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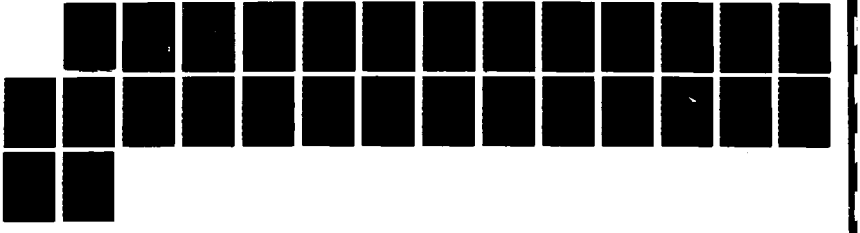

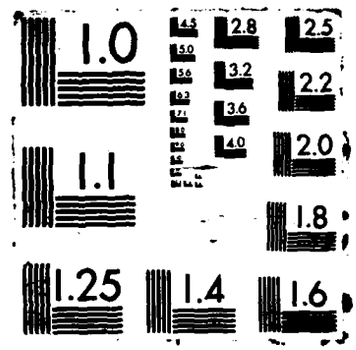
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Error Estimation Using the Simplex Method in Nonlinear Least Squares Data Analysis

by

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ABSTRACT

The simplex method is a widely-used technique in analytical chemistry. Although primarily viewed as a technique for experimental optimization, this method is also used for mathematical modeling, such as nonlinear least squares curve fitting. Acceptable methods of chemical data analysis require estimates of both the parameter values and their errors - something which is not provided by current simplex algorithms. This paper proposes a procedure for obtaining error estimates of the fitted parameters. The proposed method can be easily implemented on a laboratory minicomputer, greatly enhancing the utility of the simplex method to analytical chemists. This procedure is first described for a general function, and then illustrated using a data set from the literature.

INTRODUCTION

Many chemical and physical problems involve locating the position of an optimum (e.g., a maximum or minimum response) which is a function of several variables. By simultaneously varying several factors, the simplex method is a much more efficient technique for finding such an optimum than traditional methods of varying one factor at a time(1). This technique was introduced in 1962 by Spendley et al.(2) for optimizing either physical processes or mathematical functions. Nelder and Mead(3) modified the original work to allow the simplex to expand or contract according to the layout of the response surface, greatly increasing the potential utility of the method.

In an early application to analytical chemistry, Long(4) used the simplex method to optimize the colorimetric determination of sulfur dioxide. However, it was not until Deming and Morgan(1) began to promote the procedure in 1973 that the simplex method began to find widespread use among analytical chemists. Largely as a result of their work, this technique is now widely used by analytical chemists(5). Among its many applications, simplex optimization finds extensive use in the development of analytical methods and in optimizing the performance of analytical instruments(6).

Although primarily used by chemists for experimental optimization, the simplex method has also been used for mathematical modeling, such as nonlinear least squares curve fitting(7). In fact, Nelder and Mead(3) emphasized function minimization in their work on the simplex method. A simplex algorithm for nonlinear data analysis has recently been published as part of a work on computer applications in chemistry(8). However, most analytical chemists use nonlinear least squares routines based on gradients (first-order derivatives) or on the Hessian matrix (second-order derivatives). The advantages and disadvantages of these methods when

compared to the simplex method depend largely on the type of information being sought. In experimental optimization the functional relationship between variables is usually not known; the simplex technique performs excellently while derivative-based methods fail completely.

The simplex method does have some advantages even when the mathematical model is known. One advantage is the absence of evaluation of partial derivatives. Despite its apparent simplicity, the calculation of derivatives can be a source of problems. Incorrect differentiation or errors in programming the calculation of derivatives has been shown to be one of the most common causes of failure in nonlinear least squares algorithms(9). As the function being minimized becomes more complex, this advantage becomes more attractive. The size of the algorithm is significantly reduced by the absence of derivatives; the remaining calculations are simple and can be easily programmed on a laboratory minicomputer. Probably the most significant advantage of the simplex method is its robustness with respect to starting values. All nonlinear fitting routines, including the simplex algorithm, require initial estimates of the (unknown) parameters. The simplex method will converge from almost any starting values. (Of course poor initial estimates require more computational time.) Derivative-based methods, on the other hand, require starting values close to the unknown parameters. This consideration becomes especially important in the analysis of multidimensional data.

When compared to derivative-based methods, the simplex method has two major disadvantages: lack of speed and the absence of error estimation. The simplex method is much slower than Hessian methods, and becomes even slower as the number of variables increases. Problems with long computational times can be mitigated, but not eliminated, by efficient coding in a language such

as FORTRAN. In particularly bad cases, calculations can be run overnight and the results examined the next day. The absence of error estimates is not a significant problem for experimental optimization, particularly if a parametric model does not exist for the response surface. However, when fitting data to theoretical models the lack of error estimates is a fundamental problem. Analytical results are incomplete without a measure of uncertainty in addition to an estimate for the unknown quantity. This is illustrated in Figure 1, where absorbance versus time data from reference 1 have been modeled using a simplex algorithm. The data in Figure 2 were obtained from Figure 1 by a 200% increase in the residuals. The parameter estimates are the same for both cases. However the results are clearly not equally reliable.

The simplex method first attracted our interest during an ultrasonic absorption study of metal ion complexation kinetics. To maximize the information obtained from our kinetic measurements, we explored the possibility of using existing theoretical models for a multidimensional fit of the acoustic absorption coefficient as a function of acoustic frequency, temperature, and concentration. A Levenburg-Marquardt nonlinear least squares algorithm(10) has normally been used in our work; however, application of this routine would require evaluation of the partial derivatives of a complex function and, more importantly, "good" initial estimates of the unknown parameters. The simplex algorithm provides a method of avoiding these problems, but lacks error estimates.

This paper is concerned with the estimation of errors in the calculated parameters when using the simplex method for curve fitting. A proposal by Nelder and Mead has been incorporated into a subroutine which can be implemented with only minor modifications to an existing simplex algorithm.

Although this proposal is conceptually simple, our experience has shown that problems can arise in its implementation unless care is taken. These problems, our solutions to them, and improvements to the original proposal are discussed below; our experiences may be beneficial to others. The procedure is first outlined for a general function, and then illustrated for the data set in Figure 1.

EXPERIMENTAL

The calculations reported below were performed on a DEC LSI 11/23 computer with 32K words of memory. A variable-size simplex algorithm coded in FORTRAN by O'Neill(11) was used with minor modifications(12-14). Matrix inversion was accomplished using subroutines from the LINPACK library(15), although other statistical packages or locally developed programs should also be satisfactory.

The algorithm by O'Neill was converted to single precision, except for variance calculations. Most chemical data are not sufficiently precise to warrant the additional computer memory and time required by double precision calculations. These requirements are particularly important when computations are done on a laboratory minicomputer such as the LSI. For instance, kinetic data are obtained in our laboratory with an 8 bit ADC (Tektronix 7D20) and have a precision of 1 part in 256. Double precision arithmetic with a precision of 1 part in 10^{16} is clearly not justified.

The objective function being minimized is the sum of squares between the measured and predicted observations. Following Bevington's notation, this function will be referred to as χ^2(16). At convergence the variance between the best k vertices of the simplex is less than a preset tolerance, where k equals the number of unknown parameters. This criterion was

suggested by Nelder and Mead(3) as being particularly advantageous for least squares function minimization. The exact value of this tolerance can significantly affect the estimated errors unless the precautions outlined below are followed.

DESCRIPTION OF METHOD

The simplex procedure derives its name from the geometrical figure which moves across the error surface in search of the minimum: a simplex is a figure defined by one more point than the number of unknown parameters in the function. For example, if experimental data are being fit to a function with three unknown parameters, the simplex will consist of four vertices in a three-dimensional space. Each point represents a set of parameter values, and is associated with a vector in parameter space. The vertex with the highest value of the error function is eliminated and replaced by its reflection in the hyperspace defined by the remaining vertices. The rules governing this action have been discussed elsewhere(1,6) and will not be repeated here. This paper will confine its attention to the estimation of errors in the fitted parameters.

For purposes of discussion, assume one is trying to fit n experimental observations to a nonlinear function, f, with k unknown parameters. The quantity being minimized is

$$\chi^2 = \Sigma_i \, w_i(y_i - f_i)^2 \qquad (1)$$

where y_i and f_i are the i^{th} observed and predicted data points, respectively, and w_i is the weight due to nonconstant variance. (In cases

of constant variance, w_i is unity for all observations.) Once χ^2 has been minimized the "standard" simplex algorithm is complete; however errors in the parameter estimates have not yet been determined.

A brief review of error estimation in nonlinear least squares is appropriate at this point. Most error estimates are derived from the curvature matrix evaluated at the minimum in the error surface(16). Qualitatively, if the curvature with respect to a parameter, θ_i, is small, then χ^2 is relatively insensitive to the variation in that parameter. Therefore, θ_i is not well defined and will have a large uncertainty. Conversely, if the curvature is large, that parameter will be well defined and have a small uncertainty. The curvature matrix, α, contains the second partial derivatives of χ^2. The ij^{th} element of α is given by

$$\alpha_{ij} = \frac{\partial^2 \chi^2}{\partial\theta_i \partial\theta_j} \qquad (2)$$

The variance-covariance matrix contains estimates of the errors in the parameters, and is given by $\varepsilon = s^2\ \alpha^{-1}$. The quantity s^2 is the mean square error, and equals $\chi^2/(n-k)$. The estimated standard deviation in the i^{th} parameter is given by

$$\sigma_{\theta_i} = s\ \sqrt{\varepsilon_{ii}} \qquad (3)$$

where ε_{ii} is the i^{th} diagonal element of ε.

This suggests that the simplex estimates can be used to calculate partial derivatives and form the curvature matrix. This matrix can then be inverted and used to compute the variance-covariance matrix. Martin and

Hackbarth(17) followed a similar approach, using a commercial software package to calculate the statistical properties of the simplex estimates. The size of the commercial package used required that these calculations be done on a large, centrally located computer. The current popularity of laboratory computers results in large part from their ability to provide experimental control (including data acquision) as well as to analyze data. Consequently, the simplex algorithm should be capable of both curve fitting and the estimation of errors in fitted parameters.

The simplex method does not yield any estimate of the curvature matrix of second derivatives at the minimum. In their article, Nelder and Mead briefly discuss a method of constructing this matrix without the evaluation of derivatives. A detailed mathematical proof of their approach is beyond the scope of this article; the interested reader is referred to the original work(2,3). A flow chart of the procedure, including our modifications, is presented in Figure 3.

The final simplex consists of k+1 vertices in k-dimensional parameter space. Let these vertices be denoted by V_0, ..., V_k, with χ_i^2 denoting the value of the error surface at vertex V_i. Further, let V_0 be the vertex with the lowest error, χ_0^2. Finally, let $\vec{\theta}_i^t = (\theta_{i,1}, \ldots, \theta_{i,k})$ be the parameter vector corresponding to vertex V_i. As usual the superscript "t" denotes transpose.

A quadratic approximation can be used to fit the error surface in the vicinity of the final simplex. The k+1 points of the final simplex are combined to form "half-way points" $\vec{\theta}_{ij}=(\vec{\theta}_i+\vec{\theta}_j)/2$, $i \neq j$. The value of χ^2 at θ_{ij} is denoted by χ_{ij}. The combined set of $(k+1)(k+2)/2$ points are then used to calculate χ^2 near the minimum:

$$\chi^2 = \chi_0^2 + \vec{a}^t Q^{-1} \vec{\Delta} + \frac{1}{2} \vec{\Delta}^t (Q^{-1})^t B Q^{-1} \vec{\Delta} \qquad (4)$$

Table I defines the quantities in the above equation in terms of the values of χ^2. Initially equation 4 may appear to be needlessly complex and no improvement over more conventional approaches. The importance of this equation lies in its ability to define the gradient ($(Q^{-1})^t \vec{a}$) and the curvature matrix ($0.5\ (Q^{-1})^t B Q^{-1}$) as simple functions of the error surface.

In using this approach, it is necessary to avoid two extremes: (1) allowing the final simplex to become so small that the elements of the B matrix are largely the result of rounding errors in the calculation of χ^2, or (2) a simplex so large that the quadratic approximation is not valid. Our experience with a variable size simplex algorithm suggests the first extreme presents the greater hazard. This is particularly true when an overly strict convergence criterion is applied. The curvature of the error surface decreases as the final simplex becomes smaller. The elements of the B matrix are a measure of this curvature, and hence become poorly defined. The seriousness of this hazard will, of course, depend on the shape of the error surface and the function being fit.

To protect against a lack of curvature, Nelder and Mead(3) suggested that the difference $\chi_1^2 - \chi_0^2$ should be at least 10^3 times greater than the roundoff error in the calculation of χ^2. Our experience has been that the relative difference, $(\chi_1^2 - \chi_0^2)/\chi_0^2$, gives superior performance. If this condition is not satisfied, the distance between V_1 and the centroid is doubled and the condition checked again. This process is repeated for each vertex until the inequality is satisfied. Our work has indicated that use of the relative difference along with realistic estimates of the roundoff error provides protection against both extremes.

Once the final vertices have been checked for sufficient curvature, "half-way points" V_{ij} are computed for $i \neq j$. With these points, sufficient values of the error surface exist to construct the quadratic surface given in equation 4. The parameter vector corresponding to the minimum in the error surface is easily calculated:

$$\vec{\theta}_{min} = \vec{\theta}_0 - QB^{-1}\vec{a} \tag{5}$$

The inequality

$$\vec{a}^t B^{-1} B^{-1} \vec{a} < 1/4 \tag{6}$$

provides a check on the validity of the quadratic approximation. If this inequality is not valid, $\vec{\theta}_0$ is replaced by $\vec{\theta}_{min}$ in Table I, the elements of $\vec{a}$, B, and Q are reevaluated and a new $\vec{\theta}_{min}$ calculated. Our experience to date has been that $\vec{\theta}_{min}$ and $\vec{\theta}_0$ do not differ significantly. Nonetheless, these calculations provide an additional check on the adequacy of the quadratic approximation.

Finally, using updated versions of Q and B, the error matrix can be calculated:

$$\varepsilon = s^2\, 2\, Q^t B^{-1} Q \tag{7}$$

where $s^2 = \chi^2_{min}/(n-k)$. If $\vec{\theta}_{min}$ and $\vec{\theta}_0$ are identical, the existing Q and B matrices can be used in this calculation. Given the ease of forming new matrices using $\vec{\theta}_{min}$ in place of $\vec{\theta}_0$ in Table I, we prefer to calculate updated matrices. Since function evaluations are inexpensive in terms of

computer time and memory, the only additional cost of this procedure is the inversion of the B matrix.

ILLUSTRATION

An appreciation of the preceeding discussion can be gained by estimating the errors in the parameters obtained when fitting the data in Figure 1. The calculations involved in the application of simplex minimization to this data set have been illustrated elsewhere(1,8). Our concern is limited to the calculation of error estimates after the minimization has been completed. We have analyzed this data set using simplex, Levenburg-Marquardt, and Gauss-Newton programs; as seen in Table II, the estimated parameters from each program are in agreement with those obtained by previous authors(1,8).

The data are being fit to the nonlinear model

$$A = A_{\infty}(1 - e^{-kt}) \qquad (8)$$

where A is absorbance, t is time, A_{∞} is the absorbance at infinite time, and k is the rate constant. A 3-dimensional plot of the error surface is shown in Figure 4. Cross sections of the error surface at the fitted values for A_{∞} and k are shown in Figure 5. This figure clearly demonstrates that A_{∞} is more precisely defined than k, and is a strong argument for the estimation of parameter errors in the analysis of this data set, as well as data in other areas of chemistry.

After minimizing χ^2, the final simplex consists of three vertices in a 2-dimensional parameter space. There are two unknown parameters (A_{∞} and k).

Figure 6 shows these vertices superimposed on a contour plot of the error surface in the vicinity of the minimum. As discussed in the previous section, proper error estimation requires that the curvature matrix be computed from vertices sufficiently close together in parameter space so that the quadratic approximation is valid, but sufficiently separated so that the calculations are not simply the result of rounding error. It is of interest to note that if the "final" vertices from O'Neill's simplex algorithm are used to calculate error estimates, these errors are physically unrealistic (i.e. negative numbers). Application of the procedure outlined in Figure 3 results in an "expanded" set of vertices surrounding the minimum. These "expanded" vertices and the resulting "half-way" points are included in Figure 6. Considering the distorted shape of the error surface, the ability of this procedure to envelope the minimum and produce error estimates is quite good. The validity of our error estimates can readily be appreciated when compared to more sophisticated methods (see Table II).

Workers using the simplex commonly quote the standard deviation for lack of fit, s, as an indication of precision in fitted parameters. In the above example, the relative standard deviation in k equals 275% that in A_∞, demonstrating the inadequacy of s as a measure of the uncertainties in these quantities. The importance of this problem is, of course, a function of the model being fit, and another reason why parameter estimation is not considered complete without some estimation of the parameter errors.

CONCLUSION

Much of the work involving the simplex method in analytical chemistry has involved experimental optimization(5). Error estimation is often not appropriate for methods development or the optimization of instrumental conditions. In most of these cases, there is no precise understanding of the relationship between the individual factors. One of the advantages of the simplex method is its ability to function in these types of situations. Consequently, error analysis has not received the attention it deserves.

The simplex method can also be a useful tool for data analysis in analytical chemistry(7). This technique is conceptually simple, easily programmed on laboratory minicomputers, readily applicable to complex functions, and does not require either the evaluation of derivatives or starting estimates which are close to the final (unknown) values. However, to be useful for data analysis in a quantitative science such as analytical chemistry, the simplex method must provide error estimates of the final parameters. To the best of our knowledge, currently available simplex routines for minicomputers do not provide these estimates.

This paper has discussed a method for calculating error estimates, and the important factors in its implementation. The technique has been discussed in general terms, and then illustrated using one specific data set. However, this method is applicable to all problems in which experimental data are fit to a mathematical model. It can be easily incorporated into existing simplex routines, without requiring extensive computer memory or statistical expertise from the chemist. In spite of this simplicity, this method has a sound statistical basis and can provide chemists with much useful information.

LITERATURE CITED

1. Deming, S. N.; Morgan, S. L. Anal. Chem. 1973, 45, 278A.
2. Spendley, W.; Hext, G. R.; Himsworth, F. R. Technometrics 1962, 4, 441.
3. Nelder, J. A.; Mead, R. Computer Journal 1965, 8, 308.
4. Long, D. E. Anal. Chim. Acta 1969, 46, 193.
5. Deming, S. N.; Morgan, S. L. Anal. Chim. Acta 1983, 150, 183.
6. Deming, S. N.; Parker, L. R. CRC Critical Reviews in Analytical Chemistry 1978, 7, 187.
7. See reference 5 for a survey of the applications of the simplex method in analytical chemistry.
8. Jurs, P. C. "Computer Software Applications in Chemistry"; Wiley: New York; 1986.
9. Miller, A. J. In "Interactive Statistics"; McNeil, D., Ed.; North-Holland: New York, 1979.
10. Nash, J. C. J. Inst. Maths. Applics. 1977, 19, 231.
11. O'Neill, R. Appl. Stat. 1971, 20, 338.
12. Chambers, J. M.; Ertel, J. E. Appl. Stat. 1974, 23, 250.
13. Benyon, P. R. Appl. Stat. 1976, 25, 97.
14. Hill, I. D. Appl. Stat. 1978, 27, 380.
15. Dongarra, J. J.; Moler, C. B.; Bunch, J. R.; Stewart, G. W. "Linpack User's Guide"; Society for Industrial and Applied Mathematics: Philadelphia, PA, 1979.
16. Bevington, P. R. "Data Reduction and Error Analysis for the Physical Sciences"; McGraw-Hill: New York, 1969.
17. Martin, Y. C.; Hackbarth, J. J. In "Chemometrics: Theory and Application"; Kowalski, B. R., Ed.; American Chemical Society Symposium, Ser. 52, American Chemical Society: Washington, D.C., 1977, pp 153-164.

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Table I. Matrix Elements in Equation 4.

$\vec{a}$ vector:	$a_i = 2\,\chi_{0i}^2 - (\chi_i^2 + 3\,\chi_0^2)/2$	$i=1,\ldots,k.$
B matrix:	$b_{ii} = 2\,(\chi_i^2 + \chi_0^2 - 2\,\chi_{0i}^2)$	$i=1,\ldots,k.$
	$b_{ij} = 2\,(\chi_{ij}^2 + \chi_0^2 - \chi_{0i}^2 - \chi_{0j}^2)$	$i \neq j.$
Q matrix:	$q_{ij} = \vec{\theta}_{i,j} - \vec{\theta}_{0,j}$	$i=1,\ldots,k,$ $j=1,\ldots,k.$

Table II. Nonlinear Analysis of Data in Figure 1.

Method	A_∞, absorbance at t=∞		k, rate constant	
	Estimate	Error[a]	Estimate	Error[a]
Simplex				
Reference 1	.404	[b]	.170	[b]
Reference 8	.404	[b]	.170	[b]
This work	.404	.012	.170	.013
Marquardt[c]	.404	.009	.170	.010
Newton[c]	.404	.006	.170	.007

[a]Standard deviation of the estimated parameter.

[b]Not calculated in the original work.

[c]Computed using the IMSL library.

Figure Captions

Figure 1. Absorbance versus time data from reference 1. The solid line represents the nonlinear least squares fit using a simplex algorithm.

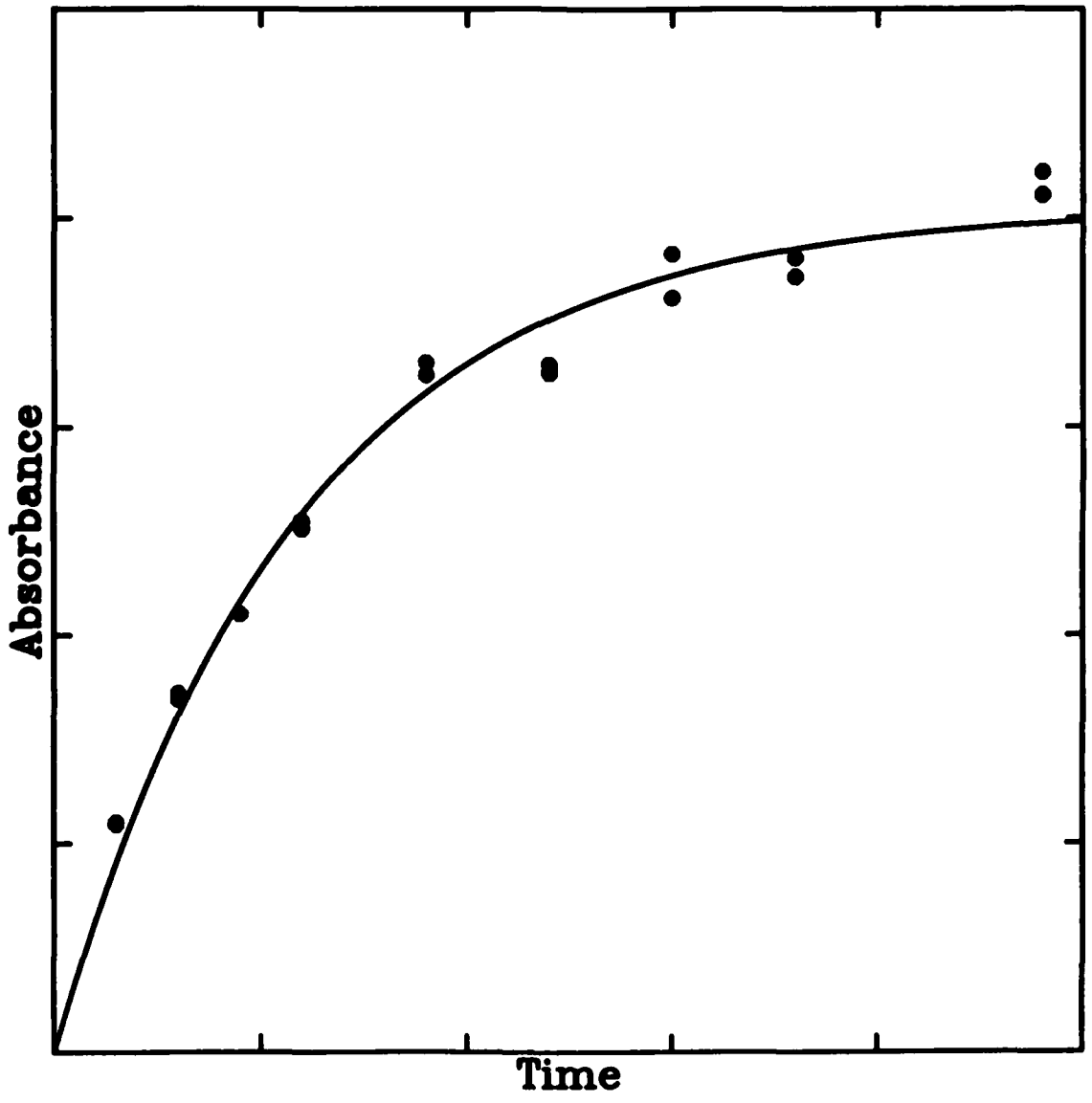
Figure 2. Absorbance versus time data obtained from Figure 1 by a 200% increase in the noise. Note that the fitted parameters are unchanged in value, but are clearly less reliable.

Figure 3. A flow chart for the estimation of errors in the parameters calculated by a simplex algorithm.

Figure 4. A 3-dimensional plot of the error surface for the data from Figure 1.

Figure 5. Cross sections of the error surface obtained when k is varied at A_∞=.40436 (—— ——), and when A_∞ is varied for k=.16968 (- - -).

Figure 6. Contour plot of the error surface in the vicinity of the minimum. Key to symbols: (o) vertices in the final simplex of the fitting routine, (*) vertices used to estimate errors, and (+) position of the minimum in parameter space. Note that the position of the final minimum coincides with one of the vertices from the simplex routine.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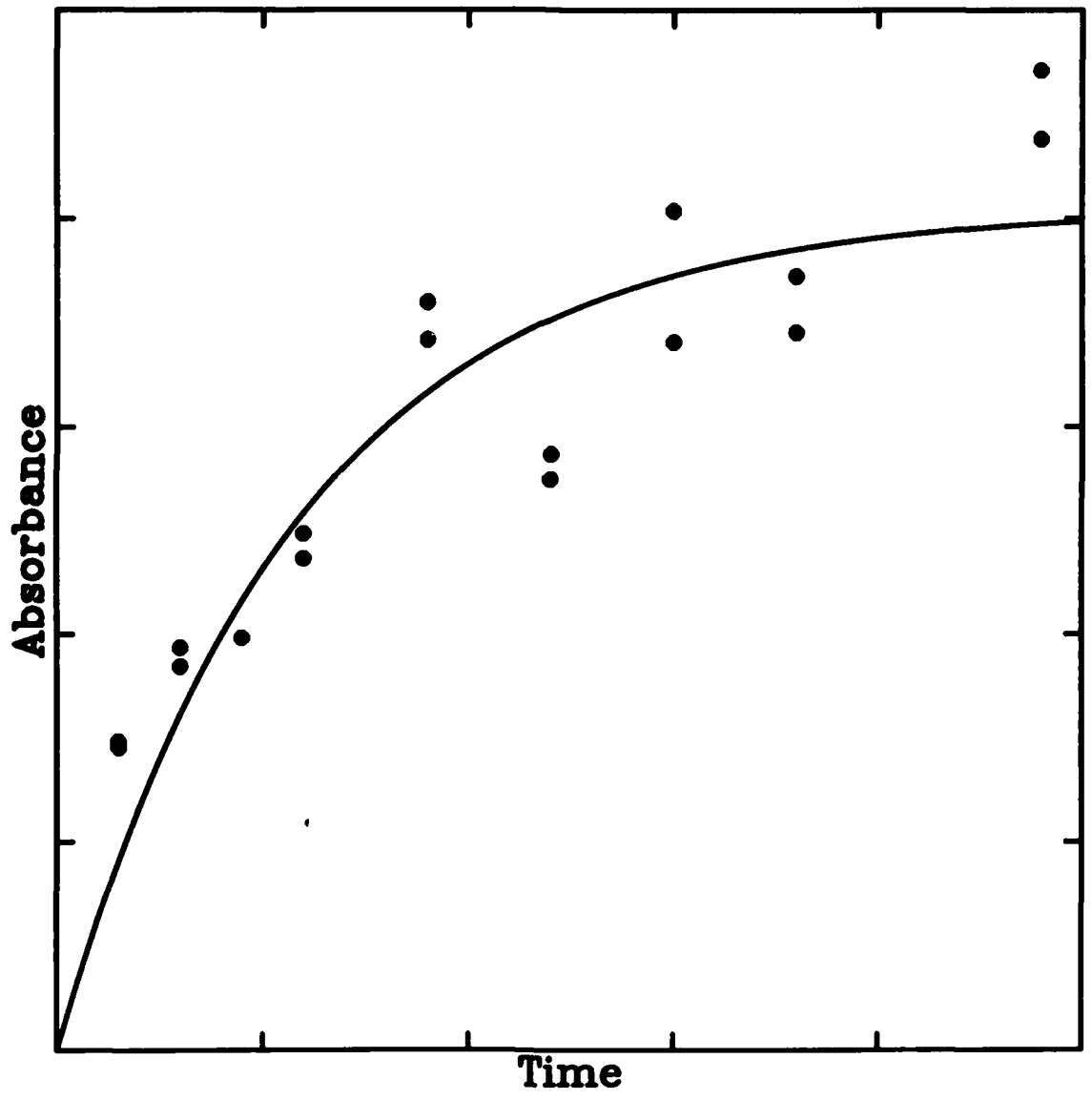
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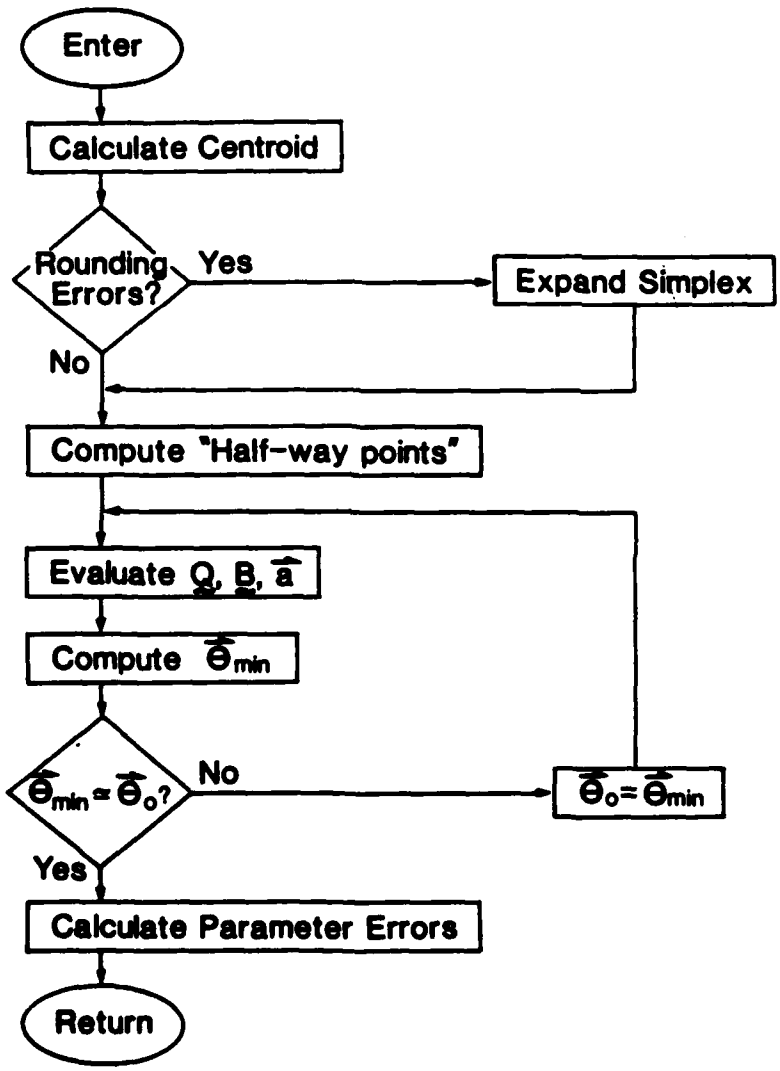
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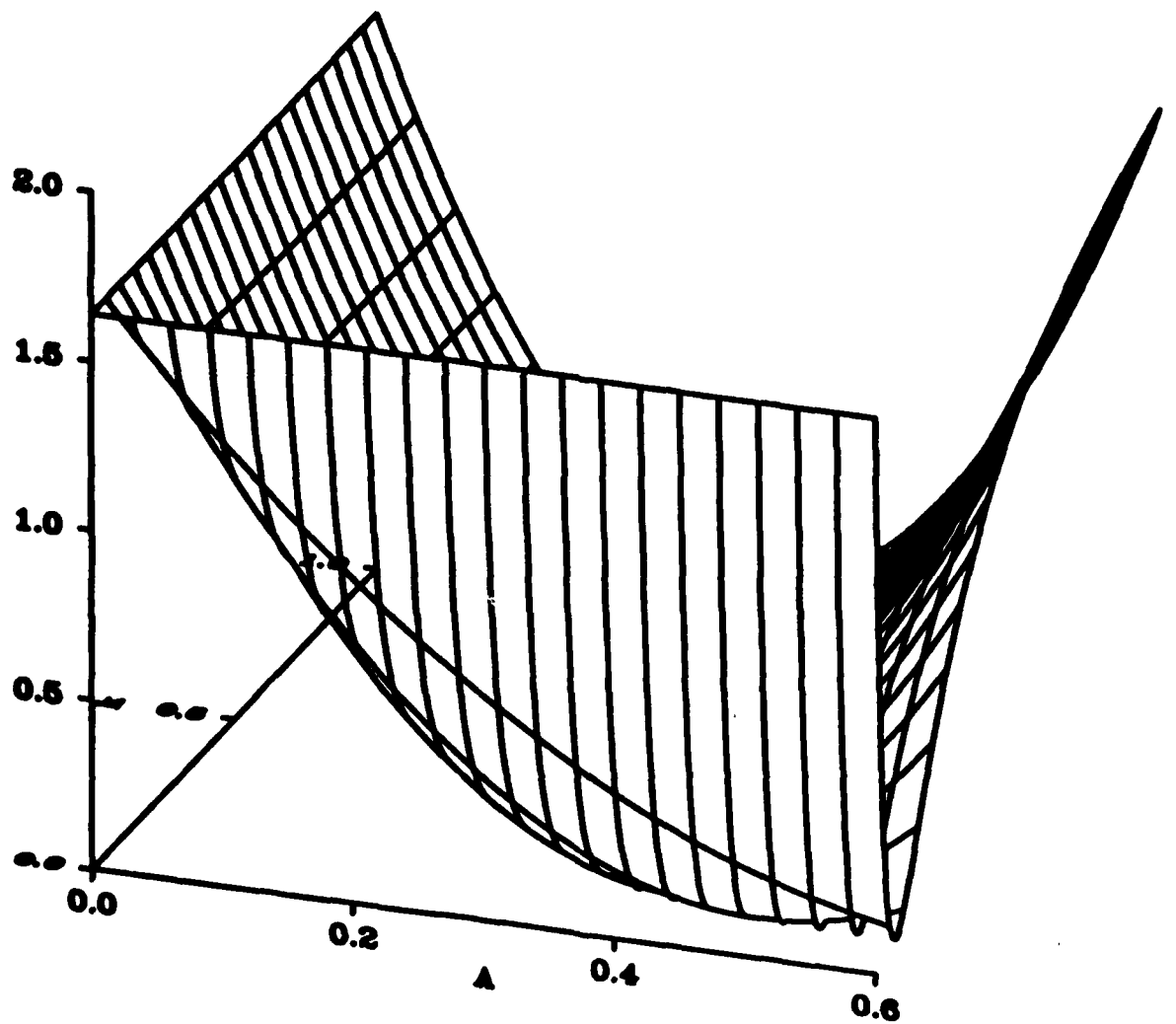
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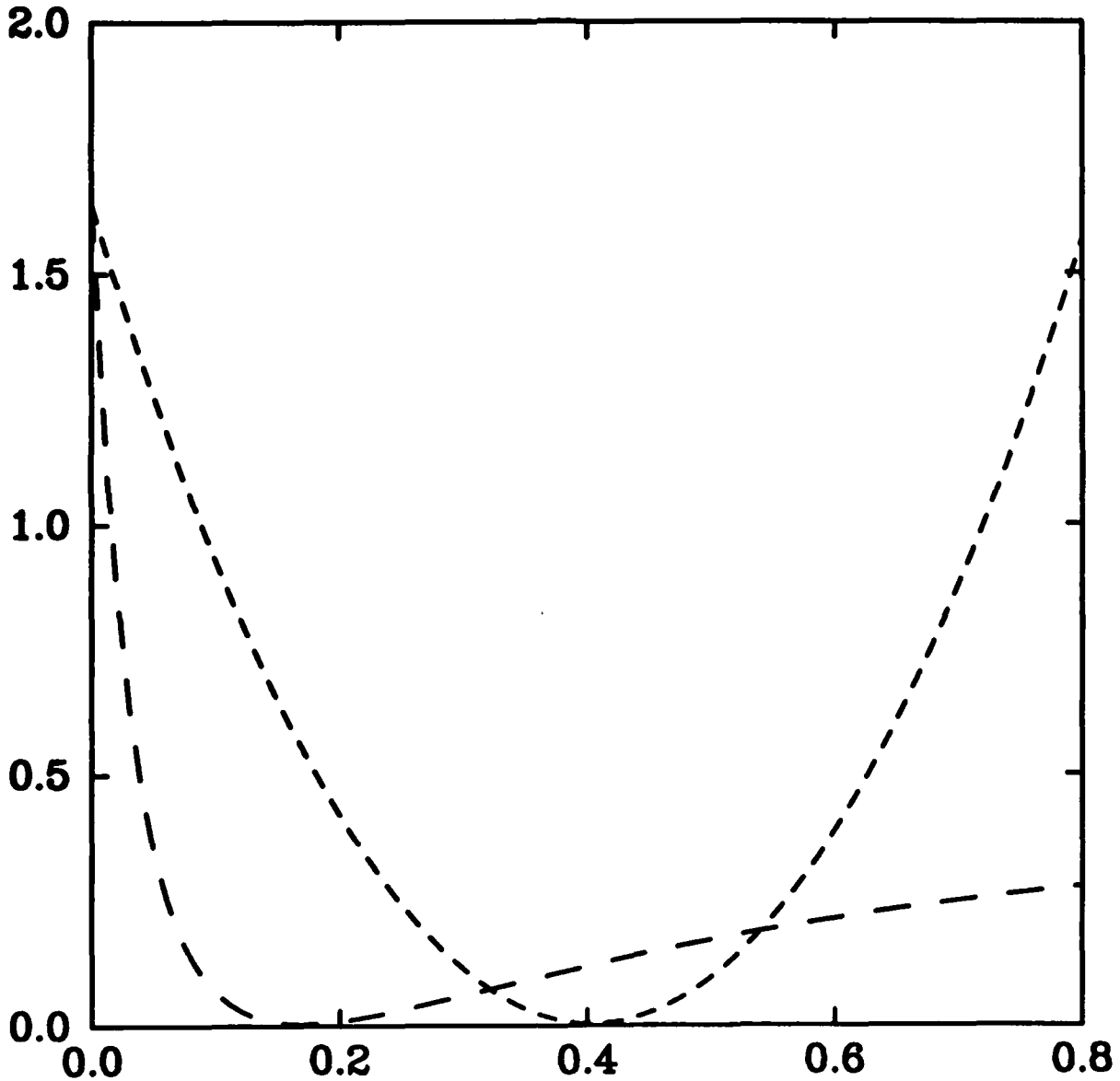
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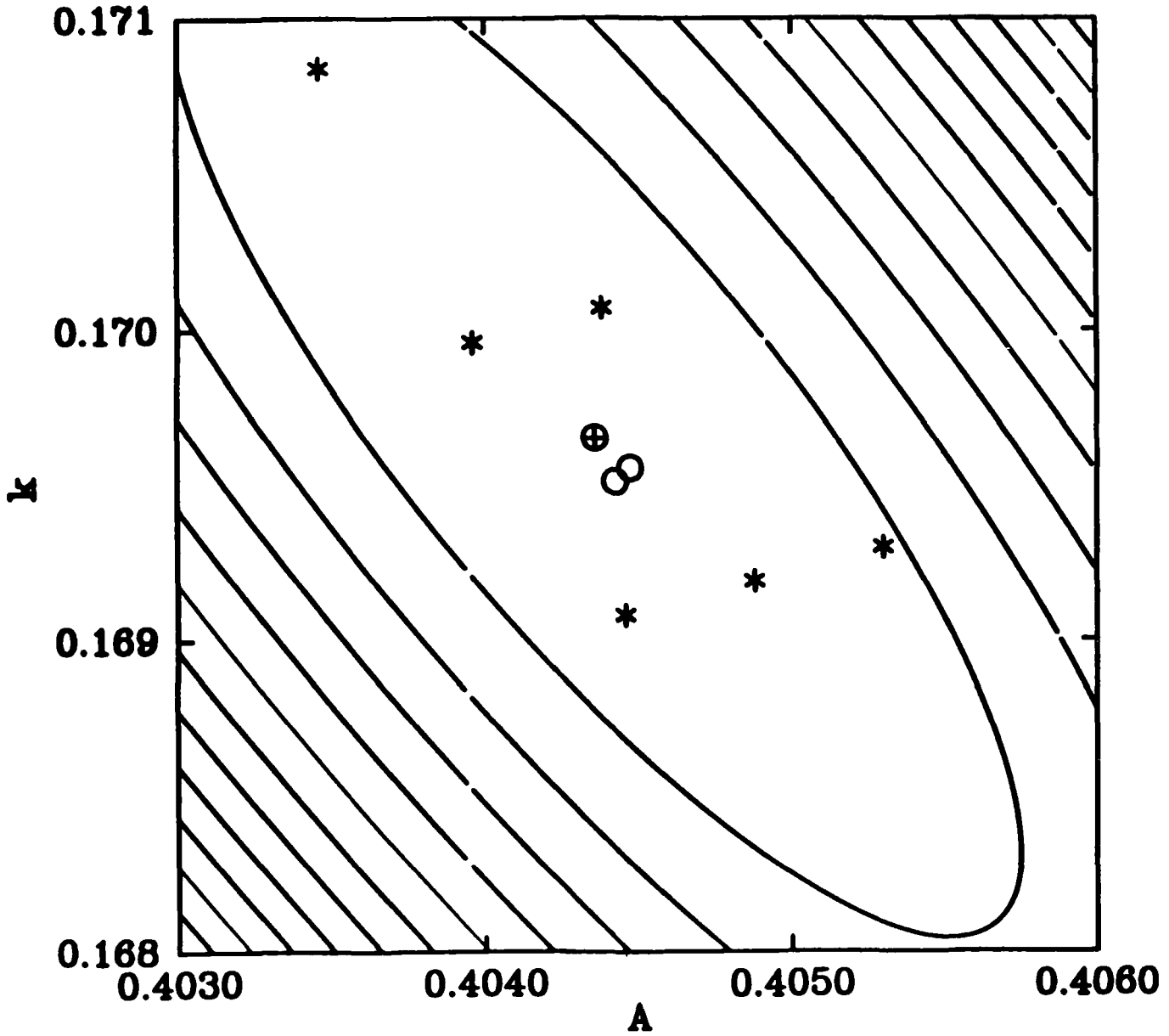
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Brief

The simplex method is frequently associated with experimental optimization. However, it is also a valuable technique for nonlinear data analysis. Current versions of the simplex algorithm do not provide error estimates of the fitted parameters. The importance of these estimates is discussed and a procedure is described for their calculation on laboratory minicomputers.

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