CHAPTER 5

Scipy : high-level scientific computing

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Scipy

The `scipy` package contains various toolboxes dedicated to common issues in scientific computing. Its different submodules correspond to different applications, such as interpolation, integration, optimization, image processing, statistics, special functions, etc.
`scipy` can be compared to other standard scientific-computing libraries, such as the GSL (GNU Scientific Library for C and C++), or Matlab's toolboxes. `scipy` is the core package for scientific routines in Python; it is meant to operate efficiently on `numpy` arrays, so that numpy and scipy work hand in hand.
Before implementing a routine, it is worth checking if the desired data processing is not already implemented in Scipy. As non-professional programmers, scientists often tend to **re-invent the wheel**, which leads to buggy, non-optimal, difficult-to-share and unmaintainable code. By contrast, `Scipy`'s routines are optimized and tested, and should therefore be used when possible.

Chapters contents

⚠ This tutorial is far from an introduction to numerical computing. As enumerating the different submodules and functions in scipy would be very boring, we concentrate instead on a few examples to give a general idea of how to use `scipy` for scientific computing.

`scipy` is composed of task-specific sub-modules:

scipy.cluster	Vector quantization / Kmeans
scipy.constants	Physical and mathematical constants
scipy.fftpack	Fourier transform
scipy.integrate	Integration routines
scipy.interpolate	Interpolation
scipy.io	Data input and output
scipy.linalg	Linear algebra routines
scipy.ndimage	n-dimensional image package
scipy.odr	Orthogonal distance regression
scipy.optimize	Optimization
scipy.signal	Signal processing
scipy.sparse	Sparse matrices
scipy.spatial	Spatial data structures and algorithms
scipy.special	Any special mathematical functions
scipy.stats	Statistics

They all depend on numpy, but are mostly independent of each other. The standard way of importing Numpy and these Scipy modules is:

```
>>> import numpy as np
>>> from scipy import stats  # same for other sub-modules
```

The main scipy namespace mostly contains functions that are really numpy functions (try scipy.cos is np.cos). Those are exposed for historical reasons only; there's usually no reason to use import scipy in your code.

5.1 File input/output: scipy.io

- Loading and saving matlab files:

```
>>> from scipy import io as spio
>>> a = np.ones((3, 3))
>>> spio.savemat('file.mat', {'a': a}) # savemat expects a dictionary
>>> data = spio.loadmat('file.mat', struct_as_record=True)
>>> data['a']
array([[ 1.,  1.,  1.],
       [ 1.,  1.,  1.],
       [ 1.,  1.,  1.]])
```

- Reading images:

```
>>> from scipy import misc
>>> misc.imread('fname.png')
array(...)
>>> # Matplotlib also has a similar function
>>> import matplotlib.pyplot as plt
>>> plt.imread('fname.png')
array(...)
```

See also:

- Load text files: numpy.loadtxt()/numpy.savetxt()
- Clever loading of text/csv files: numpy.genfromtxt()/numpy.recfromcsv()
- Fast and efficient, but numpy-specific, binary format: numpy.save()/numpy.load()

5.2 Special functions: scipy.special

Special functions are transcendental functions. The docstring of the scipy.special module is well-written, so we won't list all functions here. Frequently used ones are:

- Bessel function, such as scipy.special.jn() (nth integer order Bessel function)
- Elliptic function (scipy.special.ellipj() for the Jacobian elliptic function, ...)
- Gamma function: scipy.special.gamma(), also note scipy.special.gammaln() which will give the log of Gamma to a higher numerical precision.
- Erf, the area under a Gaussian curve: scipy.special.erf()

5.3 Linear algebra operations: scipy.linalg

The scipy.linalg module provides standard linear algebra operations, relying on an underlying efficient implementation (BLAS, LAPACK).

- The scipy.linalg.det() function computes the determinant of a square matrix:

```
>>> from scipy import linalg
>>> arr = np.array([[1, 2],
...                 [3, 4]])
>>> linalg.det(arr)
-2.0
>>> arr = np.array([[3, 2],
...                 [6, 4]])
>>> linalg.det(arr)
0.0
>>> linalg.det(np.ones((3, 4)))
Traceback (most recent call last):
...
ValueError: expected square matrix
Traceback (most recent call last):
...
ValueError: expected square matrix
```

- The scipy.linalg.inv() function computes the inverse of a square matrix:

```
>>> arr = np.array([[1, 2],
...                 [3, 4]])
>>> iarr = linalg.inv(arr)
>>> iarr
array([[-2. ,  1. ],
       [ 1.5, -0.5]])
>>> np.allclose(np.dot(arr, iarr), np.eye(2))
True
```

Finally computing the inverse of a singular matrix (its determinant is zero) will raise LinAlgError:

```
>>> arr = np.array([[3, 2],
...                 [6, 4]])
>>> linalg.inv(arr)
Traceback (most recent call last):
...
...LinAlgError: singular matrix
Traceback (most recent call last):
...
...LinAlgError: singular matrix
```

- More advanced operations are available, for example singular-value decomposition (SVD):

```
>>> arr = np.arange(9).reshape((3, 3)) + np.diag([1, 0, 1])
>>> uarr, spec, vharr = linalg.svd(arr)
```

The resulting array spectrum is:

```
>>> spec
array([ 14.88982544,   0.45294236,   0.29654967])
```

The original matrix can be re-composed by matrix multiplication of the outputs of `svd` with `np.dot`:

```
>>> sarr = np.diag(spec)
>>> svd_mat = uarr.dot(sarr).dot(vharr)
>>> np.allclose(svd_mat, arr)
True
```

SVD is commonly used in statistics and signal processing. Many other standard decompositions (QR, LU, Cholesky, Schur), as well as solvers for linear systems, are available in `scipy.linalg`.

5.4 Fast Fourier transforms: `scipy.fftpack`

The `scipy.fftpack` module allows to compute fast Fourier transforms. As an illustration, a (noisy) input signal may look like:

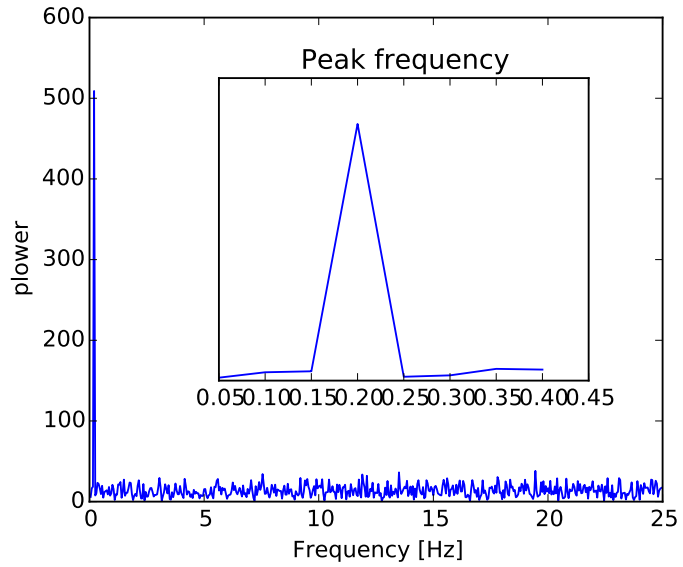
```
>>> time_step = 0.02
>>> period = 5.
>>> time_vec = np.arange(0, 20, time_step)
>>> sig = np.sin(2 * np.pi / period * time_vec) + \
...       0.5 * np.random.randn(time_vec.size)
```

The observer doesn't know the signal frequency, only the sampling time step of the signal `sig`. The signal is supposed to come from a real function so the Fourier transform will be symmetric. The `scipy.fftpack.fftfreq()` function will generate the sampling frequencies and `scipy.fftpack.fft()` will compute the fast Fourier transform:

```
>>> from scipy import fftpack
>>> sample_freq = fftpack.fftfreq(sig.size, d=time_step)
>>> sig_fft = fftpack.fft(sig)
```

Because the resulting power is symmetric, only the positive part of the spectrum needs to be used for finding the frequency:

```
>>> pidxs = np.where(sample_freq > 0)
>>> freqs = sample_freq[pidxs]
>>> power = np.abs(sig_fft)[pidxs]
```



The signal frequency can be found by:

```
>>> freq = freqs[power.argmax()]
>>> np.allclose(freq, 1./period)  # check that correct freq is found
True
```

Now the high-frequency noise will be removed from the Fourier transformed signal:

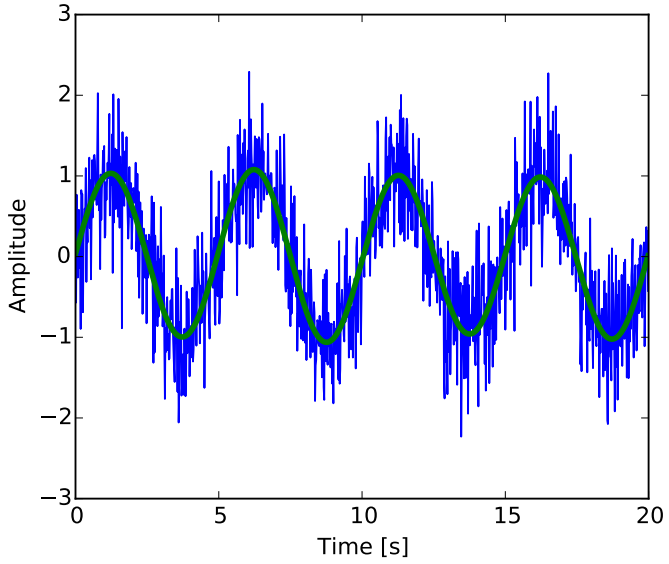
```
>>> sig_fft[np.abs(sample_freq) > freq] = 0
```

The resulting filtered signal can be computed by the `scipy.fftpack.ifft()` function:

```
>>> main_sig = fftpack.ifft(sig_fft)
```

The result can be viewed with:

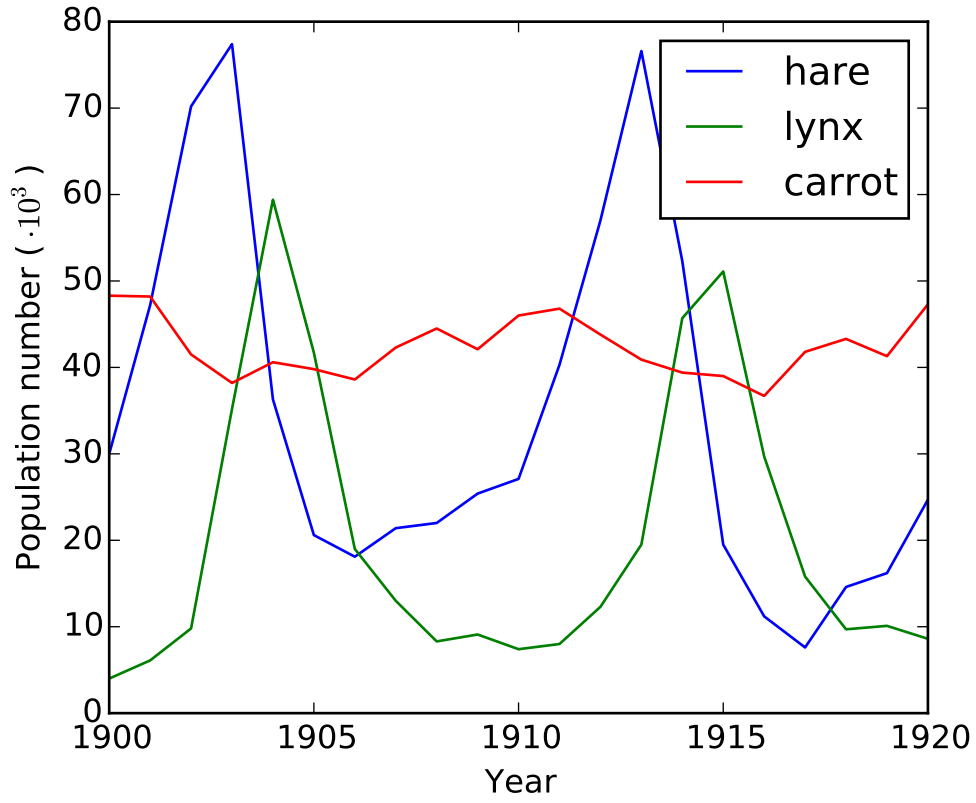
```
>>> import pylab as plt
>>> plt.figure()
<matplotlib.figure.Figure object at 0x...>
>>> plt.plot(time_vec, sig)
[<matplotlib.lines.Line2D object at 0x...>]
>>> plt.plot(time_vec, main_sig, linewidth=3)
[<matplotlib.lines.Line2D object at 0x...>]
>>> plt.xlabel('Time [s]')
<matplotlib.text.Text object at 0x...>
>>> plt.ylabel('Amplitude')
<matplotlib.text.Text object at 0x...>
```

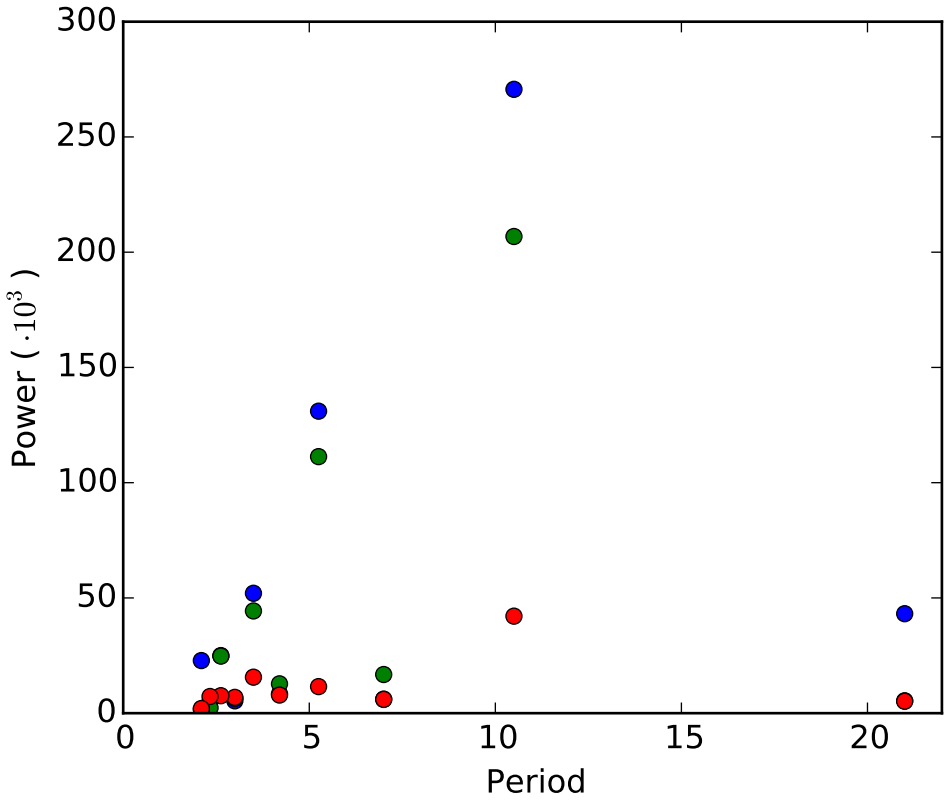


`numpy.fft`

Numpy also has an implementation of FFT (`numpy.fft`). However, in general the scipy one should be preferred, as it uses more efficient underlying implementations.

Worked example: Crude periodicity finding



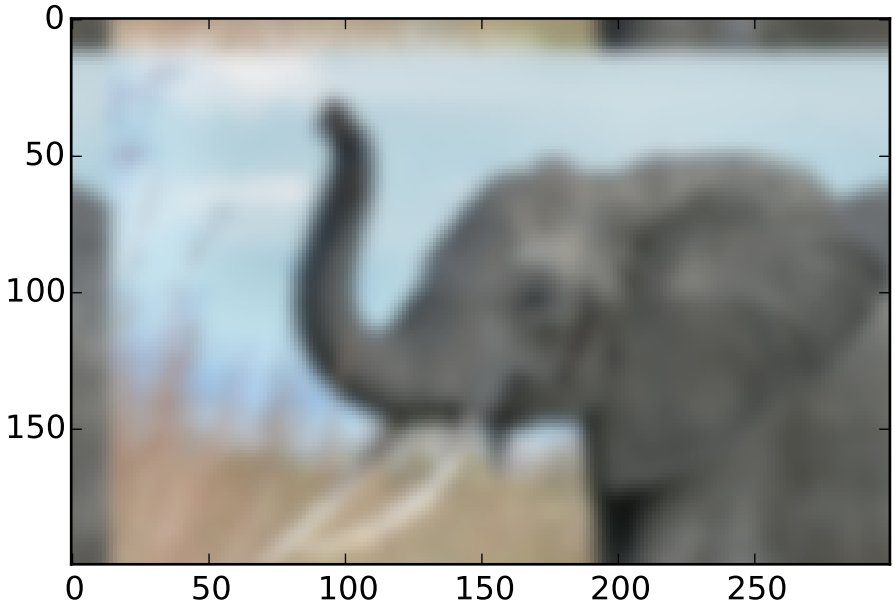


Worked example: Gaussian image blur

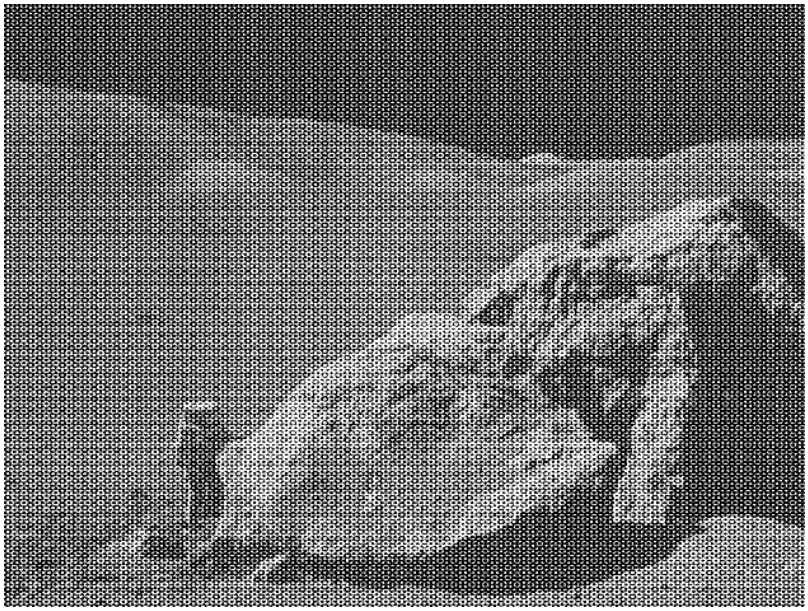
Convolution:

$$f_1(t) = \int dt' \, K(t - t') f_0(t')$$

$$\tilde{f}_1(\omega) = \tilde{K}(\omega) \tilde{f}_0(\omega)$$



Exercise: Denoise moon landing image



1. Examine the provided image moonlanding.png, which is heavily contaminated with periodic noise. In this exercise, we aim to clean up the noise using the Fast Fourier Transform.
2. Load the image using `pylab.imread()`.
3. Find and use the 2-D FFT function in `scipy.fftpack`, and plot the spectrum (Fourier transform of) the image. Do you have any trouble visualising the spectrum? If so, why?
4. The spectrum consists of high and low frequency components. The noise is contained in the high-frequency part of the spectrum, so set some of those components to zero (use array slicing).
5. Apply the inverse Fourier transform to see the resulting image.

5.5 Optimization and fit: `scipy.optimize`

Optimization is the problem of finding a numerical solution to a minimization or equality.

The `scipy.optimize` module provides useful algorithms for function minimization (scalar or multi-dimensional), curve fitting and root finding.

```
>>> from scipy import optimize
```

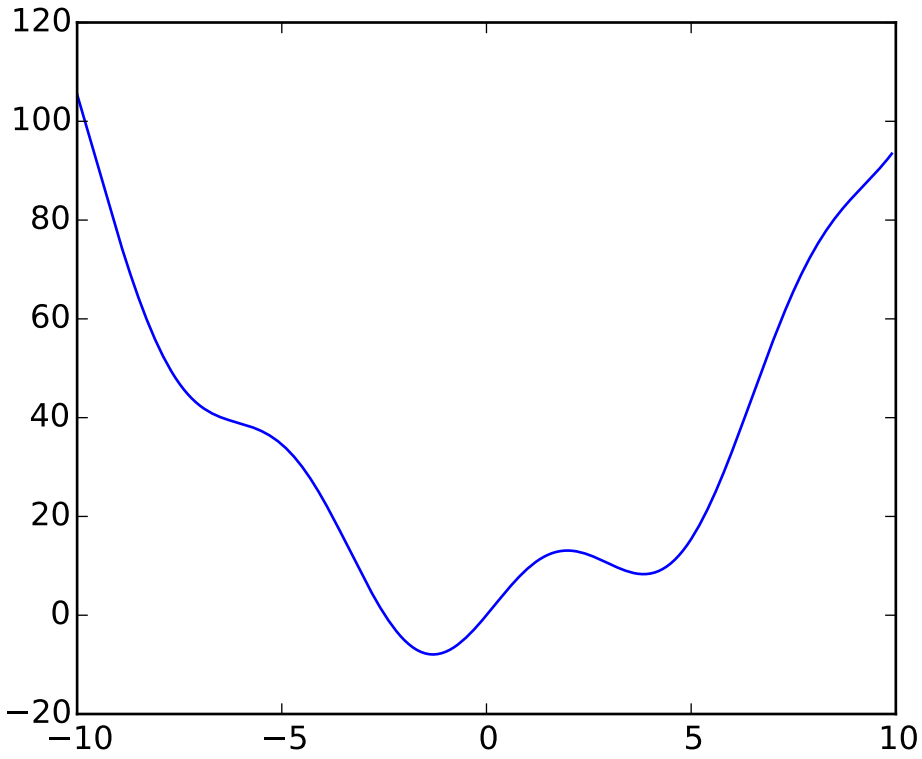
Finding the minimum of a scalar function

Let's define the following function:

```
>>> def f(x):
...     return x**2 + 10*np.sin(x)
```

and plot it:

```
>>> x = np.arange(-10, 10, 0.1)
>>> plt.plot(x, f(x))
>>> plt.show()
```



This function has a global minimum around -1.3 and a local minimum around 3.8.

The general and efficient way to find a minimum for this function is to conduct a gradient descent starting from a given initial point. The BFGS algorithm is a good way of doing this:

```
>>> optimize.fmin_bfgs(f, 0)
Optimization terminated successfully.
         Current function value: -7.945823
         Iterations: 5
         Function evaluations: 24
         Gradient evaluations: 8
array([-1.30644003])
```

A possible issue with this approach is that, if the function has local minima the algorithm may find these local minima instead of the global minimum depending on the initial point:

```
>>> optimize.fmin_bfgs(f, 3, disp=0)
array([ 3.83746663])
```

If we don't know the neighborhood of the global minimum to choose the initial point, we need to resort to costlier global optimization. To find the global minimum, we use `scipy.optimize.basinhopping()` (which combines a local optimizer with stochastic sampling of starting points for the local optimizer):

New in version 0.12.0: basinhopping was added in version 0.12.0 of Scipy

```
>>> optimize.basinhopping(f, 0)
                    nfev: 1725
 minimization_failures: 0
                     fun: -7.9458233756152845
                       x: array([-1.30644001])
                 message: ['requested number of basinhopping iterations completed successfully']
                    njev: 575
                     nit: 100
```

Another available (but much less efficient) global optimizer is `scipy.optimize.brute()` (brute force optimization on a grid). More efficient algorithms for different classes of global optimization problems exist, but this is out of the scope of `scipy`. Some useful packages for global optimization are OpenOpt, IPOPT, PyGMO and PyEvolve.

`scipy` used to contain the routine `anneal`, it has been deprecated since SciPy 0.14.0 and removed in SciPy 0.16.0.

To find the local minimum, let's constraint the variable to the interval `(0, 10)` using `scipy.optimize.fminbound()`:

```
>>> xmin_local = optimize.fminbound(f, 0, 10)
>>> xmin_local
3.8374671...
```

Finding minima of function is discussed in more details in the advanced chapter: *Mathematical optimization: finding minima of functions*.

Finding the roots of a scalar function

To find a root, i.e. a point where `f(x) = 0`, of the function `f` above we can use for example `scipy.optimize.fsolve()`:

```
>>> root = optimize.fsolve(f, 1)  # our initial guess is 1
>>> root
array([ 0.])
```

Note that only one root is found. Inspecting the plot of `f` reveals that there is a second root around -2.5. We find the exact value of it by adjusting our initial guess:

```
>>> root2 = optimize.fsolve(f, -2.5)
>>> root2
array([-2.47948183])
```

Curve fitting

Suppose we have data sampled from `f` with some noise:

```
>>> xdata = np.linspace(-10, 10, num=20)
>>> ydata = f(xdata) + np.random.randn(xdata.size)
```

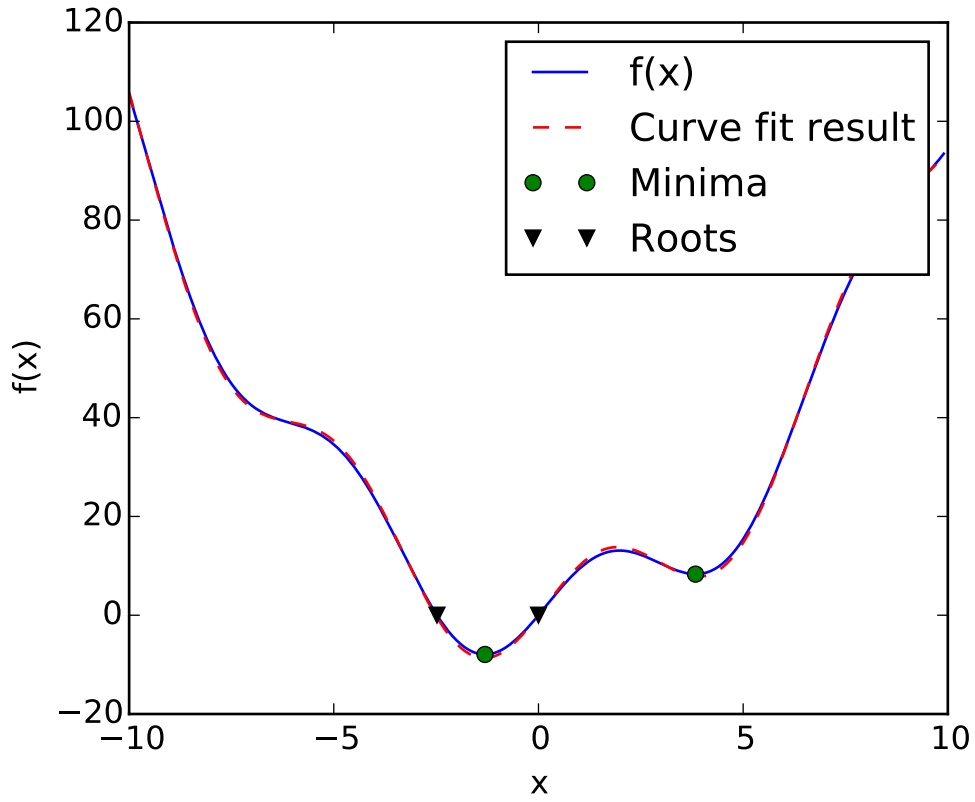
Now if we know the functional form of the function from which the samples were drawn (`x^2 + sin(x)` in this case) but not the amplitudes of the terms, we can find those by least squares curve fitting. First we have to define the function to fit:

```
>>> def f2(x, a, b):
...     return a*x**2 + b*np.sin(x)
```

Then we can use `scipy.optimize.curve_fit()` to find `a` and `b`:

```
>>> guess = [2, 2]
>>> params, params_covariance = optimize.curve_fit(f2, xdata, ydata, guess)
>>> params
array([  0.99667386,  10.17808313])
```

Now we have found the minima and roots of `f` and used curve fitting on it, we put all those resuls together in a single plot:



In Scipy >= 0.11 unified interfaces to all minimization and root finding algorithms are available: `scipy.optimize.minimize()`, `scipy.optimize.minimize_scalar()` and `scipy.optimize.root()`. They allow comparing various algorithms easily through the `method` keyword.

You can find algorithms with the same functionalities for multi-dimensional problems in `scipy.optimize`.

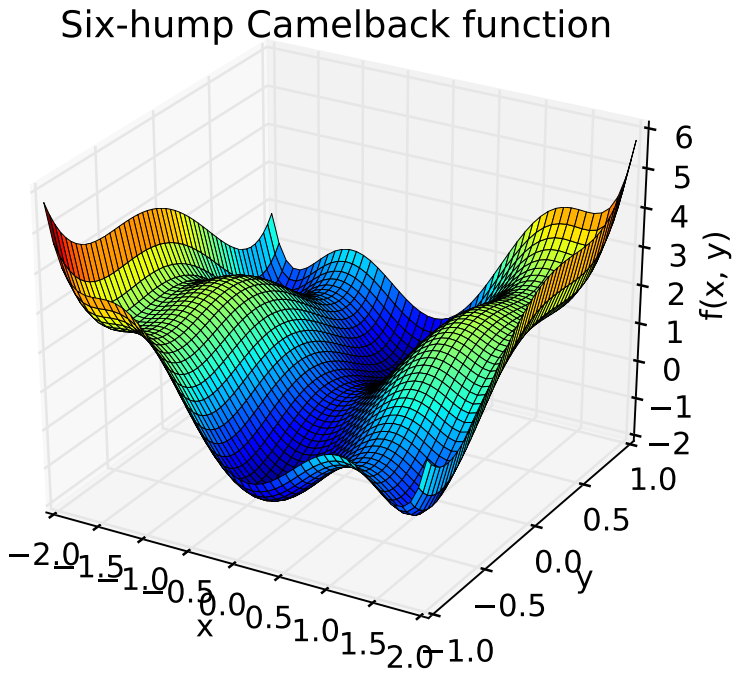
Exercise: Curve fitting of temperature data

The temperature extremes in Alaska for each month, starting in January, are given by (in degrees Celcius):

```
max:  17,  19,  21,  28,  33,  38, 37,  37,  31,  23,  19,  18
min: -62, -59, -56, -46, -32, -18, -9, -13, -25, -46, -52, -58
```

1. Plot these temperature extremes.
2. Define a function that can describe min and max temperatures. Hint: this function has to have a period of 1 year. Hint: include a time offset.
3. Fit this function to the data with `scipy.optimize.curve_fit()`.
4. Plot the result. Is the fit reasonable? If not, why?
5. Is the time offset for min and max temperatures the same within the fit accuracy?

Exercise: 2-D minimization



The six-hump camelback function

$$f(x,y) = (4 - 2.1x^2 + \frac{x^4}{3})x^2 + xy + (4y^2 - 4)y^2$$

has multiple global and local minima. Find the global minima of this function.
Hints:

- Variables can be restricted to `-2 < x < 2` and `-1 < y < 1`.
- Use `numpy.meshgrid()` and `pylab.imshow()` to find visually the regions.
- Use `scipy.optimize.fmin_bfgs()` or another multi-dimensional minimizer.

How many global minima are there, and what is the function value at those points? What happens for an initial guess of `(x, y) = (0, 0)`?

See the summary exercise on *Non linear least squares curve fitting: application to point extraction in topographical lidar data* for another, more advanced example.

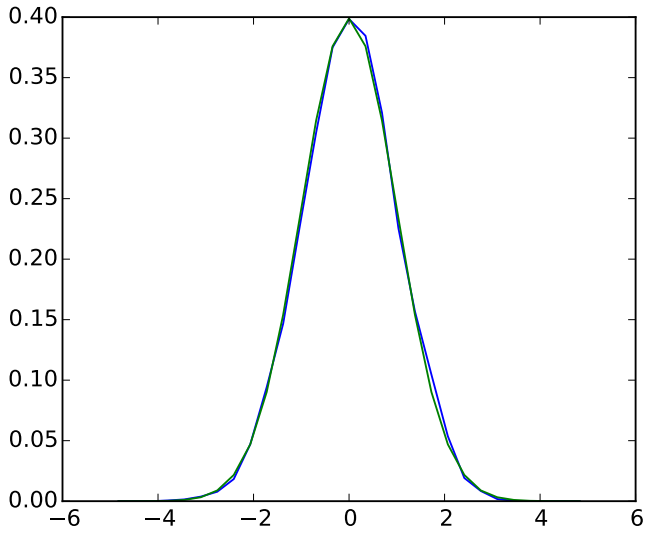
5.6 Statistics and random numbers: `scipy.stats`

The module `scipy.stats` contains statistical tools and probabilistic descriptions of random processes. Random number generators for various random process can be found in `numpy.random`.

5.6.1 Histogram and probability density function

Given observations of a random process, their histogram is an estimator of the random process's PDF (probability density function):

```
>>> a = np.random.normal(size=1000)
>>> bins = np.arange(-4, 5)
>>> bins
array([-4, -3, -2, -1,  0,  1,  2,  3,  4])
>>> histogram = np.histogram(a, bins=bins, normed=True)[0]
>>> bins = 0.5*(bins[1:] + bins[:-1])
>>> bins
array([-3.5, -2.5, -1.5, -0.5,  0.5,  1.5,  2.5,  3.5])
>>> from scipy import stats
>>> b = stats.norm.pdf(bins)  # norm is a distribution

>>> plt.plot(bins, histogram)
[<matplotlib.lines.Line2D object at ...>]
>>> plt.plot(bins, b)
[<matplotlib.lines.Line2D object at ...>]
```



If we know that the random process belongs to a given family of random processes, such as normal processes, we can do a maximum-likelihood fit of the observations to estimate the parameters of the underlying distribution. Here we fit a normal process to the observed data:

```
>>> loc, std = stats.norm.fit(a)
>>> loc
0.0314345570...
>>> std
0.9778613090...
```

Exercise: Probability distributions

Generate 1000 random variates from a gamma distribution with a shape parameter of 1, then plot a histogram from those samples. Can you plot the pdf on top (it should match)?
Extra: the distributions have a number of useful methods. Explore them by reading the docstring or by using IPython tab completion. Can you find the shape parameter of 1 back by using the `fit` method on your random variates?

5.6.2 Percentiles

The median is the value with half of the observations below, and half above:

```
>>> np.median(a)
0.04041769593...
```

It is also called the percentile 50, because 50% of the observation are below it:

```
>>> stats.scoreatpercentile(a, 50)
0.0404176959...
```

Similarly, we can calculate the percentile 90:

```
>>> stats.scoreatpercentile(a, 90)
1.3185699120...
```

The percentile is an estimator of the CDF: cumulative distribution function.

5.6.3 Statistical tests

A statistical test is a decision indicator. For instance, if we have two sets of observations, that we assume are generated from Gaussian processes, we can use a T-test to decide whether the two sets of observations are significantly different:

```
>>> a = np.random.normal(0, 1, size=100)
>>> b = np.random.normal(1, 1, size=10)
>>> stats.ttest_ind(a, b)
(array(-3.177574054...), 0.0019370639...)
```

The resulting output is composed of:

- The T statistic value: it is a number the sign of which is proportional to the difference between the two random processes and the magnitude is related to the significance of this difference.
- the *p value*: the probability of both processes being identical. If it is close to 1, the two process are almost certainly identical. The closer it is to zero, the more likely it is that the processes have different means.

See also:

The chapter on *statistics* introduces much more elaborate tools for statistical testing and statistical data loading and visualization outside of scipy.

5.7 Interpolation: `scipy.interpolate`

The `scipy.interpolate` is useful for fitting a function from experimental data and thus evaluating points where no measure exists. The module is based on the FITPACK Fortran subroutines from the netlib project.

By imagining experimental data close to a sine function:

```
>>> measured_time = np.linspace(0, 1, 10)
>>> noise = (np.random.random(10)*2 - 1) * 1e-1
>>> measures = np.sin(2 * np.pi * measured_time) + noise
```

The `scipy.interpolate.interp1d` class can build a linear interpolation function:

```
>>> from scipy.interpolate import interp1d
>>> linear_interp = interp1d(measured_time, measures)
```

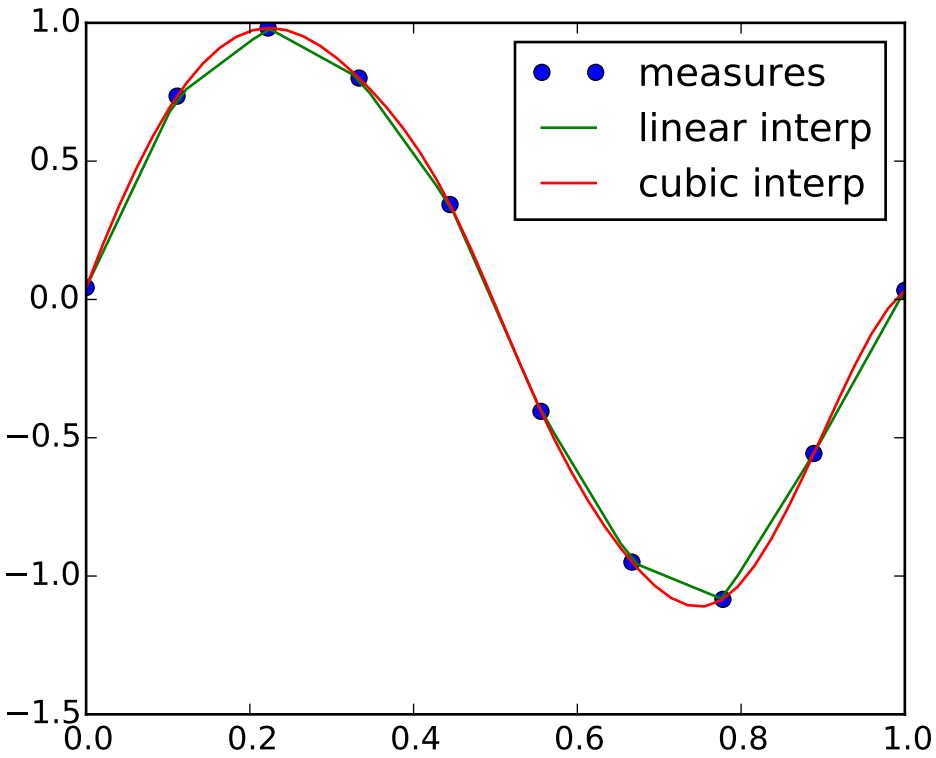
Then the `scipy.interpolate.linear_interp` instance needs to be evaluated at the time of interest:

```
>>> computed_time = np.linspace(0, 1, 50)
>>> linear_results = linear_interp(computed_time)
```

A cubic interpolation can also be selected by providing the `kind` optional keyword argument:

```
>>> cubic_interp = interp1d(measured_time, measures, kind='cubic')
>>> cubic_results = cubic_interp(computed_time)
```

The results are now gathered on the following Matplotlib figure:



`scipy.interpolate.interp2d` is similar to `scipy.interpolate.interp1d`, but for 2-D arrays. Note that for the `interp` family, the computed time must stay within the measured time range. See the summary exercise on *Maximum wind speed prediction at the Sprogø station* for a more advance spline interpolation example.

5.8 Numerical integration: `scipy.integrate`

The most generic integration routine is `scipy.integrate.quad()`:

```
>>> from scipy.integrate import quad
>>> res, err = quad(np.sin, 0, np.pi/2)
>>> np.allclose(res, 1)
True
>>> np.allclose(err, 1 - res)
True
```

Others integration schemes are available with `fixed_quad`, `quadrature`, `romberg`.

`scipy.integrate` also features routines for integrating Ordinary Differential Equations (ODE). In particular, `scipy.integrate.odeint()` is a general-purpose integrator using LSODA (Livermore Solver for Ordinary Differential equations with Automatic method switching for stiff and non-stiff problems), see the ODEPACK Fortran library for more details.

`odeint` solves first-order ODE systems of the form:

```
dy/dt = rhs(y1, y2, .., t0,...)
```

As an introduction, let us solve the ODE `dy/dt = -2y` between `t = 0..4`, with the initial condition `y(t=0) = 1`. First the function computing the derivative of the position needs to be defined:

```
>>> def calc_derivative(ypos, time, counter_arr):
...     counter_arr += 1
...     return -2 * ypos
...
```

An extra argument `counter_arr` has been added to illustrate that the function may be called several times for a single time step, until solver convergence. The counter array is defined as:

```
>>> counter = np.zeros((1,), dtype=np.uint16)
```

The trajectory will now be computed:

```
>>> from scipy.integrate import odeint
>>> time_vec = np.linspace(0, 4, 40)
>>> yvec, info = odeint(calc_derivative, 1, time_vec,
...                     args=(counter,), full_output=True)
```

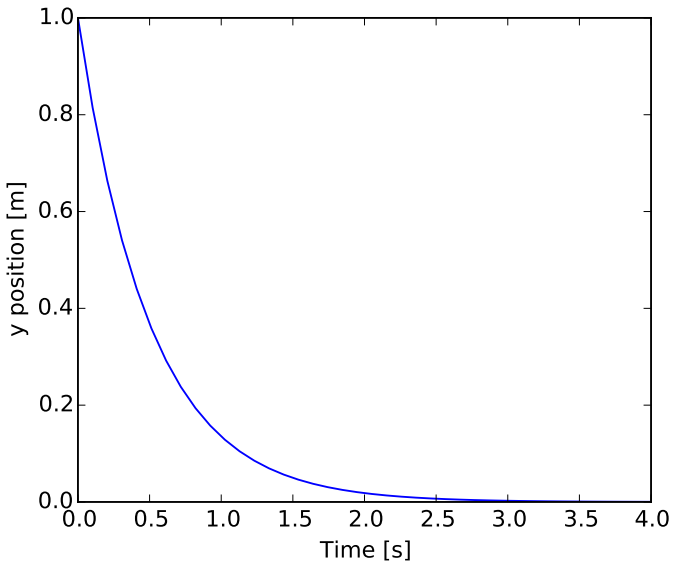
Thus the derivative function has been called more than 40 times (which was the number of time steps):

```
>>> counter
array([129], dtype=uint16)
```

and the cumulative number of iterations for each of the 10 first time steps can be obtained by:

```
>>> info['nfe'][:10]
array([31, 35, 43, 49, 53, 57, 59, 63, 65, 69], dtype=int32)
```

Note that the solver requires more iterations for the first time step. The solution `yvec` for the trajectory can now be plotted:



Another example with `scipy.integrate.odeint()` will be a damped spring-mass oscillator (2nd order oscillator). The position of a mass attached to a spring obeys the 2nd order ODE `y'' + 2 eps wo y' + wo^2 y = 0` with `wo^2 = k/m` with `k` the spring constant, `m` the mass and `eps=c/(2 m wo)` with `c` the damping coefficient. For this example, we choose the parameters as:

```
>>> mass = 0.5  # kg
>>> kspring = 4  # N/m
>>> cviscous = 0.4  # N s/m
```

so the system will be underdamped, because:

```
>>> eps = cviscous / (2 * mass * np.sqrt(kspring/mass))
>>> eps < 1
True
```

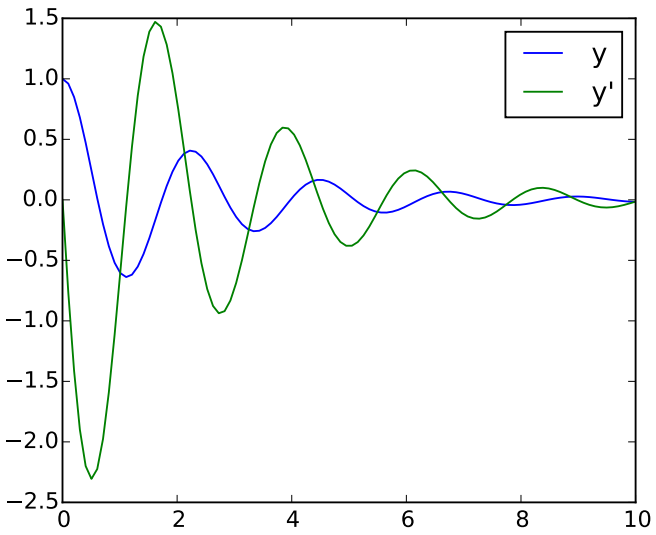
For the `scipy.integrate.odeint()` solver the 2nd order equation needs to be transformed in a system of two first-order equations for the vector `Y=(y, y')`. It will be convenient to define `nu = 2 eps * wo = c / m` and `om = wo^2 = k/m`:

```
>>> nu_coef = cviscous / mass
>>> om_coef = kspring / mass
```

Thus the function will calculate the velocity and acceleration by:

```
>>> def calc_deri(yvec, time, nuc, omc):
...     return (yvec[1], -nuc * yvec[1] - omc * yvec[0])
...
>>> time_vec = np.linspace(0, 10, 100)
>>> yarr = odeint(calc_deri, (1, 0), time_vec, args=(nu_coef, om_coef))
```

The final position and velocity are shown on the following Matplotlib figure:



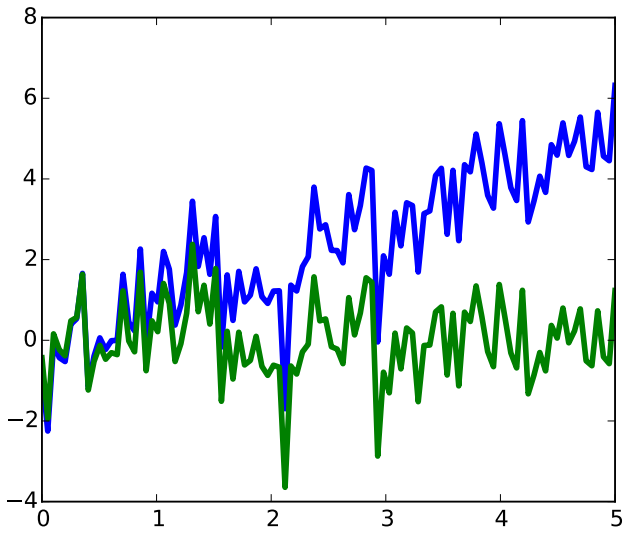
There is no Partial Differential Equations (PDE) solver in Scipy. Some Python packages for solving PDE's are available, such as fipy or SfePy.

5.9 Signal processing: `scipy.signal`

```
>>> from scipy import signal
```

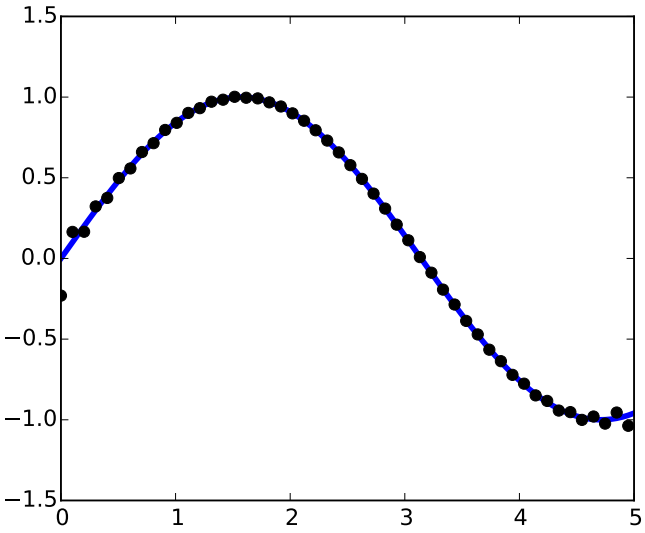
- `scipy.signal.detrend()`: remove linear trend from signal:

```
>>> t = np.linspace(0, 5, 100)
>>> x = t + np.random.normal(size=100)

>>> plt.plot(t, x, linewidth=3)
[<matplotlib.lines.Line2D object at ...>]
>>> plt.plot(t, signal.detrend(x), linewidth=3)
[<matplotlib.lines.Line2D object at ...>]
```



- `scipy.signal.resample()`: resample a signal to `n` points using FFT.

```
>>> t = np.linspace(0, 5, 100)
>>> x = np.sin(t)

>>> plt.plot(t, x, linewidth=3)
[<matplotlib.lines.Line2D object at ...>]
>>> plt.plot(t[::2], signal.resample(x, 50), 'ko')
[<matplotlib.lines.Line2D object at ...>]
```



Notice how on the side of the window the resampling is less accurate and has a rippling effect.

- `scipy.signal` has many window functions: `scipy.signal.hamming()`, `scipy.signal.bartlett()`, `scipy.signal.blackman()`...
- `scipy.signal` has filtering (median filter `scipy.signal.medfilt()`, Wiener `scipy.signal.wiener()`), but we will discuss this in the image section.

5.10 Image processing: scipy.ndimage

The submodule dedicated to image processing in scipy is scipy.ndimage.

```
>>> from scipy import ndimage
```

Image processing routines may be sorted according to the category of processing they perform.

5.10.1 Geometrical transformations on images

Changing orientation, resolution, ..

```
>>> from scipy import misc
>>> face = misc.face(gray=True)
>>> shifted_face = ndimage.shift(face, (50, 50))
>>> shifted_face2 = ndimage.shift(face, (50, 50), mode='nearest')
>>> rotated_face = ndimage.rotate(face, 30)
>>> cropped_face = face[50:-50, 50:-50]
>>> zoomed_face = ndimage.zoom(face, 2)
>>> zoomed_face.shape
(1536, 2048)
```

```
>>> plt.subplot(151)
<matplotlib.axes._subplots.AxesSubplot object at 0x...>

>>> plt.imshow(shifted_face, cmap=plt.cm.gray)
<matplotlib.image.AxesImage object at 0x...>

>>> plt.axis('off')
(-0.5, 1023.5, 767.5, -0.5)

>>> # etc.
```

5.10.2 Image filtering

```
>>> from scipy import misc
>>> face = misc.face(gray=True)
>>> face = face[:512, -512:]  # crop out square on right
>>> import numpy as np
>>> noisy_face = np.copy(face).astype(np.float)
>>> noisy_face += face.std() * 0.5 * np.random.standard_normal(face.shape)
>>> blurred_face = ndimage.gaussian_filter(noisy_face, sigma=3)
>>> median_face = ndimage.median_filter(noisy_face, size=5)
>>> from scipy import signal
>>> wiener_face = signal.wiener(noisy_face, (5, 5))
```

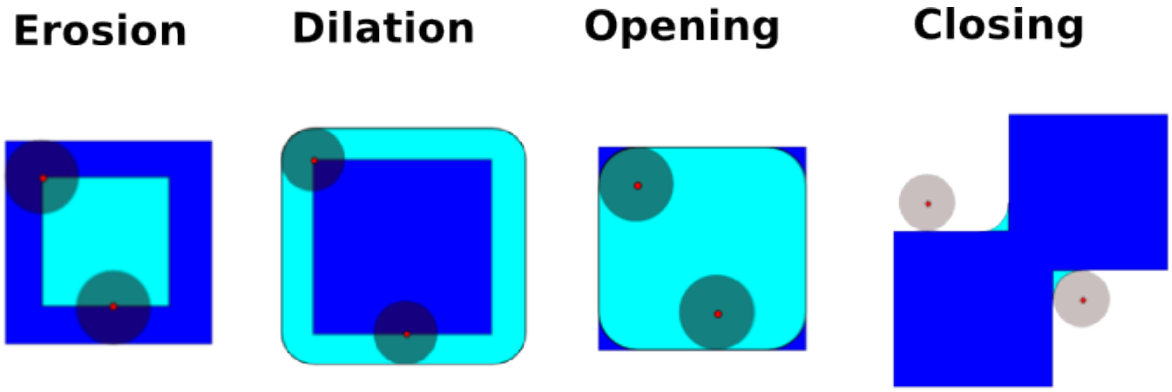
Many other filters in scipy.ndimage.filters and scipy.signal can be applied to images.

Exercise

Compare histograms for the different filtered images.

5.10.3 Mathematical morphology

Mathematical morphology is a mathematical theory that stems from set theory. It characterizes and transforms geometrical structures. Binary (black and white) images, in particular, can be transformed using this theory: the sets to be transformed are the sets of neighboring non-zero-valued pixels. The theory was also extended to gray-valued images.



Elementary mathematical-morphology operations use a *structuring element* in order to modify other geometrical structures.

Let us first generate a structuring element

```
>>> el = ndimage.generate_binary_structure(2, 1)
>>> el
array([[False, True, False],
       [...True, True, True],
       [False, True, False]], dtype=bool)
>>> el.astype(np.int)
array([[0, 1, 0],
       [1, 1, 1],
       [0, 1, 0]])
```

- **Erosion**

```
>>> a = np.zeros((7, 7), dtype=np.int)
>>> a[1:6, 2:5] = 1
>>> a
array([[0, 0, 0, 0, 0, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 0, 0, 0, 0, 0]])
>>> ndimage.binary_erosion(a).astype(a.dtype)
array([[0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0],
       [0, 0, 0, 1, 0, 0, 0],
```

```
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0]])
>>> #Erosion removes objects smaller than the structure
>>> ndimage.binary_erosion(a, structure=np.ones((5,5))).astype(a.dtype)
array([[0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0]])
```

- **Dilation**

```
>>> a = np.zeros((5, 5))
>>> a[2, 2] = 1
>>> a
array([[ 0.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  1.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.]])
>>> ndimage.binary_dilation(a).astype(a.dtype)
array([[ 0.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  1.,  0.,  0.],
       [ 0.,  1.,  1.,  1.,  0.],
       [ 0.,  0.,  1.,  0.,  0.],
       [ 0.,  0.,  0.,  0.,  0.]])
```

- **Opening**

```
>>> a = np.zeros((5, 5), dtype=np.int)
>>> a[1:4, 1:4] = 1
>>> a[4, 4] = 1
>>> a
array([[0, 0, 0, 0, 0],
       [0, 1, 1, 1, 0],
       [0, 1, 1, 1, 0],
       [0, 1, 1, 1, 0],
       [0, 0, 0, 0, 1]])
>>> # Opening removes small objects
>>> ndimage.binary_opening(a, structure=np.ones((3, 3))).astype(np.int)
array([[0, 0, 0, 0, 0],
       [0, 1, 1, 1, 0],
       [0, 1, 1, 1, 0],
       [0, 1, 1, 1, 0],
       [0, 0, 0, 0, 0]])
>>> # Opening can also smooth corners
>>> ndimage.binary_opening(a).astype(np.int)
array([[0, 0, 0, 0, 0],
       [0, 0, 1, 0, 0],
       [0, 1, 1, 1, 0],
       [0, 0, 1, 0, 0],
       [0, 0, 0, 0, 0]])
```

- **Closing:** `ndimage.binary_closing`

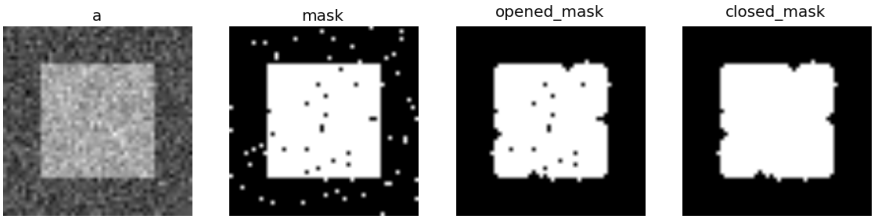
Exercise

Check that opening amounts to eroding, then dilating.

An opening operation removes small structures, while a closing operation fills small holes. Such operations

can therefore be used to "clean" an image.

```
>>> a = np.zeros((50, 50))
>>> a[10:-10, 10:-10] = 1
>>> a += 0.25 * np.random.standard_normal(a.shape)
>>> mask = a>=0.5
>>> opened_mask = ndimage.binary_opening(mask)
>>> closed_mask = ndimage.binary_closing(opened_mask)
```



Exercise

Check that the area of the reconstructed square is smaller than the area of the initial square. (The opposite would occur if the closing step was performed *before* the opening).

For *gray-valued* images, eroding (resp. dilating) amounts to replacing a pixel by the minimal (resp. maximal) value among pixels covered by the structuring element centered on the pixel of interest.

```
>>> a = np.zeros((7, 7), dtype=np.int)
>>> a[1:6, 1:6] = 3
>>> a[4, 4] = 2; a[2, 3] = 1
>>> a
array([[0, 0, 0, 0, 0, 0, 0],
       [0, 3, 3, 3, 3, 3, 0],
       [0, 3, 3, 1, 3, 3, 0],
       [0, 3, 3, 3, 3, 3, 0],
       [0, 3, 3, 3, 2, 3, 0],
       [0, 3, 3, 3, 3, 3, 0],
       [0, 0, 0, 0, 0, 0, 0]])
>>> ndimage.grey_erosion(a, size=(3, 3))
array([[0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 1, 1, 1, 0, 0],
       [0, 0, 3, 2, 2, 0, 0],
       [0, 0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0, 0]])
```

5.10.4 Measurements on images

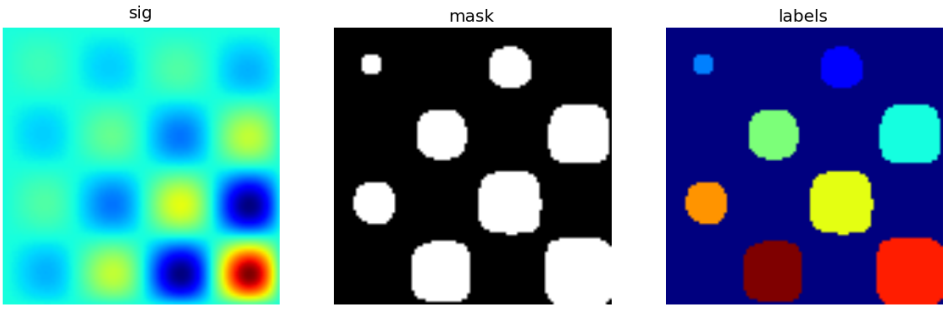
Let us first generate a nice synthetic binary image.

```
>>> x, y = np.indices((100, 100))
>>> sig = np.sin(2*np.pi*x/50.) * np.sin(2*np.pi*y/50.) * (1+x*y/50.**2)**2
>>> mask = sig > 1
```

Now we look for various information about the objects in the image:

```
>>> labels, nb = ndimage.label(mask)
>>> nb
8
>>> areas = ndimage.sum(mask, labels, range(1, labels.max()+1))
```

```
>>> areas
array([ 190.,   45.,  424.,  278.,  459.,  190.,  549.,  424.])
>>> maxima = ndimage.maximum(sig, labels, range(1, labels.max()+1))
>>> maxima
array([  1.80238238,   1.13527605,   5.51954079,   2.49611818,
         6.71673619,   1.80238238,  16.76547217,   5.51954079])
>>> ndimage.find_objects(labels==4)
[(slice(30L, 48L, None), slice(30L, 48L, None))]
>>> sl = ndimage.find_objects(labels==4)
>>> import pylab as pl
>>> pl.imshow(sig[sl[0]])
<matplotlib.image.AxesImage object at ...>
```



See the summary exercise on *Image processing application: counting bubbles and unmolten grains* for a more advanced example.

5.11 Summary exercises on scientific computing

The summary exercises use mainly Numpy, Scipy and Matplotlib. They provide some real-life examples of scientific computing with Python. Now that the basics of working with Numpy and Scipy have been introduced, the interested user is invited to try these exercises.

5.11.1 Maximum wind speed prediction at the Sprogø station

The exercise goal is to predict the maximum wind speed occurring every 50 years even if no measure exists for such a period. The available data are only measured over 21 years at the Sprogø meteorological station located in Denmark. First, the statistical steps will be given and then illustrated with functions from the scipy.interpolate module. At the end the interested readers are invited to compute results from raw data and in a slightly different approach.

Statistical approach

The annual maxima are supposed to fit a normal probability density function. However such function is not going to be estimated because it gives a probability from a wind speed maxima. Finding the maximum wind speed occurring every 50 years requires the opposite approach, the result needs to be found from a defined probability. That is the quantile function role and the exercise goal will be to find it. In the current model, it is supposed that the maximum wind speed occurring every 50 years is defined as the upper 2% quantile.

By definition, the quantile function is the inverse of the cumulative distribution function. The latter describes the probability distribution of an annual maxima. In the exercise, the cumulative probability `p_i` for a given year `i` is defined as `p_i = i/(N+1)` with `N = 21`, the number of measured years. Thus it will be possible to calculate the cumulative probability of every measured wind speed maxima. From those experimental points, the scipy.interpolate module will be very useful for fitting the quantile function. Finally the 50 years maxima is going to be evaluated from the cumulative probability of the 2% quantile.

Computing the cumulative probabilities

The annual wind speeds maxima have already been computed and saved in the numpy format in the file `examples/max-speeds.npy`, thus they will be loaded by using numpy:

```
>>> import numpy as np
>>> max_speeds = np.load('intro/summary-exercises/examples/max-speeds.npy')
>>> years_nb = max_speeds.shape[0]
```

Following the cumulative probability definition `p_i` from the previous section, the corresponding values will be:

```
>>> cprob = (np.arange(years_nb, dtype=np.float32) + 1)/(years_nb + 1)
```

and they are assumed to fit the given wind speeds:

```
>>> sorted_max_speeds = np.sort(max_speeds)
```

Prediction with UnivariateSpline

In this section the quantile function will be estimated by using the `UnivariateSpline` class which can represent a spline from points. The default behavior is to build a spline of degree 3 and points can have different weights according to their reliability. Variants are `InterpolatedUnivariateSpline` and `LSQUnivariateSpline` on which errors checking is going to change. In case a 2D spline is wanted, the `BivariateSpline` class family is provided. All those classes for 1D and 2D splines use the FITPACK Fortran subroutines, that's why a lower library access is available through the `splrep` and `splev` functions for respectively representing and evaluating a spline. Moreover interpolation functions without the use of FITPACK parameters are also provided for simpler use (see `interp1d`, `interp2d`, `barycentric_interpolate` and so on).

For the Sprogø maxima wind speeds, the `UnivariateSpline` will be used because a spline of degree 3 seems to correctly fit the data:

```
>>> from scipy.interpolate import UnivariateSpline
>>> quantile_func = UnivariateSpline(cprob, sorted_max_speeds)
```

The quantile function is now going to be evaluated from the full range of probabilities:

```
>>> nprob = np.linspace(0, 1, 1e2)
>>> fitted_max_speeds = quantile_func(nprob)
```

In the current model, the maximum wind speed occurring every 50 years is defined as the upper 2% quantile. As a result, the cumulative probability value will be:

```
>>> fifty_prob = 1. - 0.02
```

So the storm wind speed occurring every 50 years can be guessed by:

```
>>> fifty_wind = quantile_func(fifty_prob)
>>> fifty_wind
array(32.97989825...)
```

The results are now gathered on a Matplotlib figure:

Exercise with the Gumbell distribution

The interested readers are now invited to make an exercise by using the wind speeds measured over 21 years. The measurement period is around 90 minutes (the original period was around 10 minutes but the file size has been reduced for making the exercise setup easier). The data are stored in numpy format inside the file `examples/sprog-windspeeds.npy`. Do not look at the source code for the plots until you have completed the exercise.

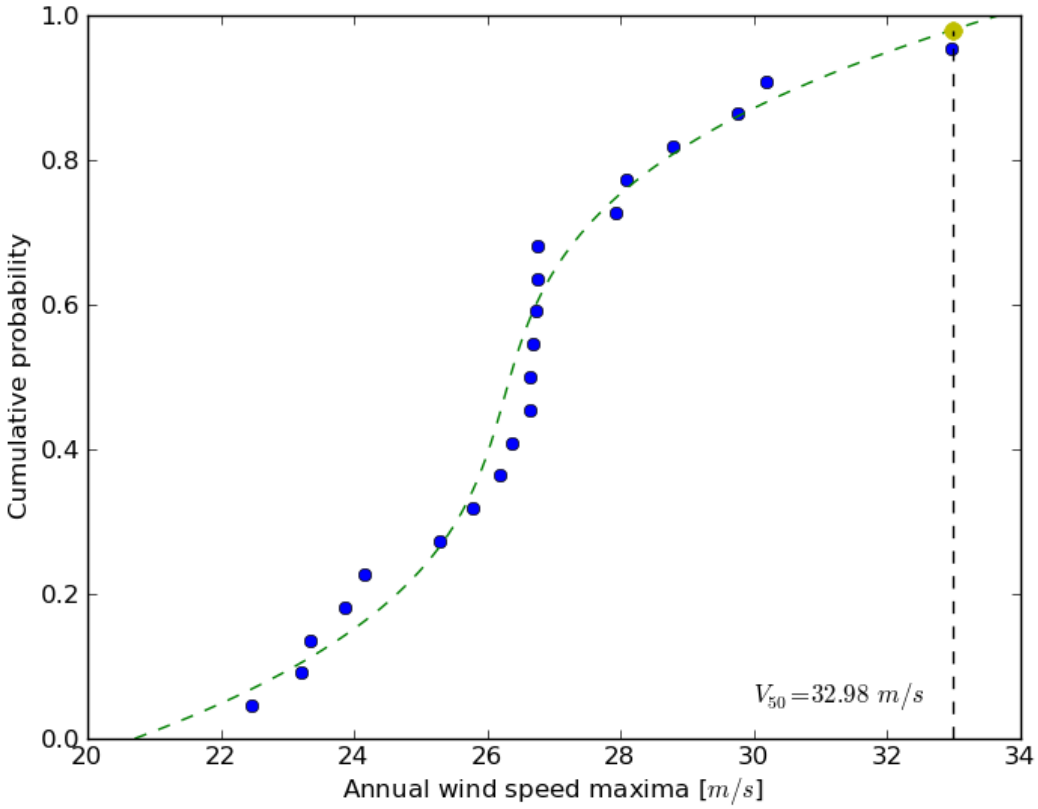


Figure 5.1: Solution: *Python source file*

- The first step will be to find the annual maxima by using numpy and plot them as a matplotlib bar figure.

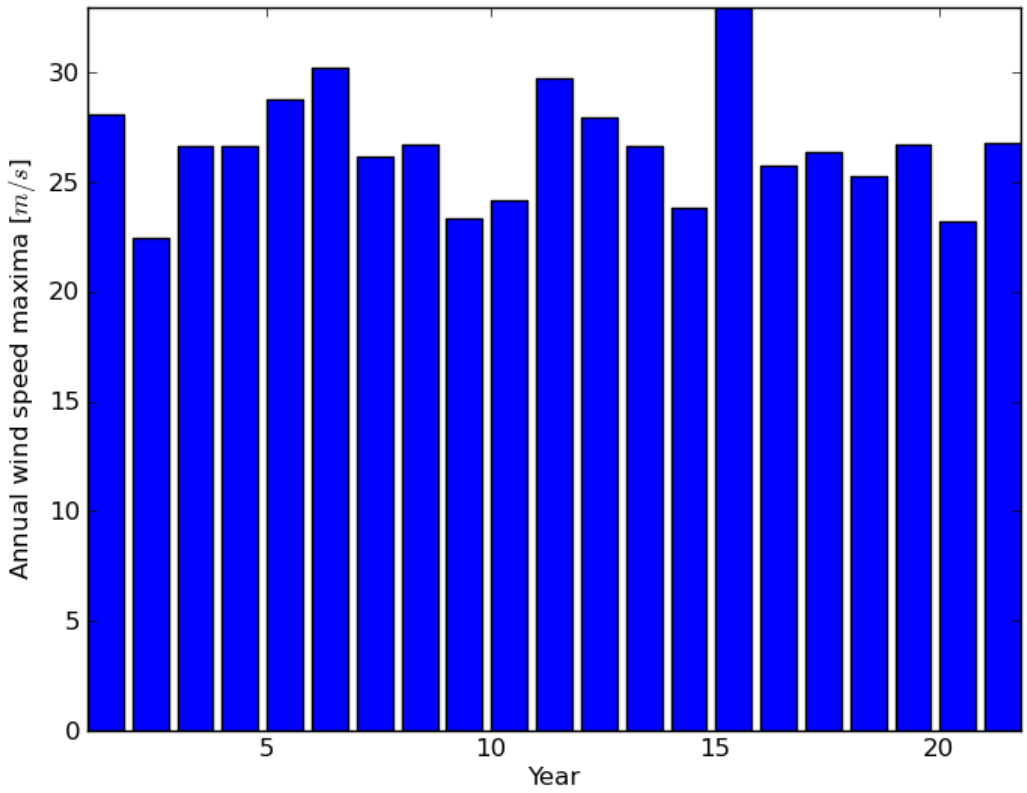


Figure 5.2: Solution: *Python source file*

- The second step will be to use the Gumbell distribution on cumulative probabilities `p_i` defined as `-log( -log(p_i) )` for fitting a linear quantile function (remember that you can define the degree of the `UnivariateSpline`). Plotting the annual maxima versus the Gumbell distribution should give you the following figure.
- The last step will be to find 34.23 m/s for the maximum wind speed occurring every 50 years.

5.11.2 Non linear least squares curve fitting: application to point extraction in topographical lidar data

The goal of this exercise is to fit a model to some data. The data used in this tutorial are lidar data and are described in details in the following introductory paragraph. If you're impatient and want to practice now, please skip it and go directly to *Loading and visualization*.

Introduction

Lidars systems are optical rangefinders that analyze property of scattered light to measure distances. Most of them emit a short light impulsion towards a target and record the reflected signal. This signal is then processed to extract the distance between the lidar system and the target.

Topographical lidar systems are such systems embedded in airborne platforms. They measure distances between the platform and the Earth, so as to deliver information on the Earth's topography (see [1] for more de-

[1] Mallet, C. and Bretar, F. Full-Waveform Topographic Lidar: State-of-the-Art. *ISPRS Journal of Photogrammetry and Remote Sensing* 64(1), pp.1-16, January 2009 http://dx.doi.org/10.1016/j.isprsjprs.2008.09.007

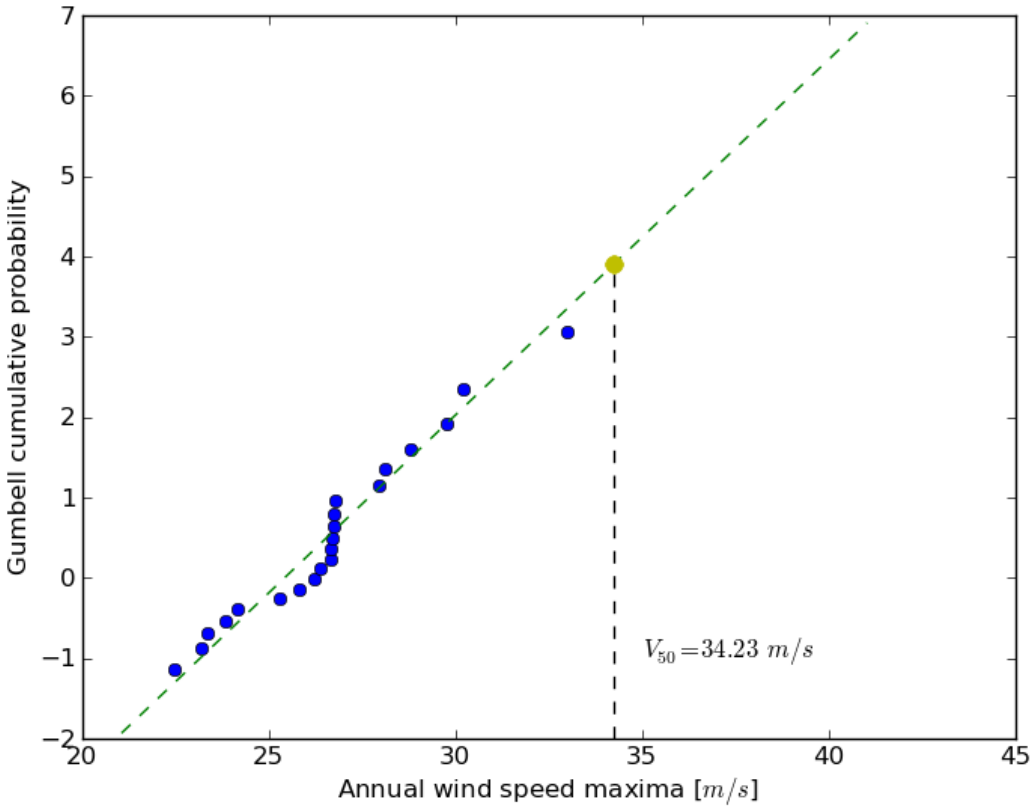


Figure 5.3: Solution: *Python source file*

tails).

In this tutorial, the goal is to analyze the waveform recorded by the lidar system [2]. Such a signal contains peaks whose center and amplitude permit to compute the position and some characteristics of the hit target. When the footprint of the laser beam is around 1m on the Earth surface, the beam can hit multiple targets during the two-way propagation (for example the ground and the top of a tree or building). The sum of the contributions of each target hit by the laser beam then produces a complex signal with multiple peaks, each one containing information about one target.

One state of the art method to extract information from these data is to decompose them in a sum of Gaussian functions where each function represents the contribution of a target hit by the laser beam.

Therefore, we use the `scipy.optimize` module to fit a waveform to one or a sum of Gaussian functions.

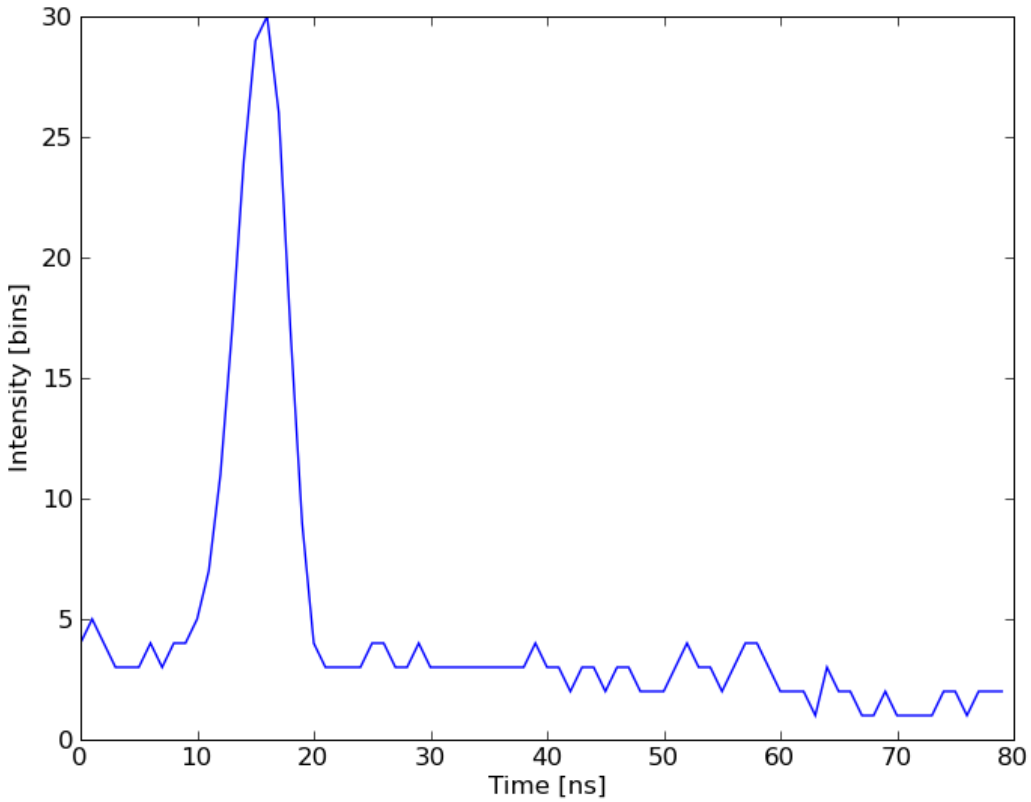
Loading and visualization

Load the first waveform using:

```
>>> import numpy as np
>>> waveform_1 = np.load('data/waveform_1.npy')
```

and visualize it:

```
>>> import matplotlib.pyplot as plt
>>> t = np.arange(len(waveform_1))
>>> plt.plot(t, waveform_1)
[<matplotlib.lines.Line2D object at ...>]
>>> plt.show()
```



As you can notice, this waveform is a 80-bin-length signal with a single peak.

[2] The data used for this tutorial are part of the demonstration data available for the FullAnalyze software and were kindly provided by the GIS DRAIX.

Fitting a waveform with a simple Gaussian model

The signal is very simple and can be modeled as a single Gaussian function and an offset corresponding to the background noise. To fit the signal with the function, we must:

- define the model
- propose an initial solution
- call `scipy.optimize.leastsq`

Model

A Gaussian function defined by

$$B + A \exp\left\{-\left(\frac{t-\mu}{\sigma}\right)^2\right\}$$

can be defined in python by:

```
>>> def model(t, coeffs):
...     return coeffs[0] + coeffs[1] * np.exp( - ((t-coeffs[2])/coeffs[3])**2 )
```

where

- `coeffs[0]` is B (noise)
- `coeffs[1]` is A (amplitude)
- `coeffs[2]` is μ (center)
- `coeffs[3]` is σ (width)

Initial solution

An approximative initial solution that we can find from looking at the graph is for instance:

```
>>> x0 = np.array([3, 30, 15, 1], dtype=float)
```

Fit

`scipy.optimize.leastsq` minimizes the sum of squares of the function given as an argument. Basically, the function to minimize is the residuals (the difference between the data and the model):

```
>>> def residuals(coeffs, y, t):
...     return y - model(t, coeffs)
```

So let's get our solution by calling `scipy.optimize.leastsq()` with the following arguments:

- the function to minimize
- an initial solution
- the additional arguments to pass to the function

```
>>> from scipy.optimize import leastsq
>>> x, flag = leastsq(residuals, x0, args=(waveform_1, t))
>>> print(x)
[  2.70363341  27.82020742  15.47924562   3.05636228]
```

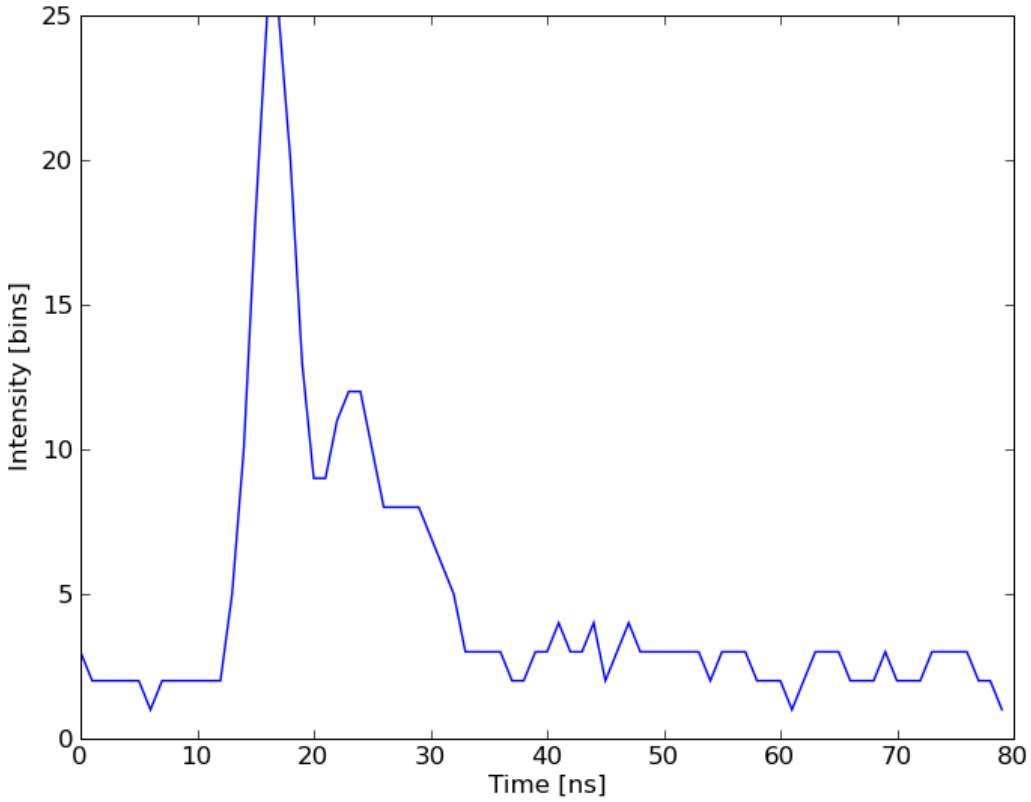
And visualize the solution:

```
>>> plt.plot(t, waveform_1, t, model(t, x))
[<matplotlib.lines.Line2D object at ...>, <matplotlib.lines.Line2D object at ...>]
>>> plt.legend(['waveform', 'model'])
<matplotlib.legend.Legend object at ...>
>>> plt.show()
```

Remark: from scipy v0.8 and above, you should rather use `scipy.optimize.curve_fit()` which takes the model and the data as arguments, so you don't need to define the residuals any more.

Going further

- Try with a more complex waveform (for instance `data/waveform_2.npy`) that contains three significant peaks. You must adapt the model which is now a sum of Gaussian functions instead of only one Gaussian peak.



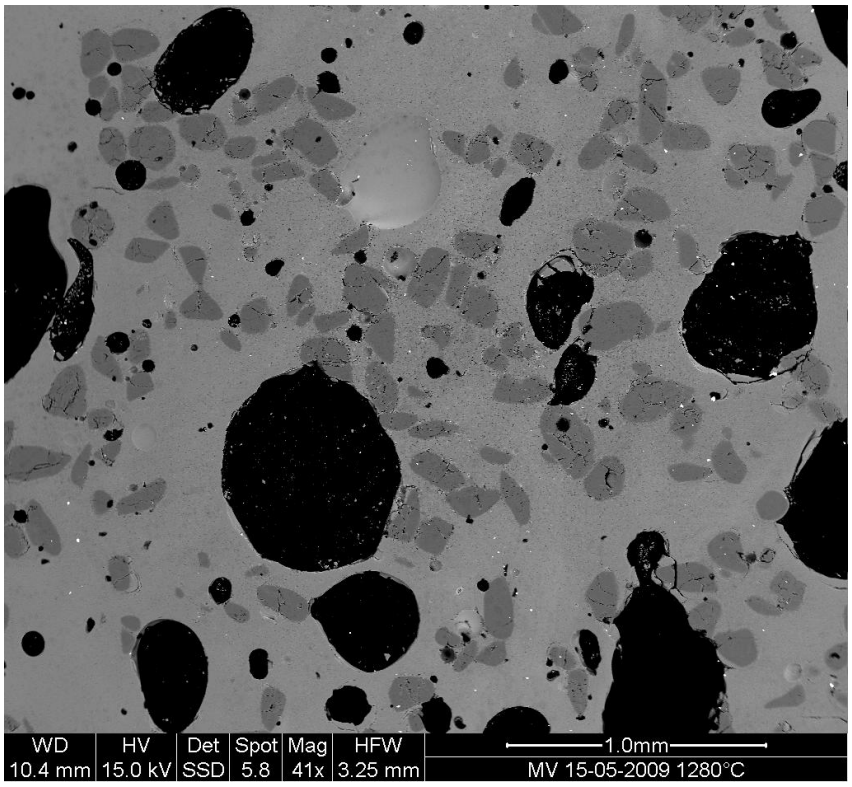
- In some cases, writing an explicit function to compute the Jacobian is faster than letting `leastsq` estimate it numerically. Create a function to compute the Jacobian of the residuals and use it as an input for `leastsq`.
- When we want to detect very small peaks in the signal, or when the initial guess is too far from a good solution, the result given by the algorithm is often not satisfying. Adding constraints to the parameters of the model enables to overcome such limitations. An example of *a priori* knowledge we can add is the sign of our variables (which are all positive).

  With the following initial solution:

```
>>> x0 = np.array([3, 50, 20, 1], dtype=float)
```

  compare the result of `scipy.optimize.leastsq()` and what you can get with `scipy.optimize.fmin_slsqp()` when adding boundary constraints.

5.11.3 Image processing application: counting bubbles and unmolten grains



Statement of the problem

1. Open the image file MV_HFV_012.jpg and display it. Browse through the keyword arguments in the docstring of `imshow` to display the image with the "right" orientation (origin in the bottom left corner, and not the upper left corner as for standard arrays).

This Scanning Element Microscopy image shows a glass sample (light gray matrix) with some bubbles (on black) and unmolten sand grains (dark gray). We wish to determine the fraction of the sample covered by these three phases, and to estimate the typical size of sand grains and bubbles, their sizes, etc.

2. Crop the image to remove the lower panel with measure information.

3. Slightly filter the image with a median filter in order to refine its histogram. Check how the histogram changes.

4. Using the histogram of the filtered image, determine thresholds that allow to define masks for sand pixels, glass pixels and bubble pixels. Other option (homework): write a function that determines automatically the thresholds from the minima of the histogram.

5. Display an image in which the three phases are colored with three different colors.

6. Use mathematical morphology to clean the different phases.

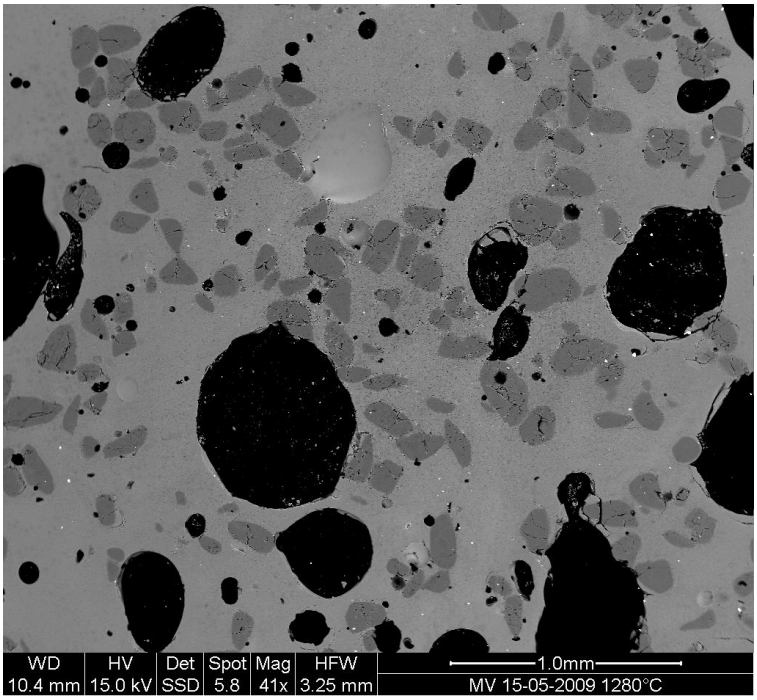
7. Attribute labels to all bubbles and sand grains, and remove from the sand mask grains that are smaller than 10 pixels. To do so, use `ndimage.sum` or `np.bincount` to compute the grain sizes.

8. Compute the mean size of bubbles.

Proposed solution

```
>>> import numpy as np
>>> import pylab as pl
>>> from scipy import ndimage
```

5.11.4 Example of solution for the image processing exercise: unmolten grains in glass



1. Open the image file MV_HFV_012.jpg and display it. Browse through the keyword arguments in the docstring of `imshow` to display the image with the "right" orientation (origin in the bottom left corner, and not the upper left corner as for standard arrays).

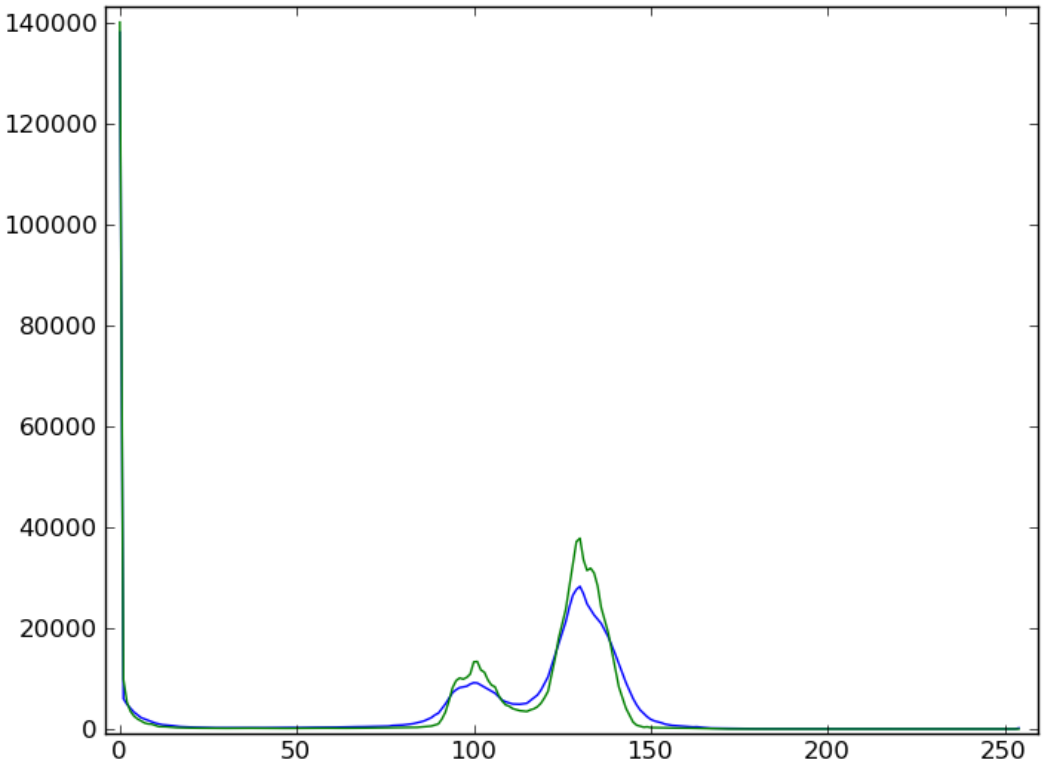
```
>>> dat = pl.imread('data/MV_HFV_012.jpg')
```

2. Crop the image to remove the lower panel with measure information.

```
>>> dat = dat[:-60]
```

3. Slightly filter the image with a median filter in order to refine its histogram. Check how the histogram changes.

```
>>> filtdat = ndimage.median_filter(dat, size=(7,7))
>>> hi_dat = np.histogram(dat, bins=np.arange(256))
>>> hi_filtdat = np.histogram(filtdat, bins=np.arange(256))
```

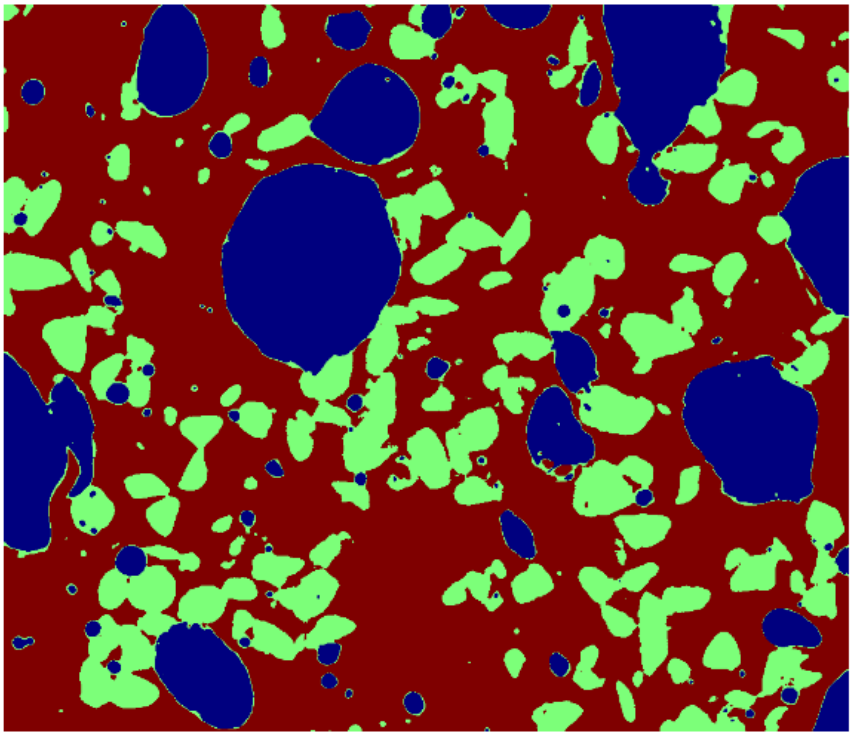


4. Using the histogram of the filtered image, determine thresholds that allow to define masks for sand pixels, glass pixels and bubble pixels. Other option (homework): write a function that determines automatically the thresholds from the minima of the histogram.

```
>>> void = filtdat <= 50
>>> sand = np.logical_and(filtdat > 50, filtdat <= 114)
>>> glass = filtdat > 114
```

5. Display an image in which the three phases are colored with three different colors.

```
>>> phases = void.astype(np.int) + 2*glass.astype(np.int) + 3*sand.astype(np.int)
```

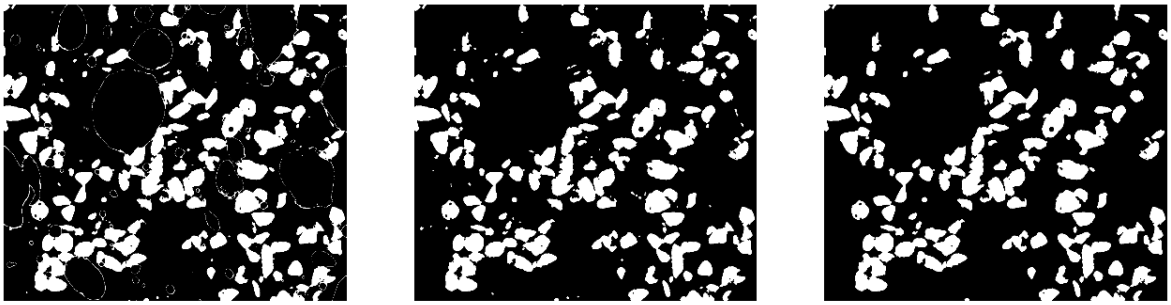


6. Use mathematical morphology to clean the different phases.

```
>>> sand_op = ndimage.binary_opening(sand, iterations=2)
```

7. Attribute labels to all bubbles and sand grains, and remove from the sand mask grains that are smaller than 10 pixels. To do so, use `ndimage.sum` or `np.bincount` to compute the grain sizes.

```
>>> sand_labels, sand_nb = ndimage.label(sand_op)
>>> sand_areas = np.array(ndimage.sum(sand_op, sand_labels, np.arange(sand_labels.max()+1)))
>>> mask = sand_areas > 100
>>> remove_small_sand = mask[sand_labels.ravel()].reshape(sand_labels.shape)
```



8. Compute the mean size of bubbles.

```
>>> bubbles_labels, bubbles_nb = ndimage.label(void)
>>> bubbles_areas = np.bincount(bubbles_labels.ravel())[1:]
>>> mean_bubble_size = bubbles_areas.mean()
>>> median_bubble_size = np.median(bubbles_areas)
>>> mean_bubble_size, median_bubble_size
```

```
    (1699.875, 65.0)
```