Numerieke methoden in de natuurwetenschappen

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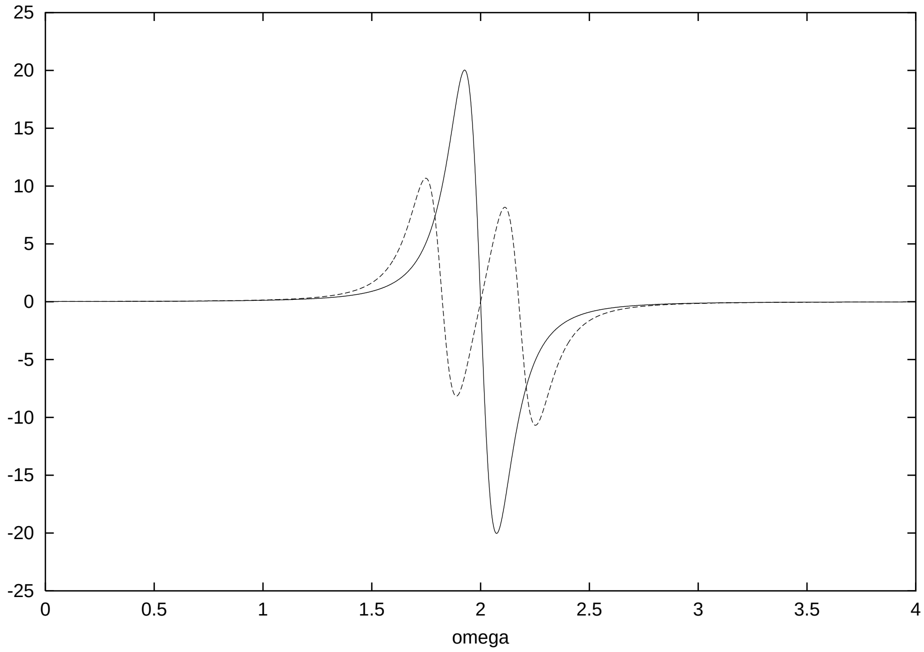
Ex. 3: General nonlinear least squares fitting

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 $\omega = 2.0$ 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 $\Delta\omega$ apart. 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:

$$f^{calc}(\omega_i, \Delta\omega) = \frac{f_0^{exp}(\omega_i + \Delta\omega/2) + f_0^{exp}(\omega_i - \Delta\omega/2)}{2} \qquad (1)$$

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

In order to facilitate comparison with the formula's given in the 'college', consider that you have only one fitting parameter so that the vector $\mathbf{a}$ has only one element $a_1 = \Delta\omega$. Consequently, the matrix M has only one element so that you have to solve just one equation iteratively. The function $f^{exp}(\omega_i)$ takes the place of y_i and $f^{calc}(\omega_i, \Delta\omega)$ that of $y(x_i, \mathbf{a})$, i running over the available experimental points. First you choose an initial guess for $\Delta\omega^0$ and for its increment $\delta\Delta\omega^0$, calculate the numerical derivative and then solve the equation $M\delta\Delta\omega = B$ to get the new value of $\delta\Delta\omega$. Add this increment (or $\sim$half of it in order to avoid large jumps in the parameters) to the initial $\Delta\omega^0$ and repeat until convergence is reached. In doing this keep track of the values $\delta\Delta\omega, \Delta\omega$, and of any other quantity of interest in successive iterations.