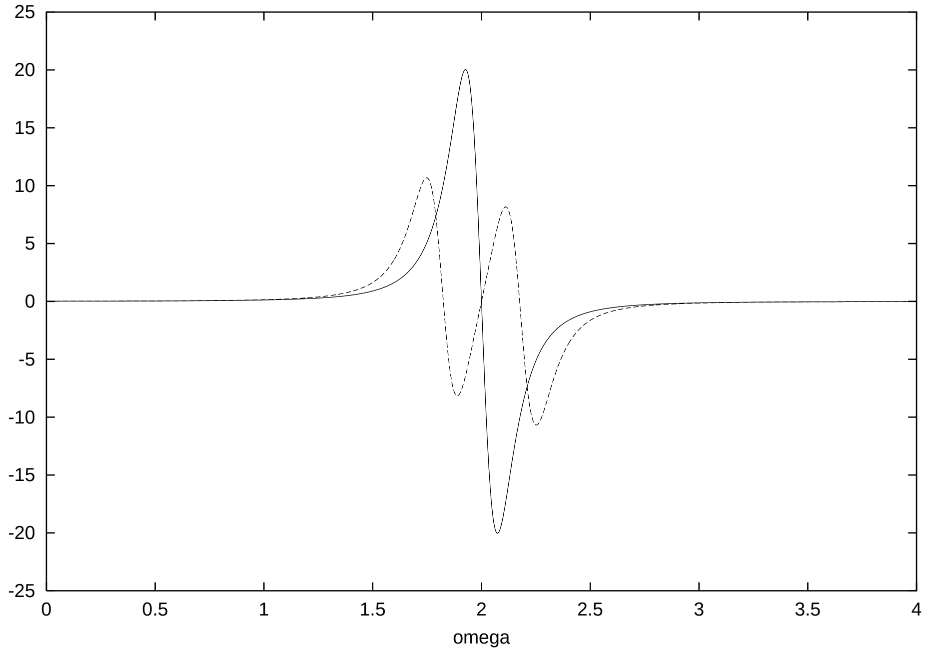
Computational Methods and Data Analysis 2002

Ex. 3: General nonlinear least squares fitting

In many experiments it happens that a given line of resonant absorption splits under the effect of a given perturbation, such as a magnetic or electric field. In this exercise the purpose is to extract the value of the splitting by applying a general nonlinear least squares fitting to the data. In figure we present a case rather simple but illustrative of a whole class of problems. The solid line is the function f_0^{exp} due to resonant absorption



at frequency $\omega = 2.0$ measured in absence of external fields, the dotted line the function f^{exp} due to a splitting of the line into two contributions of half intensity and an amount ω_s apart (the subscript s stays for splitting). Physical reasons tell us the line f^{exp} could be fitted by a function f^{calc} which can be expressed in terms of the unperturbed lineshape f_0^{exp} as:

$$f^{calc}(\omega_i, \omega_s) = \frac{1}{2}[f_0^{exp}(\omega_i + \frac{\omega_s}{2}) + f_0^{exp}(\omega_i - \frac{\omega_s}{2})] \tag{1}$$

The interesting point of this exercise is that you do not need to know the explicit form giving the shape of the absorption line but you can use the unperturbed data f_0^{exp} and formula (1) as fitting function to extract the fitting parameter ω_s by the data representing $f^{exp}(\omega_i)$.

The file splitting.dat contains 4000 values of ω, f_0^{exp} and f^{exp} in the first, second and third column respectively, that is to say ω_i, $f_0^{exp}(\omega_i)$ and $f^{exp}(\omega_i)$ for $i = 1, ..., N$ with

$N = 4000$. These values will be used to find the value of ω_s of the splitting which best describes the data with two digit precision. You can read this file with matlab and store the values in vectors with the following commands:

load		'splitting.dat'
omega	=	splitting(:,1)
f0	=	splitting(:,2)
fexp	=	splitting(:,3)

Consider that you have data in units of 0.001 and express your tentative values of ω_s and of $\delta\omega_s$ in multiples of this value. Besides, since you have to shift f_0^{exp} to evaluate $f^{calc}(\omega_i, \omega_s)$ consider you have less than 4000 points available for the fit, namely 4000-$(\omega_s/0.001)$ points.

In order to facilitate comparison with the formula's given in the notes distributed in the lecture, consider that you have only one fitting parameter so that the vector $\mathbf{p}$ has only one element $p_1 = \omega_s$. Consequently, the matrix M has only one element so that you have to solve just one equation iteratively.

The values ω_i take the place of x_i, the function $f^{exp}(\omega_i)$ takes the place of $y_i(x_i)$ and $f^{calc}(\omega_i, \omega_s)$ that of $y(x_i, \mathbf{p})$, i running over the available experimental points. First you choose an initial guess for ω_s^0 and for its increment $\delta\omega_s^0$. With this you can calculate the numerical derivative by forward difference so that you can calculate the only element E_1 of the vector $\mathbf{E}$ and M_{11} of the matrix M. Their ratio gives the new value of the increment $\delta\omega_s$. Add this increment (or better $\sim$half of it in order to avoid large jumps of the value of the parameter) to the initial ω_s^0 and repeat until convergence is reached. If you have chosen a reasonable first guess this should happen in a few iterations. If you do not reach convergance within about 10 iterations stop and try another initial value of ω_s.

To keep the iterative procedure as simple and readable as possible it is useful to define a separate function which calculates the function $f^{calc}(\omega_i, \omega_s)$ and its derivative with respect to ω_s