

Addendum to Intermediate Physics for
Medicine and Biology, 4th ed.
Fitting Exponentials

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The discussion of determining parameters in an exponential fit to experimental data needs expansion. This will be done in the next edition. In the meantime, please make these four changes in the fourth edition.

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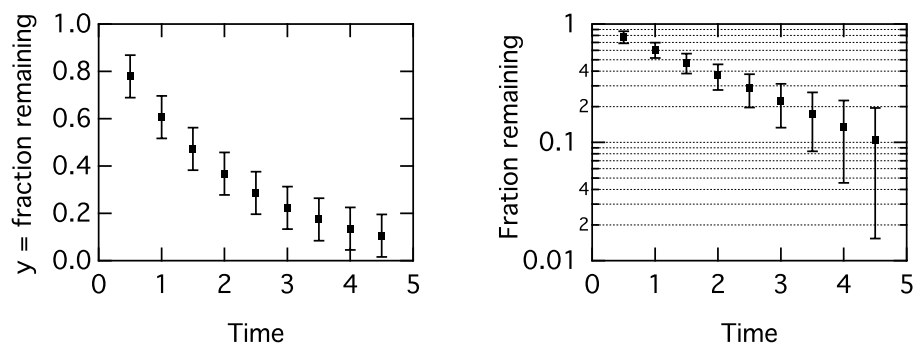


FIGURE 1. Plot of $y = e^{-0.5x}$ with error bars ± 0.09 on linear and semi-log paper.

0.1 Insert at the end of Section 2.3

When we are dealing with real data, we must consider the fact that each measurement has an experimental error associated with it. If we make several measurements of y for a particular value of the independent variable x , the values of y will be scattered. We indicate this by the error bars in Fig. 1. (Determining the size of these error bars is discussed in Chapter 11.) The data points in Fig 1 are given exactly by $y = e^{-0.5x}$, where y is the fraction remaining at time x . There is no data point for $x = 0$, but we must make sure that our fitting line passes through the point $(0,1)$. The error bars show an error of ± 0.09 . The error bars on the semi-log plot are not all the same, being much larger for long times (small values of y). If we don't plot the error bars before drawing our line, we will give too much emphasis to the data points for small y .

Equal error bars for all the points on a semi-log plot correspond to the same percentage error for each point, as shown in Fig. 2.

0.2 Insert at the end of Section 2.8

A more modern and better way to fit multiple exponentials is to use the technique of non-linear least squares. This is discussed in Sec. 11.2.

0.3 Replace Sec. 11.1.4

The least-squares technique described here gives each data point the same weight. If some points are measured more accurately than others, they should be given more weight. This can be done by assigning each data

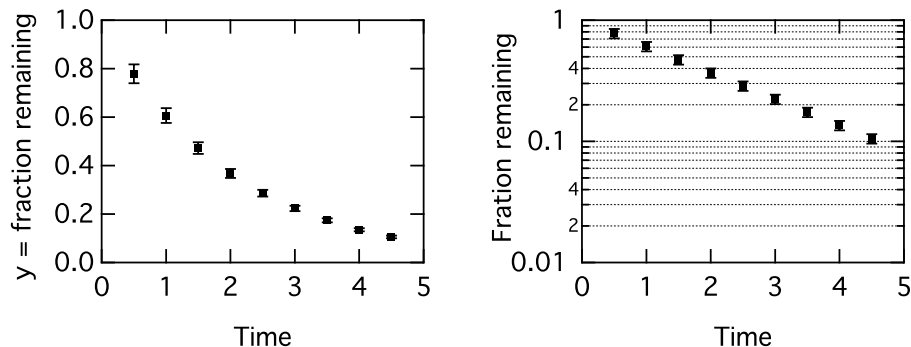


FIGURE 2. Plot of $y = e^{-0.5x}$ with error bars that are 9% of each y value.

point its own weight, replacing Eq. 11.2 by

$$Q = \frac{1}{N} \sum_{j=1}^N w_j [y_j - y(x_j)]^2. \quad (11.9)$$

For example, repeated measurements of y_j for a particular x_j might give results that are Gaussian-distributed about a mean value with standard deviation σ_j and variance σ_j^2 . (See Appendices G and I.) Then it would be appropriate to use the weight $w_j = 1/\sigma_j^2$. Setting all the weights equal to 1 as we have been doing is correct only if the variance is the same for each y_j . It is easy to show that the effect of this weighting is to add a factor of $1/\sigma_j^2$ to each term in the sums in Eqs. 11.8 [Gatland (1993)].

This analysis assumes that errors exist only in the y values. If there are errors in the x values as well, it is possible to make an approximate correction based on an effective error in the y values [Orear (1982)] or to use an iterative but exact least-squares method [Lybanon (1984)]. The treatment of unequal errors has been discussed by Gatland (1993) and by Gatland and Thompson (1993).

0.4 Replace Sec. 11.2.

If we need to fit a single exponential to a set of data, we have two choices:

Method 1. Use semi-log paper or make a linear fit to $v = \log y$.

Method 2. Use a statistical package that makes a fit directly to $y(x)$ using the method of non-linear least squares.

Both methods can be used either with uniform weighting of each data point, Eq. 11.2, or with individual weightings, Eq. 11.9.

The linear least-squares technique, Method 1, can only be used to fit data with a single exponential $y = ae^{-bx}$, where a and b are to be determined.

Take logarithms of each side of the equation:

$$\log y = \log a - bx \log e,$$

$$v = a' - b'x.$$

This is a linear equation, and constants a' and b' can be determined using Eqs. 11.5. With a sum of two or more exponentials, this method does not work. We will see below that even when it does work, Method 1 should not be used.

Method 2 can be used for any fitting function, for example $y = a^{-bx}$, $y = ae^{-bx} + c$, or even a sum of exponentials:

$$y = a_1 e^{-b_1 x} + a_2 e^{-b_2 x} + \dots$$

When we try to minimize Q by the technique of the previous section, we find that when the derivatives of this fitting function are set equal to zero, the equations in a_1, a_2 , etc., are linear if we assume that the values of the b_k are known. However, the equations for determining the b 's are transcendental equations that are quite difficult to solve.

The problem can be solved using the technique of *nonlinear least squares*. In its simplest form, one makes an initial guess for each parameter¹ $b_{10}, b_{20}, \dots, b_{k0}$ and says that the correct value of each b is given by $b_k = b_{k0} + h_k$. The calculated value of y is written as a Taylor's-series expansion with all the derivatives evaluated for b_{10}, b_{20}, \dots :

$$y(x_j; b_1, b_2, \dots) = y(x_j; b_{10}, b_{20}, \dots) + \frac{\partial y}{\partial b_1} h_1 + \frac{\partial y}{\partial b_2} h_2 + \dots$$

Since y and its derivatives can be evaluated using the current guess for each b , the expression is linear in the h_k , and the linear least-squares technique can be used to determine the values of the h_k that minimize Q . After each h_k has been determined, the revised values $b_k = b_{k0} + h_k$ are used as the initial guesses, and the process is repeated until a minimum value of Q is found. The technique is not always stable; it can overshoot and give too large a value for h_k . There are many ways to improve the process to ensure more rapid convergence. The most common is called the Levenberg–Marquardt method [see Bevington and Robinson (1992) or Press *et al.* (1992)].

Using the method of non-linear least squares used to be quite difficult. Now, however, it is available in many statistical packages, such as R (see The R Project at <http://www.r-project.org/>).

Referring back to Figure 1, we see that if each data point on a linear plot has the same weight (variance), then the weights of the log-transformed

¹The parameters a_k can either be included in the parameter list, or the values of a_k for each trial set b_k can be determined by linear least squares.

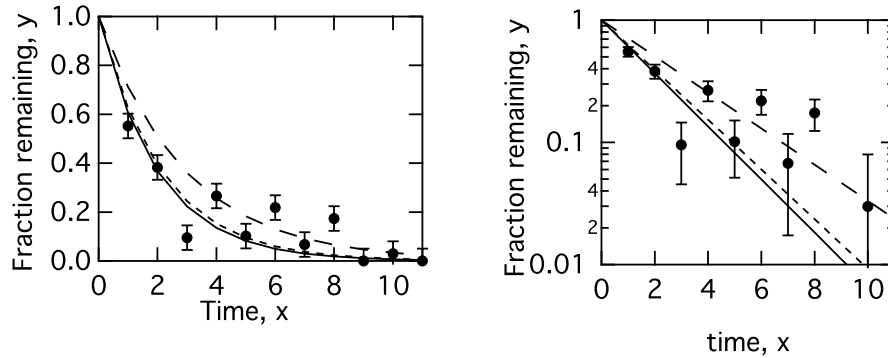


FIGURE 3. A comparison of fitting techniques when each data point has the same weight. The solid line shows the original model, $y = e^{-0.5x}$. The data points have a Gaussian-distributed random error with standard deviation 0.09. The dotted line is a non-linear least squares fit to y . The value of b is 0.47. The dashed line is a linear-least squares fit to log-transformed data, $v = \log y$. The value of b is 0.34.

data should be very different. This fact has not always been appreciated. It is very easy to use Method 1 (take the logarithm of y and make a linear least-squares fit to the transformed data) giving the same weight to each data point. This can give substantial errors in the parameters.

For example, some ecologists study the decomposition of litter on the forest floor. They make a number of porous litter bags, fill each one with the same mass of litter material $m(0)$, put them on the forest floor, and retrieve bags at various later times. If several bags are retrieved at the same time, there is much more scatter in the mass from bag to bag than there is in the original mass measurement $m(0)$. The dependent variable is the fraction of mass remaining: $y(x_j) = m(x_j)/m(0)$. A model, such as simple exponential decay, is used to fit y . There is no data point for $x = 0$ but the fit $y = ae^{-bx}$ must have $a = 1$. Sometimes there is nothing left in a litter bag and $y(x_j) = 0$.

Incorrect analyses occur frequently in the literature. Adair, Hobbie and Hobbie (2010) studied the way decomposition data have been analyzed in 498 papers. They also compared the results of using Method 1 and Method 2 on both real and artificial data.

At least forty percent of the papers used Method 1; only 15% explicitly stated that they used Method 2. The other papers were not clear about the method used. The distinction between the methods is shown in Fig. 3. The original model was simple exponential decay with $b = 0.5$: $y = e^{-0.5x}$. Gaussian-distributed random noise with standard deviation $\sigma = 0.09$ was added to each data point. (These values are typical of decomposition experiments.) When this was fit using Method 1, linear least squares on the

log-transformed data with all points weighted the same, the estimate of b was 0.34, a significant under-estimate. With Method 2, a non-linear least squares fit to the original data with equal weighting, the value of b was 0.47.

There is another problem with Method 1. If one of the values of $y(x_j) = 0$, it cannot be log-transformed. Some investigators have substituted arbitrary small values that are very far from the fit in the semi-log plot, greatly distorting the estimated value of b . It is better to delete these data points in Method 1. Zero values present no problem with Method 2.

Nearly 60% of the papers analyzed made the fit using $y = ae^{-bx}$ and adjusting a to improve the fit. This gave a smaller Q but the estimating function was not one at $x = 0$, and the value of b was quite different than if a is set equal to one.

In the simulation studies Adair *et al.* found that Method 1 gave reliable parameter estimates only when the errors were lognormally distributed (i.e., Gaussian in the log-transformed data). Method 2, however gave good parameter estimates in all cases. In the real data sets, Method 1 gave consistently larger estimates of b than Method 2. (This same effect was observed in the simulation studies.) The differences were most pronounced for rapid decay (large values of b).

The moral: use non-linear least squares, Method 2!

The same problem occurs when using log-log plots for allometric scaling (Packard, 2009).

0.5 References

Adair, E. C., S. E. Hobbie and R. K. Hobbie (2010). Single-pool exponential decomposition models: potential pitfalls in their use in ecological studies. *Ecology* 9(4): 1225-1236.

Packard,, G. C. On the use of logarithmic transformations in allometric analyses. *Journal of Theoretical Biology* 257: 515–518 (2009).