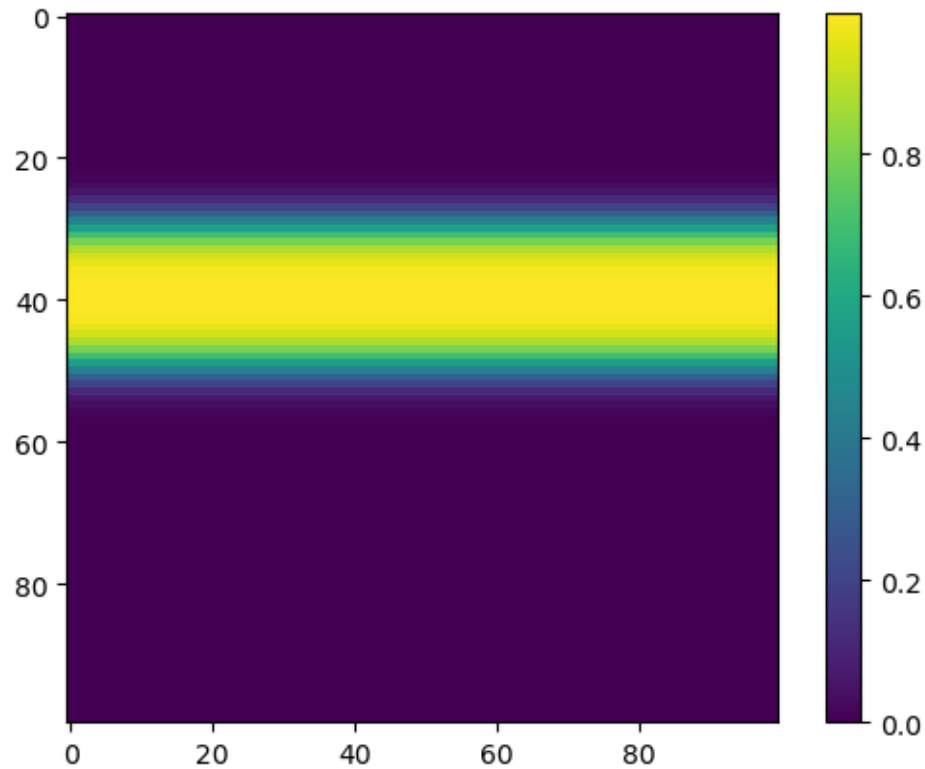
```
[ ]: # Let's define an image representing a long slit of width 10 pixels
      slit = np.zeros((100, 100))
      slit[30:50, :] = 1
```

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

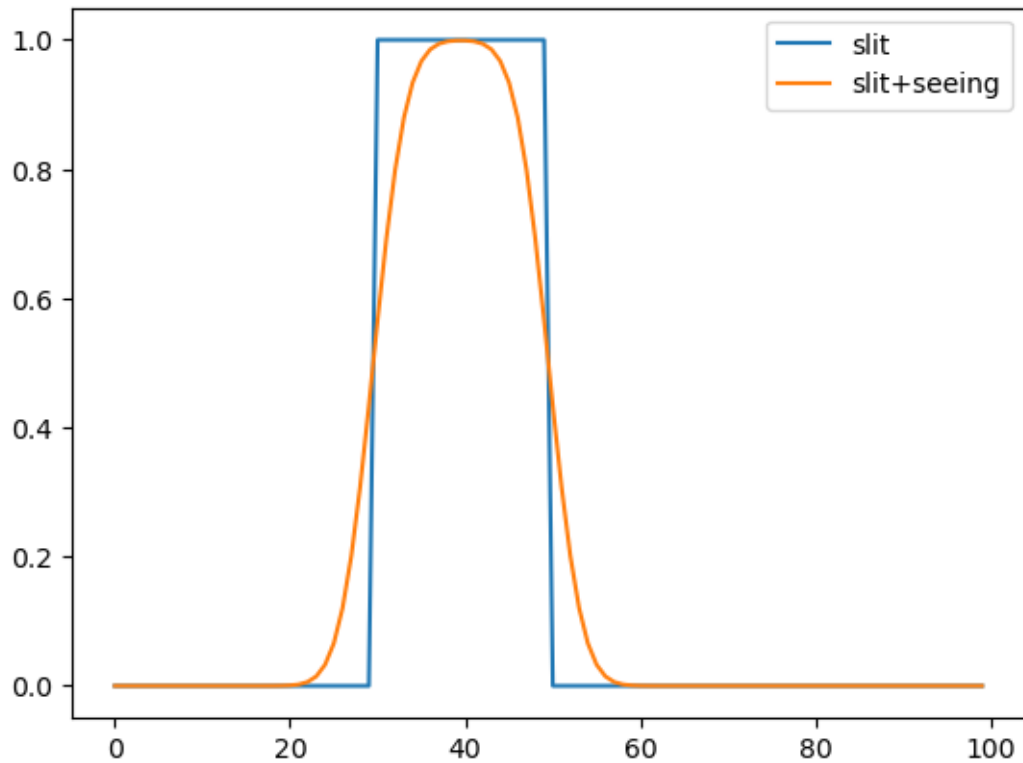


```
[ ]: # This is the routine to apply a gaussian convolution
      from scipy.ndimage import gaussian_filter
```

```
[ ]: slit_seeing = gaussian_filter(slit, 3) # Convolve with a gaussian, 3 is the
      ↪ standard deviation in pixels
      plt.imshow(slit_seeing)
      plt.colorbar();
```



```
[ ]: 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');
```

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

```
20.0 20.0
```

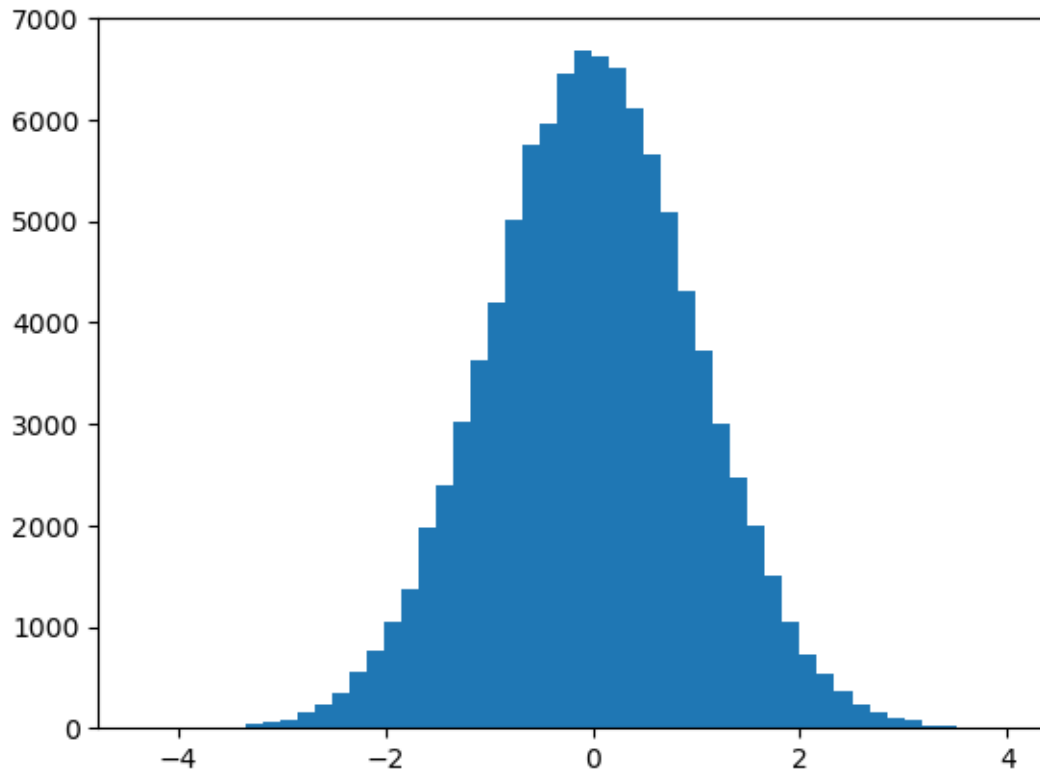
1.0.7 Quantiles

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

```
[ ]: #help(mquantiles)
```

```
[ ]: data = np.random.randn(100000)
```

```
[ ]: f, ax = plt.subplots()
      ax.hist(data, bins=50);
```



```
[ ]: mquantiles(data, [0.16, 0.5, 0.84]) # should return something close to -1, 0, 1
      ↪ (the stv of the normal distribution)
```

```
[ ]: array([-0.99458906,  0.00134218,  0.9971658  ])
```

```
[ ]: 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.]])
```

```
[ ]: mq = mquantiles(data, axis=0, limit=(0, 50))
      print(mq)
```

```
[[19.2  14.6   1.45]
 [40.   37.5   2.5 ]]
```

```
[42.8  40.05  3.55]]
```

1.0.8 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>