Determining the exponent b via Chi-sq minimization

To determine the exponent b, we use data from the disk sources at 7 energies: 3 energies from Bi^{207}, 2 energies from Na^{22}, and 2 energies from Co^{60}. The four parameters b, C_{Bi}, C_{Na} and C_{Co} need to be found that best fit the data. In this app we offer two ways to fit the data. One option is to use Newton's method in four dimensions to find the minimum of the χ^2 function, which we explain below.

There are 4 fitting parameters for the data modeled by the equations:

$$\begin{aligned} C_i &= C_{Bi} Y_i (E_i/1460)^b \qquad (i = 1, 2, 3) \\ C_i &= C_{Na} Y_i (E_i/1460)^b \qquad (i = 4, 5) \\ C_i &= C_{Co} Y_i (E_i/1460)^b \qquad (i = 6, 7) \end{aligned}$$

Note that the exponent b is the same for all the sources. There are 4 free parameters to vary to best fit the data: b, C_{Bi}, C_{Na}, and C_{Co}. For brevity, we define $C_{Bi} \equiv A$, $C_{Na} \equiv B$, and $C_{Co} \equiv C$. The equations become

$$\begin{aligned} C_i &= A Y_i (E_i/1460)^b \qquad (i = 1, 2, 3) \\ C_i &= B Y_i (E_i/1460)^b \qquad (i = 4, 5) \\ C_i &= C Y_i (E_i/1460)^b \qquad (i = 6, 7) \end{aligned}$$

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. The error of C_i is taken to be $\sqrt{C_i}$. For brevity we define $(E_i/1460) \equiv x_i$, and $w_i \equiv 1/\sqrt{C_i}$. Our χ^2 function, which for brevity be call f, is then

$$f(b, A, B, C) \equiv \sum_{i=1}^{3} w_i (A Y_i x_i^b - y_i)^2 + \sum_{i=4}^{5} w_i (B Y_i x_i^b - y_i)^2 + \sum_{i=6}^{7} w_i (C Y_i x_i^b - y_i)^2 \tag{1}$$

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:

$$
\begin{aligned}
D_1 \equiv \frac{\partial f}{\partial b} &= 0 \\
D_2 \equiv \frac{\partial f}{\partial A} &= 0 \\
D_3 \equiv \frac{\partial f}{\partial B} &= 0 \\
D_4 \equiv \frac{\partial f}{\partial C} &= 0
\end{aligned}
$$

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, C_0) and move to the next point (b_1, A_1, B_1, C_1) that will reduce the value of f. We repeat the iteration until $D_1 = D_2 = D_3 = D_4 = 0$ to the desired accuracy. We will use Newton's method in four dimensions to step through the parameter space. The steps will be small if f is near the minimum, and are defined as ϵ_i:

$$
\begin{aligned}
b_1 &= b_0 + \epsilon_1 \\
A_1 &= A_0 + \epsilon_2 \\
B_1 &= B_0 + \epsilon_3 \\
C_1 &= C_0 + \epsilon_4
\end{aligned}
$$

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

$$
f \approx f_0 + \sum_{i=1}^{4} D_i \epsilon_i + \frac{1}{2} \sum_{i=1}^{4} \epsilon_i^2 H_{ii} + \sum_{i=2}^{4} \epsilon_1 \epsilon_i H_{1i} \tag{2}
$$

where H_{ij} is the Hessian matrix:

$$
H_{11} = \frac{\partial^2 f}{\partial b^2} \qquad H_{22} = \frac{\partial^2 f}{\partial A^2} \qquad H_{33} = \frac{\partial^2 f}{\partial B^2} \qquad H_{44} = \frac{\partial^2 f}{\partial C^2}
$$
$$
H_{12} = H_{21} = \frac{\partial^2 f}{\partial b \partial A} \qquad H_{13} = H_{31} = \frac{\partial^2 f}{\partial b \partial B} \qquad H_{14} = H_{41} = \frac{\partial^2 f}{\partial b \partial C}
$$
$$
H_{23} = H_{32} = H_{24} = H_{42} = H_{34} = H_{43} = 0
$$

It is a very nice feature of our Hessian matrix that 6 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:

$$\begin{aligned}
\frac{\partial f}{\partial \epsilon_1} &= D_1 + \sum_{i=1}^{4} \epsilon_i H_{1i} = 0 \\
\frac{\partial f}{\partial \epsilon_2} &= D_2 + H_{12}\epsilon_1 + H_{22}\epsilon_2 = 0 \\
\frac{\partial f}{\partial \epsilon_3} &= D_3 + H_{13}\epsilon_1 + H_{33}\epsilon_3 = 0 \\
\frac{\partial f}{\partial \epsilon_4} &= D_4 + H_{14}\epsilon_1 + H_{44}\epsilon_4 = 0
\end{aligned}$$

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

$$\begin{aligned}
\epsilon_1 &= \frac{D_2(H_{12}/H_{22}) + D_3(H_{13}/H_{33}) + D_4(H_{14}/H_{44}) - D_1}{H_{11} - H_{12}^2/H_{22} - H_{13}^2/H_{33} - H_{14}^2/H_{44}} \\
\epsilon_2 &= (-D_2 - H_{12}\epsilon_1)/H_{22} \\
\epsilon_3 &= (-D_3 - H_{13}\epsilon_1)/H_{33} \\
\epsilon_4 &= (-D_4 - H_{14}\epsilon_1)/H_{44}
\end{aligned}$$

The four ϵ_i are added to their respective parameters to give the new values: $(b_1, A_1, B_1, C_1) = (b_0 + \epsilon_1, A_0 + \epsilon_2, B_0 + \epsilon_3, C_0 + \epsilon_4)$. The four old values are replaced by the new values for the parameters, and the process is repeated for the next step in the four parameter space. We start with the four 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:

$$
\begin{aligned}
D_1 &= \sum_{i=1}^{3} 2w_i(AY_ix_i^b - y_i)AY_ix_i^b ln(x_i) + \sum_{i=4}^{5} 2w_i(BY_ix_i^b - y_i)BY_ix_i^b ln(x_i) + \\
&\quad \sum_{i=6}^{7} 2w_i(CY_ix_i^b - y_i)CY_ix_i^b ln(x_i) \\
D_2 &= \sum_{i=1}^{3} 2w_i(AY_ix_i^b - y_i)Y_ix_i^b \\
D_3 &= \sum_{i=4}^{5} 2w_i(BY_ix_i^b - y_i)Y_ix_i^b \\
D_4 &= \sum_{i=6}^{7} 2w_i(CY_ix_i^b - y_i)Y_ix_i^b \\
H_{11} &= \sum_{i=1}^{3} 2w_i(2(AY_i ln(x_i)x_i^b)^2 - Ay_iY_i(ln(x_i))^2x_i^b) \\
&\quad + \sum_{i=4}^{5} 2w_i(2(BY_i ln(x_i)x_i^b)^2 - By_iY_i(ln(x_i))^2x_i^b) \\
&\quad + \sum_{i=6}^{7} 2w_i(2(CY_i ln(x_i)x_i^b)^2 - Cy_iY_i(ln(x_i))^2x_i^b) \\
H_{22} &= \sum_{i=1}^{3} 2w_iY_i^2x_i^{2b} \\
H_{33} &= \sum_{i=4}^{5} 2w_iY_i^2x_i^{2b} \\
H_{44} &= \sum_{i=6}^{7} 2w_iY_i^2x_i^{2b} \\
H_{12} &= \sum_{i=1}^{3} 2w_iY_ix_i^b ln(x_i)(2AY_ix_i^b - y_i) \\
H_{13} &= \sum_{i=4}^{5} 2w_iY_ix_i^b ln(x_i)(2BY_ix_i^b - y_i) \\
H_{14} &= \sum_{i=6}^{7} 2w_iY_ix_i^b ln(x_i)(2CY_ix_i^b - y_i)
\end{aligned}
$$