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Criteria for Choosing a Linearized Least-Squares Technique for the Exponential Model $\exp(A_1 + A_2 x)$

R. G. MUNRO

Center for Materials Science, National Measurement Laboratory, National Bureau of Standards, Washington, D.C. 20234

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A user-oriented discussion of the determination of the parameters A_1 and A_2 in the exponential model $\exp(A_1 + A_2 x)$ is presented in the context of four linear least-squares techniques. Among these four, the best method to use is found to be dependent on several criteria, of which the most important are: (1) the objective of the fit, (2) the range of data, and (3) the type of error contained in the data. Given the optimal method according to these criteria, the improvement in the estimated values of A_1 and A_2, obtained by extending either the range of data or the density of data, is also determined.

1. INTRODUCTION

The exponential model, $z(x) = \exp(A_1 + A_2 x)$, is frequently encountered in the analysis of experimental data. The model, whatever its application, requires that the values of A_1 and A_2 be estimated according to some subjectively chosen criteria using an observed set of experimental data. Most commonly, the choice made is to minimize the sum of the squared residuals. For the exponential model, this results in a nonlinear treatment of the data. While numerical techniques are now widely available to perform these nonlinear computations rather routinely, often the linearized model, $y = \ln z = A_1 + A_2 x$, is used because of its greater simplicity and convenience. In this note, attention is given to the linearized model, and a comparison is made among four possible methods of determining values for A_1 and A_2. Emphasis is placed on a special problem of the linearized least-squares model.

In general, there are many fine discussions readily available describing the least-squared-error technique of fitting a smooth curve through experimental data [1–6]. In the case of the exponential model, though, the use of a logarithm in the data analysis requires supplementary discussion. For example, it is well known [1, p. 252ff; 2, p. 180ff; 3, p. 673ff] that the process of linearization effectively changes the weight factors of the observed data. Suppose $[(x_i, z_i), i = 1, N]$ is a set of data where x is the independent variable and z is the dependent variable. Then, the linearization effectively yields a greater weight for the smaller values of z. To compensate for this effect, a modified weight factor is commonly recommended according to the reasoning that if the weight factor w_i for the ith point in the data set is inversely

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proportional to the variance of the value z_i, then the modified weight w_i' should be inversely proportional to the variance of $\ln z_i$. Hence, $w_i' \sim w_i z_i$. What is not widely realized is that this procedure can affect, seriously and deleteriously, the estimated values of A_1 and A_2 in some circumstances.

The difficulty is that there are two distinguishable objectives involved in the fitting of data by models, and standard discussions of the least-squares method address only one of these. For the exponential model, this is:

(I) Best smooth curve: Through the given data, obtain an exponential curve that most closely represents the trend of the observed data.

It has already been noted that the customary measure of the goodness of a fit to data is the value of the sum of the squared residuals,

$$\sigma^2 = (N-2)^{-1} \sum_i (z_i - \exp(A_1 + A_2 x_i))^2. \tag{1}$$

An alternative objective can also be stated:

(II) Best parameter values: On the basis of the observed data, obtain values for A_1 and A_2 that deviate from their true values by as little as possible.

A dimensionless measure of the goodness of a pair of values (A_1, A_2) can be given by the squared relative error,

$$\delta^2 = (A_1 - \alpha_1)^2/\alpha_1^2 + (A_2 - \alpha_2)^2/\alpha_2^2, \tag{2}$$

where (α_1, α_2) is the corresponding pair of ideal parameter values.

It might be thought, at first, that these two objectives are equivalent, but they are not. The first objective is applicable when a smooth curve is desired for the purpose of interpolation. This is the case to which theoretical statistics has devoted much effort, and in this case, the actual values of the parameters A_1 and A_2 may have no significance. The second objective is applicable when the parameters are physically meaningful, for example, as transition rates or bandgap energies.

It is quite easy to imagine a case in which the two objectives represent dfferent interests. Suppose that a set of data $[x_i, z_i]$ is given with the uncertainty of any z being, e.g., ± 10 %. The independent variable x is assumed to have no error. Suppose also that the values of z range over several orders of magnitude such that $0 < \delta_i^2 < \delta_{i+1}^2$ and $\delta_1^2 \ll \delta_N^2$, where δ_i is the estimated error at the ith point of the data. In this case, the equal percentage uncertainty of all the data implies that all points should have an equal effect on the estimated values of the parameters, yet, per force, δ_N^2 must influence those values much more strongly than δ_1^2, in the prescription of objective I. In other words, it is conceivable that the relative errors at the smaller, though equally good, values of z could be exaggerated compared to the relative errors at the larger, but not better, values of z. Necessarily, the values of the parameters suffer an error from this procedure.

To guard against an unwarranted bias in favor of the values of z with the larger magnitudes, it is sometimes thought that the data should be weighted so that, effec-

tively, it is the relative squared error that is minimized. In this case, while $\delta_1^2 \ll \delta_N^2$, the relative values $(\delta_i/z_i)^2$ are comparable for all points in the data. For the present problem, it can be seen in Section 3 that this procedure has only limited value. For the sake of greater generality, this alternative is considered here, as well as the use of the modified weight factor, w_i'.

Specifically, consideration is given to a choice among four linearized versions of Eq. (1) which can be minimized with respect to A_1 and A_2 by the simpler linear least-squares methods. These are:

$$S_{\mathrm{U}}^2 = \sum_i w_i(\ln z_i - A_1 - A_2 x_i)^2, \tag{3}$$

$$S_{\mathrm{M}}^2 = \sum_i w_i z_i(\ln z_i - A_1 - A_2 x_i)^2, \tag{4}$$

$$S_{\mathrm{UR}}^2 = \sum_i w_i(1 - (A_1 + A_2 x_i)/\ln z_i)^2, \tag{5}$$

$$S_{\mathrm{MR}}^2 = \sum_i w_i z_i(1 - (A_1 + A_2 x_i)/\ln z_i)^2, \tag{6}$$

where the subscripted letters are intended to suggest the meanings U = unmodified, M = modified, and R = relative. The methods denoted by the letters U and M are the most widely used procedures. Method U, with $W_i = 1$, is available on many pocket calculators and is often used because of this convenience. Table 1 provides an illustration of the differences that result from the different procedures. (Details of the computation are deferred until Section 2.) In this example, method U yields the best values of the parameters as judged by objective II, but method *M* yields the best smooth curve through the data as judged by objective I. In general, it can be seen that the type of error in the data, the method of analysis, and the objective of the analysis are all significant considerations. Further, the criteria of smallest standard error and best parameter values can be nonequivalent to a significant degree. Other examples in the form of Table 1 would show that the performances of the four methods yield

TABLE 1

A Simple Example of Variable Results in the Relative Performances of Four Least-Squares-Fitting Procedures for the Model $f(x) = \exp(A_1 + A_2 x)$[a]

Method	$\lvert\%$ Err. $A_1\rvert$	$\lvert\%$ Err. $A_2\rvert$	Parameter ranking	Standard error	Stnd. err. ranking
U	0.6	0.1	1	97	3
M	17	3	4	66	1
UR	8	0.4	3	123	4
MR	6	0.6	2	82	2

[a] For this example, $A_1 = 1.0$, $A_2 = -0.1$. A relative random error ε is associated with $f(x)$ such that $z = (1 + \varepsilon)f(x)$ and $|\varepsilon| \leqslant 0.25$. Methods U, M, UR, MR are specified by Eqs. (3)–(6).

variable rankings, according to the type of error, the range of data, and the density of data.

The observations on Table 1 indicate that the most that should be expected for the methods represented by Eqs. (3)–(6) is a statistical basis for selecting the appropriate method for a given problem. The most commonly followed procedure for laboratory work is to use an unweighted data set in which case the w_i may all be set equal to unity in Eqs. (3)–(6). Since any other nonequivalent choice for the w_i requires a knowledge of the experimental details, only the case $w_i = 1$, for all i, is considered in this note. In Sections 2 and 3, a discussion of the relative performance of the four methods, for each of the two objectives, under a variety of conditions, is presented. Based on these results, the improvement in the determined values of the parameters, that can be achieved by increasing the density or the range of data, is examined in Section 3.

2. Approach

The present determination of the relative performances of the least-squares methods represented by Eqs. (3)–(6) follows from a simple pedestrian approach. It has already been noted that there are at least three important considerations: the objective, the method, and the nature of the error. In addition to these, it was noted that the range of the data and the magnitude of the errors must also be considered. All of these points can be examined statistically by analyzing a collection of simulated data sets. If the ideal parameters α_1 and α_2 are known, then a set of data can be generated according to the equation

$$z_i = (1 + \varepsilon_i) \exp(\alpha_1 + \alpha_2 x_i), \tag{7}$$

where ε_i is a computer-generated random number representing the relative error of the ith element of the data set. (The random-number generator used for this simulation produced a normally distributed error with a mean value of zero. The magnitude of the error was controlled by the choice of the variance of the normally distributed error.) The nature of the error can also be varied, and in this note, five types of error are examined. To be definite, let the data set be ordered such that, for ideal values, $z_1 < z_2 < \cdots < z_N$. With respect to this ordering, the types of error can be denoted as follows.

(A) $\sigma(\varepsilon_i) = \sigma_0$. All data points have comparable percentage error.

(B) $\sigma(\varepsilon_i) = \sigma_1$ for $i < N/2$ and $\sigma(\varepsilon_i) = \sigma_2 < \sigma_1$ for $i \geqslant N/2$. The data set is composed of two parts obtained under different experimental conditions. Each part is individually of type A.

(C) Same as B except $\sigma_2 > \sigma_1$.

(D) $\sigma(\varepsilon_i) > \sigma(\varepsilon_{i+1})$. The percentage error decreases steadily with increasing z.

(E) $\sigma(\varepsilon_i) < \sigma(\varepsilon_{i+1})$. The percentage error increases steadily with increasing z.

For error type A, the optimal least-squares method can be anticipated theoretically. When all $\sigma(\varepsilon_i)$ are equal and the squared residuals are weighted by the reciprocal variances of the z_i, the minimum variance estimation of the parameters is produced by method U. Often the individual variances of the z_i are not known experimentally, and then a further estimate is made which, in practice, sets $\text{var}(z_i) = \sigma_0^2$ for all i. This is equivalent to setting all $w_i = 1$ as is done here. Consequently, to the extent that the second approximation can be applied, the optimal method for error type A should be method U.

In all cases, the data were generated using Eq. (7) according to the following scheme. The independent variable, x, was chosen to be equally spaced such that there were n points of data for each decade in the range of z-values. The ideal independent variable, z, was chosen to cover the range $10^{-1} - 10^{N-1}$, where N is the number of decades in the range of z. The total number of points in a given data set was then the product nN. (As a practical note for computer computations, when other values of x are encountered, it could be desirable to scale the dependent variable to bring the data into a range equivalent to what was used here. This would be useful as a means of avoiding underflow, overflow, and extreme round-off errors in the computations.)

The values of the ideal parameters α_1 and α_2 were selected as follows. First, as a result of several trial cases, it was found that there was a quantitative variation in the results depending on the algebraic signs of the parameters. Consequently, the four combinations $(\text{sgn}\,\alpha_1, \text{sgn}\,\alpha_2) = (-,+)$, $(+,-)$, $(-,-)$, and $(+,+)$ were treated separately. Second, it was then found that quantitative variations among widely varying pairs of values of (α_1, α_2) having the same $(\text{sgn}\,\alpha_1, \text{sgn}\,\alpha_2)$ were negligible. Third, the quantitative variations among cases of different $(\text{sgn}\,\alpha_1, \text{sgn}\,\alpha_2)$ did not produce qualitative differences except in the case of error type D in the range of five to seven decades of data. Consequently, the numerical values of the ideal parameters were selected to sample the ranges of values that can be expected in laboratory applications.

For example, one of the more extreme cases of parameter values occurs in the study of transient capacitance time constants versus reciprocal temperature for deep-level impurities in semiconductor materials. In this case, $\alpha_1 \gtrsim -25$ and $\alpha_2 \lesssim 6.5$ are typical values. A second example is the study of viscosity. Under temperature or pressure variations, the viscosity of a liquid can be driven through one of the widest range of values of any property characterizing a material substance. Viscosities of liquids can vary from about 10^{-3} to 10^{13} P with the variation being roughly exponential in either pressure or reciprocal temperature. The pressure variations are usually larger and have parameter values on the order of $\alpha_1 \geqslant -10$ and $\alpha_2 \lesssim 4$ GPa^{-1}.

From such observations, the kth values of 25 pairs of values were assigned as follows:

$$(-,+) \qquad \alpha_1(K) = -25 + 2(K-1)/3, \qquad \alpha_2(K) = 6.5 - 0.125(K-1), \tag{8}$$

$$(+,-) \qquad \alpha_1(K) = 25 - 2(K-1)/3, \qquad \alpha_2(K) = -6.5 + 0.125(K-1), \tag{9}$$

$$(-,-) \qquad \alpha_1(K) = -2 - (K-1)/3, \qquad \alpha_2(K) = -2 - (K-1)/12, \tag{10}$$

$$(+,+) \qquad \alpha_1(K) = 2 + (K-1)/6, \qquad \alpha_2(K) = 2 + (K-1)/12. \tag{11}$$

For given values of the ideal parameters and the independent variable x, Eq. (7) was used to generate the data for a simulated experiment. In each case, 100 replications of the experiment were performed; i.e., 100 sets of random relative errors were generated. Thus, for each commbination of $(\operatorname{sgn}\alpha_1, \operatorname{sgn}\alpha_2)$, results were obtained for 2500 least-squares fits. The normally distributed random relative errors had a mean value of zero. The variance $\sigma^2(\varepsilon)$ was chosen to simulate the typical experimental situation in which the uncertainty in the data is not worse than about 10 %. For the five error types A through E designated above, (A) $\sigma_0 = 0.1$, (B) $\sigma_1 = 0.1$, $\sigma_2 = 0.025$, (C) $\sigma_1 = 0.025$, $\sigma_2 = 0.1$, (D) $\sigma(\varepsilon_i) = (N + 1 - i)\,0.1/N$, (E) $\sigma(\varepsilon_i) = 0.1i/N$, where N = total number of data points and where the ordering of the ideal values of z was given above.

3. Numerical Results

All numerical computations were performed in a double-precision mode, and test calculations were made with all errors set equal to zero to observe the performance of the numerical routines under optimum conditions. The largest relative error obtained in these cases was about 2×10^{-16} for either parameter.

The two objectives were each examined with respect to the four methods of fitting and five error cases. For objective I, the best smooth curve through the data, the results were nearly unanimous. With only a few isolated exceptions, the modified method, represented by Eq. (4), produced significantly better results. As noted in the introduction, this was expected. The results for objective II were less straightforward.

To determine the best-fitting method for objective II, the rms relative parameter error, obtained as in Eq. (2) and averaged over all fits, was plotted for each method as a function of the number of decades of data and the number of points of data per decade. As an example, Fig. 1 illustrates the average results for error type B. For only one decade of data, the curves show a slight preference for method UR. However, for more than one decade, the relative methods rapidly become significantly worse than methods U and M and, therefore, are not shown for the other decades. From one to three decades, method M is the best, but at three decades, the curves of U and M cross. Thereafter, method U is best. By 10 decades, the error of method M is about five times that of method U.

The precise location of the crossing of the curves is necessarily uncertain in itself because of the statistical nature of the study. To measure the significance of the separation of two curves, the 95 % confidence limit for the value of δ for each ideal parameter pair was determined on the basis of the 100 replications of the experiment. The largest of these, for all the parameter values, was used for the error bars in Fig. 1.

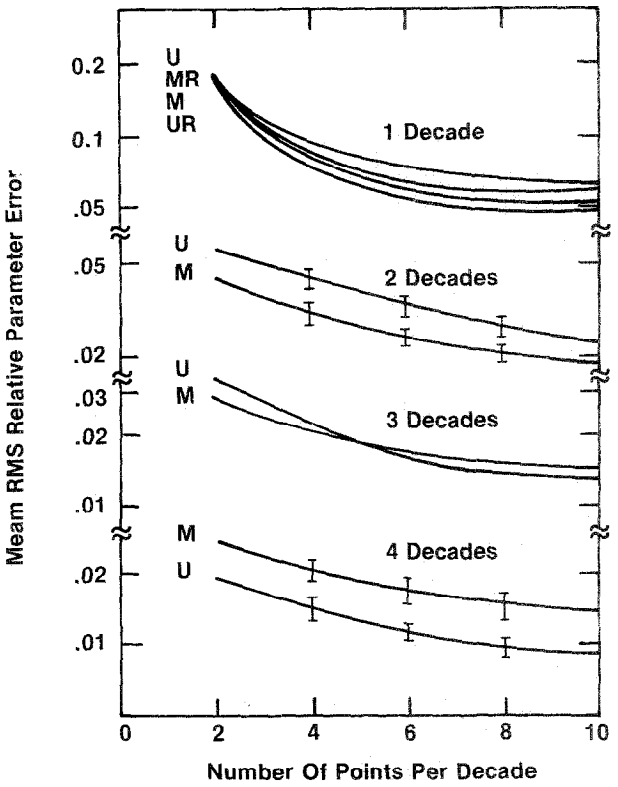

Fig. 1. Mean rms relative parameter error [see Eq. (2)] as a function of the range and density of data for error type B, illustrating the procedure for determining the best least-squares method for obtaining the best parameter values.

Following this procedure for each of the five types of error, the overall results are illustrated by Fig. 2, with one exception, which is detailed in Table 2. The numerical values of Fig 2 were obtained for the case $(\operatorname{sgn}\alpha_1, \operatorname{sgn}\alpha_2) = (-, +)$, and the values were scaled to represent in each case an average experimental error of about 10 %. Since there were quantitative variations among the four combinations of $(\operatorname{sgn}\alpha_1, \operatorname{sgn}\alpha_2)$, Fig. 2 is intended only to illustrate the relative importance of different ranges and densities of data and as a comparison of the different error types. The table inset of Fig. 2 gives the qualitative results which were the same for all cases of $(\operatorname{sgn}\alpha_1, \operatorname{sgn}\alpha_2)$.

As suggested in Section 2, method U was always optimal for error type A and objective II. Additionally, method U was always the best method for objective II applied to error types C and E. For error types B and D, the best method varied with the number of decades, as indicated in the figure.

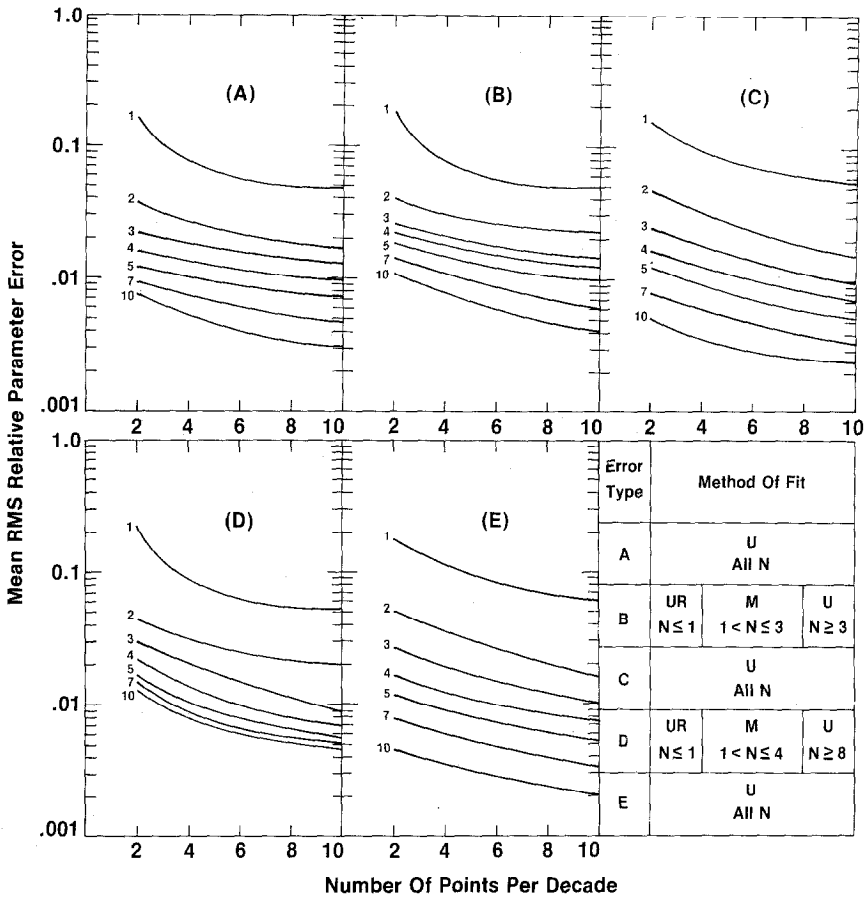

FIG. 2. The best curves of the mean rms relative parameter error [see Eq. (2)] as a function of the range and density data for error types A through E. The average standard deviation of the normally distributed input error is 0.10. The numbers beside the curves denote values of N = number of decades of data. The methods U, M, UR, and MR are specified by Eqs. (3)–(6). The table inset identifies the method of fit as determined by the procedure of Fig. 1.

TABLE 2

For Error Type D and Objective II, the Best Least-Squares Method Showed a Variation with (sgn α_1, sgn α_2), as Given Here[a]

(sgn α_1, sgn α_2)	5 dec.	6 dec.	7 dec.
(−, +)	M	U	U
(+, −)	M	M	M, U
(−, −)	M	U	U
(+, +)	U	U	U

[a] These cases had nonoverlapping error bars except for (+, −) at seven decades of data. In the latter case, the curves crossed at a density of about five points per decade.

4. Conclusion

The present statistical examination of four linear least-squares methods of fitting the exponential model $\exp(A_1 + A_2 x)$ to experimental data has the following conclusions. (1) The best smooth curve through the given data is almost always given by the well-known technique of using a modified weight factor. (2) The best values of A_1 and A_2, as determined by Eqs. (3)–(6), frequently do not produce the smallest standard error when Eq. (1) is subsequently used for its evaluation. (3) The range and density of data and the type of error determine a statistically best linear method for evaluating A_1 and A_2. (4) Increasing the range of data is generally more effective for improving the parameter values than is increasing the density of data.

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