Classifying radioactive isotopes with Monte Carlo

Patrick Green

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1 Introduction

This report will outline how a maximum likelihood fitting can be used to extract both decay constants from an isotope of two decay components. It will also outline whether the method of fitting is bias and whether is resembles a good representation of the experimental data.

2 Maximum Likelihood Fitting

The experimental data given contained a series of decay times for an isotope with two decay components. The decay time for each component will be referred to as t_a and t_b consecutively and the ratio of atoms that are of component a as f. To fit a model the method of maximum likelihood fitting was used. For any data point with decay time t the probability of that value occurring is $p(t/t_a, t_b, f)$. For this isotope the probability is:

$$p(t/t_a, t_b, f) = f(1/t_a)exp^{-t/t_a} + (1-f)(1/t_b)exp^{-t/t_b}$$

A model can be fitted to the data by minimizing the value of LL. As every data point is independent the probability for this experiment occurring is:

$$L = \prod_i p(t_i/t_a, t_b, f)$$

To maximize this value is the same as to maximize the $log(L)$ and therefore the solution is the most minimal value for the Negative Linear Likelihood which is:

$$LL = -\sum_i log(p(t_i/t_a, t_b, f))$$

The minimizing was done using the **scipy.optimize** function **minimize** with the *Nelder-Mead* algorithm.

3 Parameter Estimation

As the likelihood is posed as a probability the resulting parameters will lie in a Normal distribution given by the equation of a Gaussian:

$$p(x_j) = \frac{1}{\sqrt{2\pi\sigma_j^2}} exp^{-\frac{1}{2\sigma_j^2}(x_j - \widehat{x}_j)^2}$$

Using this probability distribution the value for the LL function is given by:

$$-LL = \sum_j \frac{1}{2} ln(2\pi) + ln(\sigma_i) + \frac{1}{2\sigma_j^2}(x_j - \widehat{x}_j)^2$$

Assuming the measurement errors σ_j are constant the LL function differs only with the value of $\chi = \sum_j \frac{1}{\sigma_j^2}(x_j - \widehat{x}_j)^2$ by 0.5 and therefore an increase in the LL function by 0.5 corresponds to an increase in σ of the estimated parameter.

By fitting the model to 10000 experimental measurements and analyzing the distribution of possible parameter values to find the parameter value σ above and σ below, the following results were attained:

Parameters	Estimate	$+\sigma$	$-\sigma$	Error
t_a	0.19783951	0.195	0.201	0.003
t_b	1.3072256	1.279	1.337	0.03
f	0.7484944	0.742	0.755	0.013

Below are the distribution of parameter values for t_a, t_b and f consecutively plotted in the region -3σ to 3σ where the values for $-\sigma$ and σ are marked:

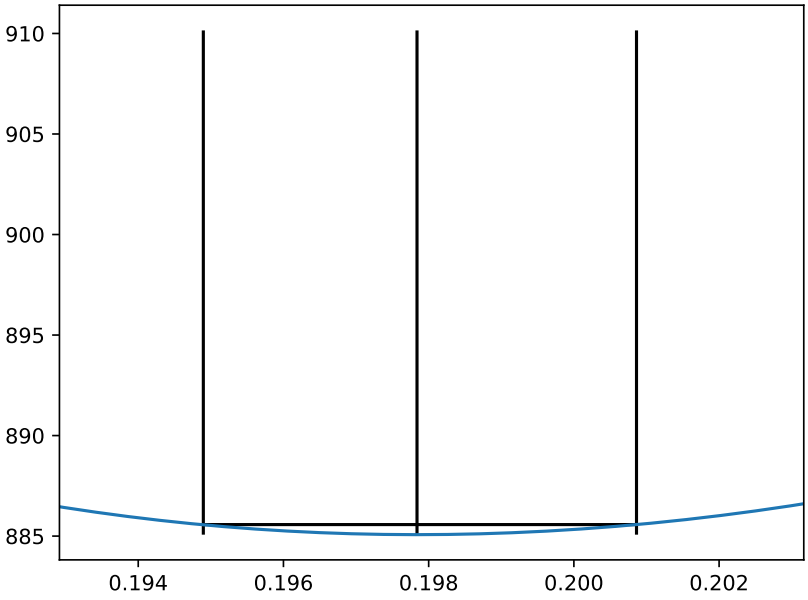


Figure 1: The value of t_a at $-\sigma$ is 0.195 and the value at $+\sigma$ is 0.201

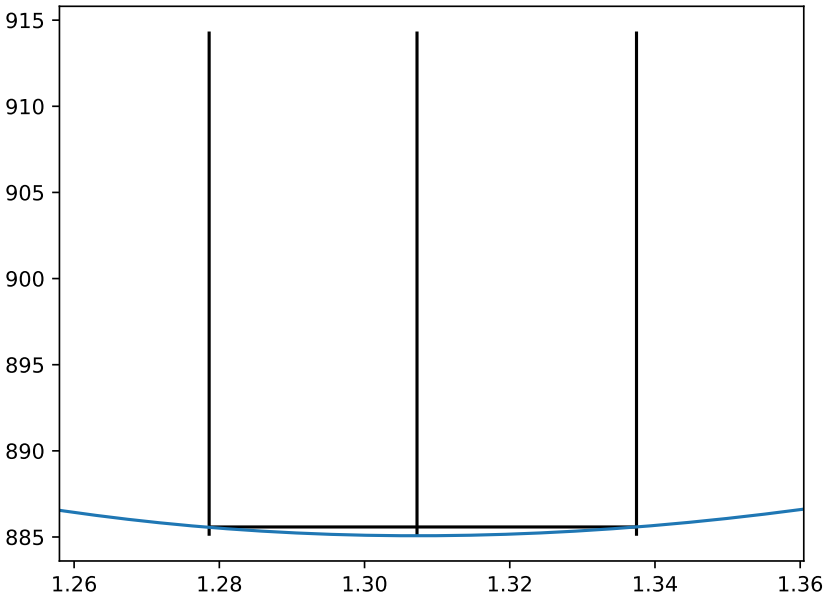


Figure 2: The value of t_b at $-\sigma$ is 1.279 and the value at $+\sigma$ is 1.337

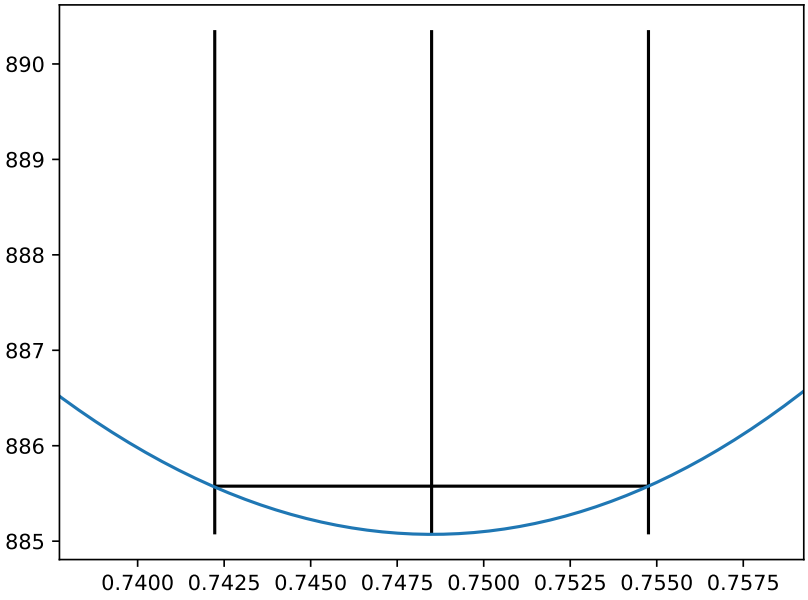


Figure 3: The value of f at $-\sigma$ is 0.742 and the value at $+\sigma$ is 0.755

4 Experimental Error

To test whether a parameter estimation method using log likelihood was a good representation of the experiment the model was simulated using a Monte Carlo method. This was done by sampling random decay time values in the range of $0 : 7$ seconds and then either including that value in the test set or excluding it depending on whether a generated random number is less than the

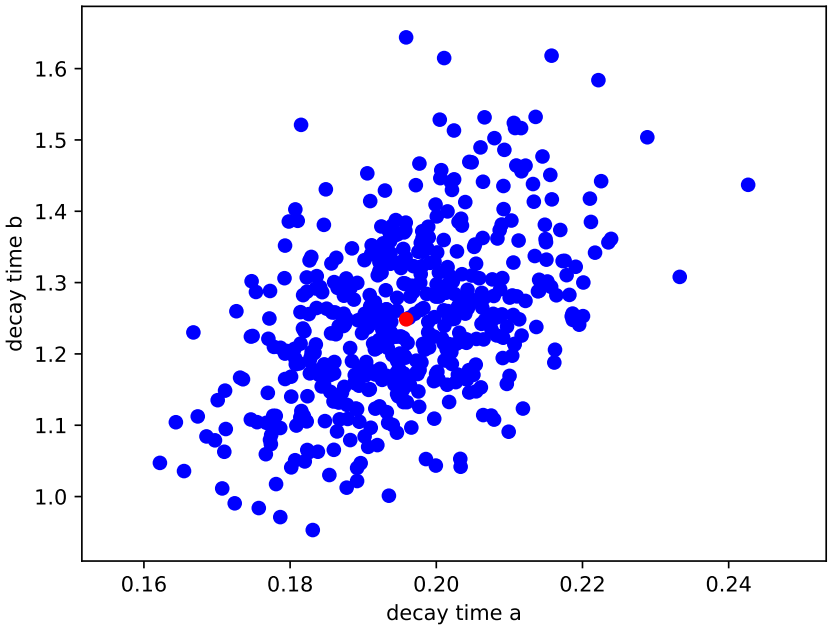
evaluated probability for that decay time. As each independent atom in the simulation required a probability in which it would decay or not given the model parameters. For this I normalized the probability used in the previous section so that its integral over t resulted in zero. The probability in which any atom would decay:

$$p(t/t_a, t_b, f) = A(f(1/t_a)exp^{-t/t_a} + (1-f)(1/t_b)exp^{-t/t_b}) \qquad A = \frac{(t_a t_b)^2}{1 + f(t_b^2 - t_a^2)}$$

As the Monte Carlo simulation uses the generation of a random number with a uniform distribution the fitted parameters will vary through a normal distribution. A normal distribution will generate a value in the region of its mean with a standard deviation equal to 1 over the square root of the size of the sample. The following results are obtained from 500 Monte Carlo runs each with 10000 data points therefore the result of the simulation will vary by $\frac{1}{\sqrt{500}}$ percent of the estimated value which is 0.045.

Parameter	Mean	Stdev	Error as %
t_a	0.195	0.013	0.067
t_b	1.250	0.117	0.093
f	0.740	0.033	0.044

The estimated errors for the simulation for each parameter are 0.067, 0.093 and 0.044 respectively and were calculated as the $\frac{mean}{standarddeviation}$ across each of the 500 Monte Carlo experiments. It appears the method is biased as both the error for t_a and t_b are above the estimate for the error in a normal distribution of 500 predictions which is 0.045. A plot of the estimated parameters for both decay times of each component is plotted bellow. It is clear the larger error is induced by the method overestimating t_b given t_a is high and vice versa as there appears to be positive correlation in the graph and not a true normal distribution.



Furthermore the error estimated by varying the LL function in the fitting process in section 3 is a lot lower than the error calculated in the Monte Carlo simulations. This is most likely due to the model not following the exact behavior of the isotopes. Also possibly the measurement error σ_j is not constant and affected by the background radiation as the values fitting the original experimental measurements estimate each parameter as a lot higher than the estimates from the Monte Carlo simulations. Below is a graph of the frequency of each decay time for the experimental measurements in blue and the Monte Carlo model in red. It is clear that the Monte Carlo model

overestimates the error that occurs in an actual experiment as the randomness of it doesn't seem to match entirely. This is understandable as the assumption that every atom is independent used in the derivation of the LL function is incorrect. Therefore a method without that assumption might be required to estimate the parameters