Determining the exponent b via Chi-sq minimization

To determine the exponent b and the two activity parameters, $A_I\epsilon_{1460}$ and $A_{II}\epsilon_{1460}$ one can use linear regression or minimize a Chi-square function. Here, we explain the Chi-square minimizaton method. The advantage of this method is that one can weight the data with the uncertainy in the Counts/Yield. The method explained below uses Newton's method in three dimensions.

There are 3 fitting parameters for the data from the two decay series modeled by the equations:

$$\begin{aligned} (C/Y)_{1i} &= A_I\epsilon_{1460}(E_{1i}/1460)^b \qquad (i = 1 \rightarrow N_I) \\ (C/Y)_{2i} &= A_{II}\epsilon_{1460}(E_{2i}/1460)^b \qquad (i = 1 \rightarrow N_{II}) \end{aligned}$$

Note that the exponent b is the same for all the sources. There are 3 free parameters to vary to best fit the data: b, $A_I\epsilon_{1460}$, and $A_{II}\epsilon_{1460}$. For brevity, we define $A_I\epsilon_{1460} \equiv A$, $A_{II}\epsilon_{1460} \equiv B$, $N_I \equiv na$ and $N_{II} \equiv n2$. We also define $(C/Y)_{1i} \equiv y_{1i}$, $(C/Y)_{2i} \equiv y_{2i}$, $E_{1i}/1460 \equiv x_{1i}$, and $E_{2i}/1460 \equiv x_{2i}$ With these definitons, the equations become

$$\begin{aligned} y_{1i} &= Ax_{1i}^b \qquad (i = 1 \rightarrow n1) \\ y_{2i} &= Bx_{2i}^b \qquad (i = 1 \rightarrow n2) \end{aligned}$$

To determine the "best fit" values we define a chi-square function χ^2 as the difference between the data and the modeling equations divided by the error in the data. We label the error of $(C/Y)_i$ as Δ_{1i} and Δ_{2i} for the respective decay series. Defining the weights $w_{1i} \equiv 1/\Delta_{1i}^2$ and $w_{2i} \equiv 1/\Delta_{2i}^2$, Our χ^2 function, which for brevity be call f, is then

$$f(b, A, B) \equiv \sum_{i=1}^{n1} w_{1i}(Ax_{1i}^b - y_{1i})^2 + \sum_{i=1}^{n2} w_{2i}(Bx_{2i}^b - y_{2i})^2 \qquad (1)$$

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

$$
\begin{aligned}
D_1 \equiv \frac{\partial f}{\partial b} &= 0 \\
D_2 \equiv \frac{\partial f}{\partial A} &= 0 \\
D_3 \equiv \frac{\partial f}{\partial B} &= 0
\end{aligned}
$$

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, B_0) and move to the next point (b_1, A_1, B_1) that will reduce the value of f. We repeat the iteration until $D_1 = D_2 = D_3 = 0$ to the desired accuracy. We will use Newton's method in three dimensions to step through the parameter space. The steps will be small if f is near the minimum, and are defined as ϵ_i:

$$
\begin{aligned}
b_1 &= b_0 + \epsilon_1 \\
A_1 &= A_0 + \epsilon_2 \\
B_1 &= B_0 + \epsilon_3
\end{aligned}
$$

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

$$
f \approx f_0 + \sum_{i=1}^{3} D_i \epsilon_i + \frac{1}{2} \sum_{i=1}^{3} \epsilon_i^2 H_{ii} + \sum_{i=2}^{3} \epsilon_1 \epsilon_i H_{1i} \tag{2}
$$

where H_{ij} is the Hessian matrix:

$$
H_{11} = \frac{\partial^2 f}{\partial b^2} \qquad H_{22} = \frac{\partial^2 f}{\partial A^2} \qquad H_{33} = \frac{\partial^2 f}{\partial B^2}
$$

$$
H_{12} = H_{21} = \frac{\partial^2 f}{\partial b \partial A} \qquad H_{13} = H_{31} = \frac{\partial^2 f}{\partial b \partial B}
$$

$$
H_{23} = H_{32} = 0
$$

It is a very nice feature of our Hessian matrix that 2 elements are zero. With this approximate expression, i.e. the Taylor expansion of f to second order, we can find the minimum of this paraboloid by solving for where the first derivatives equal zero:

$$
\begin{aligned}
\frac{\partial f}{\partial \epsilon_1} &= D_1 + \sum_{i=1}^{4} \epsilon_i H_{1i} = 0 \\
\frac{\partial f}{\partial \epsilon_2} &= D_2 + H_{12}\epsilon_1 + H_{22}\epsilon_2 = 0 \\
\frac{\partial f}{\partial \epsilon_3} &= D_3 + H_{13}\epsilon_1 + H_{33}\epsilon_3 = 0
\end{aligned}
$$

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

$$
\begin{aligned}
\epsilon_1 &= \frac{D_2(H_{12}/H_{22}) + D_3(H_{13}/H_{33}) - D_1}{H_{11} - H_{12}^2/H_{22} - H_{13}^2/H_{33}} \\
\epsilon_2 &= (-D_2 - H_{12}\epsilon_1)/H_{22} \\
\epsilon_3 &= (-D_3 - H_{13}\epsilon_1)/H_{33}
\end{aligned}
$$

The three ϵ_i are added to their respective parameters to give the new values: $(b_1, A_1, B_1) = (b_0 + \epsilon_1, A_0 + \epsilon_2, B_0 + \epsilon_3)$. The three old values are replaced by the new values for the parameters, and the process is repeated for the next step in the three parameter space. We start with the three values from the linear regression formulas. Since these initial values are close to the true minimum, the function f 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 are:

$$
\begin{aligned}
D_1 &= \sum_{i=1}^{n1} 2w_{1i}(Ax_{1i}^b - y_{1i})Ax_{1i}^b ln(x_{1i}) + \sum_{i=1}^{n2} 2w_{2i}(Bx_{2i}^b - y_{2i})Bx_{2i}^b ln(x_{2i}) \\
D_2 &= \sum_{i=1}^{n1} 2w_{1i}(Ax_{1i}^b - y_{1i})x_{1i}^b \\
D_3 &= \sum_{i=1}^{n2} 2w_{2i}(Bx_{2i}^b - y_{2i})x_{2i}^b \\
H_{11} &= \sum_{i=1}^{n1} 2w_{1i}(2(Aln(x_{1i})x_{1i}^b)^2 - Ay_{1i}(ln(x_{1i}))^2 x_{1i}^b) \\
&\quad + \sum_{i=1}^{n2} 2w_{2i}(2(Bln(x_{2i})x_{2i}^b)^2 - By_{2i}(ln(x_{2i}))^2 x_{2i}^b) \\
H_{22} &= \sum_{i=1}^{n1} 2w_{1i}x_{1i}^{2b} \\
H_{33} &= \sum_{i=1}^{n2} 2w_{2i}x_{2i}^{2b} \\
H_{12} &= \sum_{i=1}^{n1} 2w_{1i}x_{1i}^b ln(x_{1i})(2Ax_{1i}^b - y_{1i}) \\
H_{13} &= \sum_{i=1}^{n2} 2w_{2i}x_{2i}^b ln(x_{2i})(2Bx_{2i}^b - y_{2i})
\end{aligned}
$$