Determining the fitting parameters in Curvefit

In this curvefitting program we offer two ways to fit 3 different types of functions to data. The three types of functions are: linear $y = a + bx$, exponential $y = ae^{bx}$ and a power law function $y = ax^b$. The two ways to fit the data are via linear regression and minimizing a chi-square function.

For the linear regression option, we use the standard formulas for "Least-Squares Fitting" found in Chapter 8 of "An introduction to Error Analysis" (Second Edition) by John Taylor. For the exponential and power fits, the equations are linearized. The uncertainty in the fitting parameters a and b are determined from Eqs. 8.15, 8.16, and 8.17.

For the chi-square search method, we find values of a and b that minimize a chi-square function χ^2 which is defined to be the difference between the data and the modeling equations divided by the error in the data. For example, for the exponential fit,

$$\chi^2(a, b) = \sum_i^N \left(\frac{ae^{bx_i} - y_i}{\sigma_i} \right)^2 \tag{1}$$

where σ_i is the error in y_i. For convenience we call $1/\sigma_i^2 \equiv w_i$. The χ^2 function becomes

$$\chi^2(a, b) = \sum_i^N w_i \left(ae^{bx_i} - y_i \right)^2 \tag{2}$$

For the power function, we have

$$\chi^2(a, b) = \sum_i^N w_i \left(ax_i^b - y_i \right)^2 \tag{3}$$

We want to find values of a and b for which the function χ^2 is a miminum.

The function χ^2 will be an extremum (i.e. a minimum) when the partial derivative with respect to each of the two parameters equals zero:

$$\begin{aligned} D_1 \equiv \frac{\partial \chi^2}{\partial b} &= 0 \\ D_2 \equiv \frac{\partial \chi^2}{\partial a} &= 0 \end{aligned}$$

A closed form expression for the solution to these equations is not possible. We will find a solution using an iterative process. We start from one point (b_0, a_0) and move to the next point (b_1, a_1) that will reduce the value of χ^2. We repeat the iteration until $D_1 = D_2 = 0$ to the desired accuracy. We use Newton's method in two dimensions to step through the parameter space. The steps will be small if χ^2 is near the minimum, and are defined as ϵ_i:

$$\begin{aligned} b_1 &= b_0 + \epsilon_1 \\ a_1 &= a_0 + \epsilon_2 \end{aligned}$$

We expand χ^2, via a Taylor expansion, up to order 2:

$$\chi^2(a_1, b_1) \approx \chi^2(a_0, b_0) + \sum_{i=1}^{2} D_i \epsilon_i + \frac{1}{2} \sum_{i=1}^{2} \epsilon_i^2 H_{ii} + \epsilon_1 \epsilon_2 H_{12} \tag{4}$$

where H_{ij} is the Hessian matrix:

$$H_{11} = \frac{\partial^2 \chi^2}{\partial b^2} \qquad H_{22} = \frac{\partial^2 \chi^2}{\partial a^2} \qquad H_{12} = H_{21} = \frac{\partial^2 \chi^2}{\partial b \partial a}$$

With this approximate expression, i.e. the Taylor expansion of χ^2 to second order, we can find the minimum of this paraboloid by solving for where the first derivatives equal zero:

$$\begin{aligned} \frac{\partial \chi^2}{\partial \epsilon_1} &= D_1 + H_{11}\epsilon_1 + H_{12}\epsilon_2 = 0 \\ \frac{\partial \chi^2}{\partial \epsilon_2} &= D_2 + H_{12}\epsilon_1 + H_{22}\epsilon_2 = 0 \end{aligned}$$

These two equations can be solved for the ϵ_i using substitution with the result:

$$\begin{aligned} \epsilon_1 &= \frac{D_2 H_{12} - D_1 H_{22}}{H_{11} H_{22} - H_{12}^2} \\ \epsilon_2 &= \frac{D_1 H_{12} - D_2 H_{11}}{H_{11} H_{22} - H_{12}^2} \end{aligned}$$

The two ϵ_i are added to their respective parameters to give the new values: $(b_1, a_1) = (b_0 + \epsilon_1, a_0 + \epsilon_2)$. The two old values are replaced by the new values for the parameters, and the process is repeated for the next step in the two parameter space. We start with the two values (b_0, a_0) from the linear regression formulas. Since these initial values are close to the true minimum, the function χ^2 is nearly a paraboloid, and convergence is obtained in only a few iterations.

The partial derivatives and the Hessian matrix are determined from the sums by differentiating the χ^2 formula. The results for the exponential fit are:

$$
\begin{aligned}
D_1 &= \sum_{i=1}^{N} 2w_i(ae^{bx_i} - y_i)ae^{bx_i}x_i \\
D_2 &= \sum_{i=1}^{N} 2w_i(ae^{bx_i} - y_i)e^{bx_i} \\
H_{11} &= \sum_{i=1}^{N} 2w_i(2a^2x_i^2e^{2bx_i} - ay_ix_i^2e^{bx_i}) \\
H_{22} &= \sum_{i=1}^{N} 2w_ie^{2bx_i} \\
H_{12} &= \sum_{i=1}^{N} 2w_i(2ax_ie^{2bx_i} - y_ix_ie^{bx_i})
\end{aligned}
$$

The derivatives and Hessian matrix results for the power fit are:

$$
\begin{aligned}
D_1 &= \sum_i^N 2w_i(ax_i^b - y_i)ax_i^b ln(x_i) \\
D_2 &= \sum_i^N 2w_i(ax_i^b - y_i)x_i^b \\
H_{11} &= \sum_i^N 2w_i(2a^2x_i^{2b}(ln(x_i))^2 - Ay_ix_i^b(ln(x_i))^2 \\
H_{22} &= \sum_i^N 2w_i x_i^{2b} \\
H_{12} &= \sum_i^N 2w_i(2ax_i^{2b}ln(x_i) - y_ix_i^b ln(x_i))
\end{aligned}
$$

For the errors in the fitting parameters a and b for the linear regression fits, we use the formulas in Taylor's book. Also for the Chi-square fit for the linear form we use the formula in his book. However, for the Chi-square fit for the exponential and power forms we use as errors the square root of the diagonal elements of the inverse Hessian matrix (H^{-1}), which is also refered to as the error matrix:

$$
\Delta b = \sqrt{\frac{H_{22}}{H_{11}H_{22} - H_{12}^2}}
$$

$$
\Delta a = \sqrt{\frac{H_{11}}{H_{11}H_{22} - H_{12}^2}}
$$

We note that these errors are different than the ones determined using gnuplot. In gnuplot, these errors are multiplied by $\sqrt{2\chi^2/(degrees\ of\ freedom)}$ so that the chi-square per degree of freedom is normalized to one. We print out the chi-square per degree of freedom, χ^2/df so you can check if this number is between one and two. If it is too small, then your Δy errors are too large. If χ^2/df is too large, then your Δy errors are either too small, or the fitting function is incorrect.

As a final note, if the fitting function is not a good representation of the data, the Newton's method we use might not converge. To avoid this possible problem, we use a grid search if the χ^2 starts to increase.