

A NOTE ON PARAMETER-EFFECTS CURVATURE

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ABSTRACT

The parameter-effects curvature measure of nonlinearity of Bates and Watts (1980) is examined for two models: a growth model and the Fieller-Creasy model. Exact confidence regions are constructed and are compared to linear approximation regions. For the first model the agreement between the regions is good despite high curvature. For the Fieller-Creasy model it is shown that the agreement can be quite poor despite low curvature.

Key Words: Nonlinear Regression; Curvature; Exact Confidence Regions.

1. INTRODUCTION

Bates and Watts (1980) propose relative measures of intrinsic and parameter-effects curvature for nonlinear regression models. The usefulness of these measures stems, in part, from the claim that they can be used to assess the adequacy of inferences based on the usual tangent plane approximation of the solution locus: Relatively small values for both the maximum intrinsic curvature Γ^N and the maximum parameter-effects curvature Γ^T indicate that the tangent plane approximation is reasonable, while relatively large values for either Γ^N or Γ^T indicate that this approximation is untenable.

In practice it is usual to find that Γ^N is relatively small while Γ^T is relatively large (Bates and Watts, 1980; Ratkowsky, 1983). In such situations, reparameterization may improve matters, but the best parameterization is known for only one-parameter models (Hougaard, 1983) and trial and error is a time consuming and often unrewarding method (Ratkowsky, 1983).

Using the two parameter Michaelis-Menten model, Bates and Watts (1981) give a dramatic example of what can be achieved through reparameterization when Γ^N is relatively small and Γ^T is relatively large. In the original parameterization, the exact and tangent plane 95% confidence regions for the unknown parameters differ drastically while these regions are quite close when based on the expected-value reparameterization (Ross, 1970).

Perhaps the most common methods for analyzing data from a nonlinear model are based on the tangent plane approximation. The clear implication of the recent work is that this approximation must not be used when Γ^T is large relative to the cutoffs given by Bates and Watts (1980, 1981); otherwise, the tangent plane approximation should be reasonable. Because of

the potential practical impact of the current work, particularly the recent book by Ratkowsky (1983), we expect that this note on our experiences with the Bates-Watts methodology will be of some value to the practitioner.

In Section 2 we briefly review relevant background material, describe methods for obtaining exact confidence regions and show by example that confidence regions based on the tangent plane can be reasonably accurate when the maximum parameter-effects curvature Γ^T is large.

In Section 3 we investigate the implications of the Bates-Wates methodology for the Fieller-Creasy problem. This problem was chosen because it is of considerable importance on its own (Wallace, 1980) and has several useful aspects that enable us to focus on key issues. In addition, it is hoped that the study of a particular problem will furnish some useful insight about Γ^T .

2. CURVATURES AND CONFIDENCE REGIONS

The standard nonlinear regression model can be represented as

$$y_i = f(\underline{x}_i, \underline{\theta}) + \varepsilon_i \quad , \quad i=1,2,\dots,n \quad (1)$$

where \underline{x}_i is a vector of known explanatory variables associated with the i -th observable response y_i , $\underline{\theta}$ is a $p \times 1$ vector of unknown parameters with true value $\underline{\theta}^*$, the response function f is assumed to be known, continuous and twice differentiable in $\underline{\theta}$, and the errors ε_i are assumed to be independent, identically distributed normal random variables with mean zero and variance σ^2 .

Let \underline{V} denote the $n \times p$ matrix with elements $\partial f(\underline{x}_i, \underline{\theta}) / \partial \theta_j$ $i=1,2,\dots,n$, $j=1,2,\dots,p$, and let \underline{P} denote the projection operator for the column space

of \underline{V} . In what follows, a "hat" added to any quantity indicates evaluation at the maximum likelihood estimate $\hat{\underline{\theta}}$, while a "star" indicates evaluation at $\underline{\theta}^*$. Finally, let $F(\alpha; p, \nu)$ denote the upper α probability point of the F distribution with p and ν degrees of freedom.

The reader is assumed to be familiar with the construction and properties of Γ^N and Γ^T as discussed in Bates and Watts (1980, 1981) and Hamilton, Watts and Bates (1982). In particular, recall that values of Γ^N and Γ^T less than $1/\sqrt{F(\alpha; p, \nu)}$ should indicate that the tangent plane approximation is reasonable; otherwise this approximation is to be judged untenable. Here, ν is the number of degrees of freedom associated with s^2 , the estimate of σ^2 used for constructing confidence regions for $\underline{\theta}^*$.

Let $\underline{\varepsilon}(\underline{\theta})$ denote the $n \times 1$ vector with elements $y_i - f(x_i, \underline{\theta})$, $i = 1, 2, \dots, n$, partition $\underline{\theta}^T = (\underline{\theta}_1^T, \underline{\theta}_2^T)$ and let $\underline{V} = (V_1, V_2)$ denote the conforming partition of \underline{V} . Potential pivots for constructing exact confidence regions for $\underline{\theta}_2^*$ can be obtained from the work of Gallant (1975) who shows that the likelihood ratio test statistic T_2 for the hypothesis $\underline{\theta}_2^* = \underline{\theta}_{20}$ can be represented as $T_2 - 1 = Z_2 + a_n$ where na_n converges to zero in probability and, under the null hypothesis,

$$Z_2 = \underline{\varepsilon}^T(\underline{\theta}^*) (\underline{P}^* - \underline{P}_1^*) \underline{\varepsilon}(\underline{\theta}^*) / \underline{\varepsilon}^T(\underline{\theta}^*) (\underline{I} - \underline{P}^*) \underline{\varepsilon}(\underline{\theta}^*). \quad (2)$$

Here, \underline{P}_1^* is the projection operator for the column space of \underline{V}_1^* . Under the null hypothesis $\underline{\theta}_2^* = \underline{\theta}_{20}$, $(n-p)Z_2/q$ is an F random variable with q and $n-p$ degrees of freedom, where q is the dimension of $\underline{\theta}_2$. Thus, whenever Z_2 is free of $\underline{\theta}_1$ it can be used as a pivot for constructing an exact (in the sense that the level is exact) confidence region for $\underline{\theta}_2^*$.

Of course, Z_2 will not be free of $\underline{\theta}_1$, in general. However, Z_2 can always be used to construct exact confidence regions for the full parameter vector ($P_1 = 0$) and for certain subsets of $\underline{\theta}$ that can be described as follows. Repartition $\underline{\theta}^T = (\underline{\alpha}^T, \underline{\beta}^T)$ and consider response functions that can be represented as

$$f(\underline{x}_i, \underline{\theta}) = \sum_{j=1}^r \alpha_j g_j(\underline{x}_i, \underline{\beta}) \quad (3)$$

where the α_j 's are the elements of the $r \times 1$ vector $\underline{\alpha}$. Clearly, the α_j 's enter \underline{V} only as column multipliers so that the projection operators \underline{P} and \underline{P}_1 in (2) will be free of $\underline{\alpha}$. It follows that (2) can be used to construct an exact confidence region for any subset of $\underline{\theta}$ that includes $\underline{\beta}$.

All exact confidence regions in the following examples correspond to subsets of this form.

Our interest in assessing the value of using curvature measures as indicators of the accuracy of the tangent plane approximation stems from a set of experimental data on the effects of amino acid supplements to turkey diets. For brevity, we discuss the analysis of only a portion of these data. The response y_i is pen weight and the response function, which has independent theoretical support (Parks, 1982), is

$$f(x_i, \underline{\theta}) = \theta_1 + \theta_2(1 - e^{0.3x_i}) \quad (4)$$

with supplementation levels $x_i = 0, .04, .1, .16, .28$ and $.44$. The basal level $x_i = 0$ was replicated 10 times and the remaining levels were each replicated 5 times so that there are a total of $n = 35$ observations.

The ordinary least squares estimate of $\underline{\theta}$ from (4) is $\hat{\underline{\theta}}^T = (622.96, 178.25, -7.12)$, $s = 19.66$, $\Gamma^N = .14$ and $\Gamma^T = 1.14$. Although the intrinsic curvature is small, the parameter-effects curvature is large.

In view of the discussions in the literature, we would expect little agreement between exact and tangent plane confidence regions. However, this is evidently not the case: Figures 1 and 2 give the exact and approximate 95% confidence regions for (θ_1^*, θ_3^*) and (θ_2^*, θ_3^*) , respectively. The approximations are not perfect, of course, but they are close enough to the exact regions that there must be a large subjective component in assessments of their adequacy. In this case, we judge the approximations to be reasonable.

The approximate and exact 95% intervals for θ_3^* are $(-9.58, -4.67)$ and $(-9.68, -5.06)$, respectively. Again, we judge the approximation to be reasonable. In this experiment, interest centers almost exclusively on (θ_2, θ_3) so that the tangent plane approximation does seem to provide a reasonable method of analysis, even though the parameter-effects curvature is larger than that in the example of Bates and Watts (1981).

We have found similar occurrences in a variety of other situations. Such examples are certainly informative, but cannot provide much useful insight since the precise connection between the model/data and Γ^T is generally intractable. For certain special cases, however, this connection can be developed in detail. We study such a case in the next section.

3. THE FIELLER-CREASY PROBLEM

The nonlinear model for the usual two-sample problem in which the ratio of the population means is of interest can be written as

$$f(x_i, \theta) = \theta_1 x_i + \theta_1 \theta_2 (1 - x_i) \quad (5)$$

where x_i is an indicator variable that takes the values 1 and 0 for populations 1 and 2, respectively. Let n_1 and n_2 denote the sample sizes for populations 1 and 2 and without loss of generality assume that σ^2 is known.

For model (5), $\Gamma^N = 0$ and a little algebra will verify that

$$\Gamma^T = \frac{\sigma\sqrt{n_2} \{(\hat{\theta}_2^2 + n_1/n_2)^{\frac{1}{2}} + |\hat{\theta}_2|\}}{n_1 |\hat{\theta}_1|} \quad (6)$$

which reduces to

$$\Gamma^T = \frac{\sqrt{2} \sigma \{(\hat{\theta}_2^2 + 1)^{\frac{1}{2}} + |\hat{\theta}_2|\}}{|\hat{\theta}_1| \sqrt{n}} \quad (7)$$

when $n_1 = n_2 = n/2$. Since σ is assumed to be known, we used the standard radius $\rho = \sigma$ when constructing Γ^T . The corresponding cutoff for assessing the adequacy of the tangent plane approximation is $1/\sqrt{\chi(\alpha; 2)}$ where $\chi(\alpha; p)$ is the upper α probability point of the chi-squared distribution with p degrees of freedom. For the remainder of this discussion, we will assume equal sample sizes, $n_1 = n_2$.

3.1 Joint Confidence Regions

Using the numerator of (2), we find an exact $(1-\alpha)$ joint confidence region for (θ_1^*, θ_2^*) to be

$$E_\alpha^-(\theta_1, \theta_2) = \{(\theta_1, \theta_2) | (\theta_1 - \hat{\theta}_1)^2 + (\theta_1 \theta_2 - \hat{\theta}_1 \hat{\theta}_2)^2 \leq c\} \quad (8)$$

where $c = 2\sigma^2 \chi(\alpha; 2)/n$. Alternatively, this can be expressed as a region centered on $(\hat{\theta}_1, \hat{\theta}_2)$,

$$E_\alpha(\theta_1, \theta_2) = \{(k_1, k_2) | k_1^2 + (\hat{\theta}_2 k_1 + \hat{\theta}_1 k_2 + k_1 k_2)^2 \leq c\} \quad (9)$$

where $k_1 = \theta_1 - \hat{\theta}_1$ and $k_2 = \theta_2 - \hat{\theta}_2$. For this problem, the exact confidence region given by (8) or (9) is the same as the usual likelihood region.

The corresponding approximate region based on the tangent plane at $\hat{\theta}$ is obtained by deleting the term $k_1 k_2$ that occurs in (9),

$$A_\alpha(\theta_1, \theta_2) = \{(k_1, k_2) | k_1^2 + (\hat{\theta}_2 k_1 + \hat{\theta}_1 k_2)^2 \leq c\} \quad (10)$$

Evidently, Γ^T should reflect the difference between A_α and E_α . In essence, Γ^T measures this difference by comparing the term $k_1 k_2$ to the linear approximation:

$$\Gamma^T = \sigma\sqrt{n}/2 \max |k_1 k_2| / \{k_1^2 + (\hat{\theta}_2 k_1 + \hat{\theta}_1 k_2)^2\} \quad (11)$$

where the maximum is taken over all directions (k_1, k_2) in R^2 .

From (9) it can be seen that when $k_1 = -\hat{\theta}_1$ and $\hat{\theta}_1^2(1+\hat{\theta}_2^2) < c$, all $k_2 \in R^1$ are contained in E_α . The cutoff $\Gamma^T < 1/\sqrt{\chi(\alpha; 2)}$ successfully indicates such drastic occurrences since, from (7), a necessary condition for $\Gamma^T < 1/\sqrt{\chi(\alpha; 2)}$ is $\hat{\theta}_1^2 > c$.

Further insight can be gained by inspecting the faces \underline{A}_1 and \underline{A}_2 of the 2x2x2 parameter-effects curvature array,

$$\underline{A}_1 = (a_{1ij}) = \frac{\sigma \hat{\theta}_2}{\hat{\theta}_1} \left\{ \frac{2}{(1+\hat{\theta}_2^2)n} \right\}^{\frac{1}{2}} \begin{pmatrix} 0 & 1 \\ 1 & -2\hat{\theta}_2 \end{pmatrix} \quad (12)$$

and

$$\underline{A}_2 = (a_{2ij}) = \underline{A}_1 / \hat{\theta}_2 \quad (13)$$

Let $\hat{\underline{V}} = \underline{Q}\underline{R}$ denote the QR-factorization of $\hat{\underline{V}}$ where the $n \times p$ matrix \underline{Q} has orthogonal columns and the $p \times p$ matrix \underline{R} is upper triangular with positive diagonal elements. The elements of \underline{A}_1 and \underline{A}_2 reflect the behavior of the tangent plane parameter curves in terms of the transformed parameter space coordinates $\underline{\phi} = (\phi_i) = \underline{R}(\underline{\theta} - \hat{\underline{\theta}})$, as described in detail by Bates and Watts (1981).

The ϕ_1 compansion term $a_{111} = 0$, so that the ϕ_2 parameter curves will be spaced uniformly on the tangent plane. The remaining compansion term (a_{222}) and the terms that correspond to arcing (a_{122} and a_{211}) and fanning

$(a_{121}$ and $a_{212})$ can be large or small depending on the values of $\hat{\theta}_1, \hat{\theta}_2, n$ and σ .

When $\hat{\theta}_2 = 0$, $a_{212} = a_{221} = (2/n)^{\frac{1}{2}} \sigma / \hat{\theta}_1$ and all remaining terms are zero. In this case, there will be no comparison or arcing, but there may be considerable fanning of the ϕ_1 parameter curves. For example, the confidence regions $E_{.05}$ and $A_{.05}$ are displayed in Figure 3 for $\hat{\theta}_1 = 3$, $\hat{\theta}_2 = 0$ and $c = 6$. The substantial fanning effect is clearly evident. Although the Bates-Watts condition indicates that the tangent plane approximation should be reasonable in this case, $\Gamma^T = .33 < .41 = \chi^{-\frac{1}{2}}(.05; 2)$, our reaction to Figure 3 leads to the opposite conclusion.

The visual impact of displays such as that in Figure 3 seems to be well-reflected by $E(|l_1|/l_2)$ where l_1 and l_2 are the lengths indicated in Figure 3 and the expectation is with respect to a uniform distribution over the portion of the x-axis contained in A_α . When $\hat{\theta}_2 = 0$ we find

$$E(|l_1|/l_2) = -\hat{\theta}_1 \log (1 - c/\hat{\theta}_1^2) / 2\sqrt{c}. \quad (14)$$

Under the conditions of Figure 3, $E(|l_1|/l_2) = .67$, indicating that as we move along the x-axis $E_{.05}$ and $A_{.05}$ differ by 67% on the average. Using (14) we find that Γ^T must be substantially less than the cutoff if $E_{.05}$ and $A_{.05}$ are to be in reasonable agreement, say $E(|l_1|/l_2) < .15$.

When $\hat{\theta}_1$ and $\hat{\theta}_2$ are both large, arcing will be the only important effect since all elements of A_1 and A_2 will be small except for a_{122} . The regions $A_{.05}$ and $E_{.05}$ are displayed in Figure 4 for $\hat{\theta}_1 = 62$, $\hat{\theta}_2 = 32$ and $c = 6$. For clarity, the axes in Figure 4 correspond to the axes of the ellipse $A_{.05}$. The arcing of the parameter lines is clearly evident and the large curvature $\Gamma^T = 1.03$ correctly indicates our reaction to the figure.

For further illustration, Figures 5a - 5d give the regions $A_{.05}$ and $E_{.05}$ for $\hat{\theta}_1 = 8$, $\hat{\theta}_2 = 1.2(.6)3$ and $c = 6$. Before continuing, the reader may wish to inspect these figures and decide which, if any, of the approximations are acceptable. We have shown an expanded series of such figures to several people; few agree with the Bates-Watts cutoff and most would be willing to use the linear approximation when Γ^T is somewhat larger than the cutoff. Of the four figures in question, only one (5a) corresponds to an acceptable approximation according to the Bates-Watts criterion.

3.2 Marginal Confidence Regions for θ_2

We next consider marginal regions for θ_2 . The usual exact region for θ_2^* is (Wallace, 1980)

$$E_{\alpha}(\theta_2) = \{\theta_2 | \hat{\theta}_1^2 (\hat{\theta}_2 - \theta_2)^2 / (1 + \theta_2^2) \leq c_1\} \quad (15)$$

where $c_1 = 2\sigma^2 \chi(\alpha; 1)/n$. This region can be obtained from the pivotal (2) modified to accommodate the case when σ^2 is known and is the same as the marginal likelihood region discussed in Cox and Hinkley (1974, p.343). It is well known that $E_{\alpha}(\theta_2)$ will be an interval only if $\hat{\theta}_1^2 > c_1$; otherwise, $E_{\alpha}(\theta_2)$ will be the complement of an interval or the entire real line. Recall that a necessary condition for the Bates-Watts criterion to hold is $\hat{\theta}_1^2 > c > c_1$ so that following this guideline will insure that $E_{\alpha}(\theta_2)$ will be an interval when the tangent plane approximation is used. Thus, under the constraint $r = c/\hat{\theta}_1^2 < 1$, $E_{\alpha}(\theta_2)$ can be represented as

$$[\hat{\theta}_2 \pm \{r_1(1-r_1) + r_1 \hat{\theta}_2^2\}^{1/2}] / (1-r_1) \quad (16)$$

where $r_1 = c_1/\hat{\theta}_1^2 < r < 1$.

The interval $A_{\alpha}(\theta_2)$ computed from the tangent plane approximation is

$$\hat{\theta}_2 \pm (r_1 + r_1 \hat{\theta}_2^2)^{1/2}. \quad (17)$$

When $\hat{\theta}_2 = 0$, both intervals (16) and (17) are symmetric about the estimate and the ratio of their lengths is $E_\alpha/A_\alpha = (1-r_1)^{-\frac{1}{2}}$ so that the exact interval will always be longer than the approximate interval. Under the conditions of Figure 3, this ratio has the value 1.32 which seems less than adequate.

When $\hat{\theta}_2$ is large it can happen that the Bates-Watts condition is violated even though (16) and (17) are very close. From (7) it can be seen that the Bates-Watts condition will be violated whenever $r_1 \hat{\theta}_2^2 \geq 1$. It is clearly possible to make (16) and (17) arbitrarily close while maintaining $r_1 \hat{\theta}_2^2 \geq 1$. Consider, for example, the case when $2\sigma^2/n = 1$, $\alpha = .05$ and $\hat{\theta}_2^2 = r_1^{-1} = 1000$. These conditions force $c_1 = 3.84$, $\hat{\theta}_1 = 61.97$, $\Gamma^T = 1.02 > 1/\sqrt{\chi(.05;2)} = .409$,

$$E_{.05}(\theta_2) = (30.653, 32.656) \quad (18)$$

and

$$A_{.05}(\theta_2) = (30.622, 32.623). \quad (19)$$

4. DISCUSSION

Our general conclusion from this study is that the Bates-Watts criterion has merit, but it falls short of being a reliable indicator of the accuracy of the tangent plane approximation. In the Fieller-Creasy problem, use of the Bates-Watts criterion precludes use of the tangent plane approximation when the exact confidence region is unbounded and, depending on the value of $\hat{\theta}_2$, may serve as a useful guide (see Figures 5a - 5d). On the other hand, Γ^T may be relatively large when the approximation is reasonable (see Figures 1 and 2, and equations 18 and 19), or Γ^T may be relatively small when the approximation seems untenable (see Figure 3).

This conclusion is based on a series of examples such as those described in Section 2 and on a detailed study of the Fieller-Creasy problem. This problem was chosen for several reasons: First, it is important in its own right and the associated curiosities make it a useful test case. Second, since $\Gamma^N = 0$ the problem reflects the small intrinsic curvatures often encountered in practice. Third, the derivation of the curvatures is based on a quadratic expansion of the response function. For the Fieller-Creasy problem this expansion is exact so that we need not be concerned about the potential complications associated with ignoring higher order terms (Linsen, 1980). Fourth, use of the exact confidence regions as a standard is reasonable since they coincide with the likelihood regions in the situation studied. Finally, the problem is simple enough to allow the parameter-effects array and the associated curvature to be displayed as explicit functions of the data.

The mean square parameter-effects curvature (Beale, 1960; Bates and Watts, 1980) is an alternative to Γ^T and for the Fieller-Creasy problem can be written as an explicit function of the data by using (12) and (13). Generally, we have found little to indicate that the mean square curvature should be preferred to Γ^T or vice versa.

Finally, like Bates and Watts (1980, 1981), our assessments of the accuracy of the tangent plane approximation have not made full use of the statistical structure of the problem. It may be of interest, for example, to compare regions using probability or likelihood content. Such comparisons, which must entail the development of new measures of accuracy, are outside the scope of this report.

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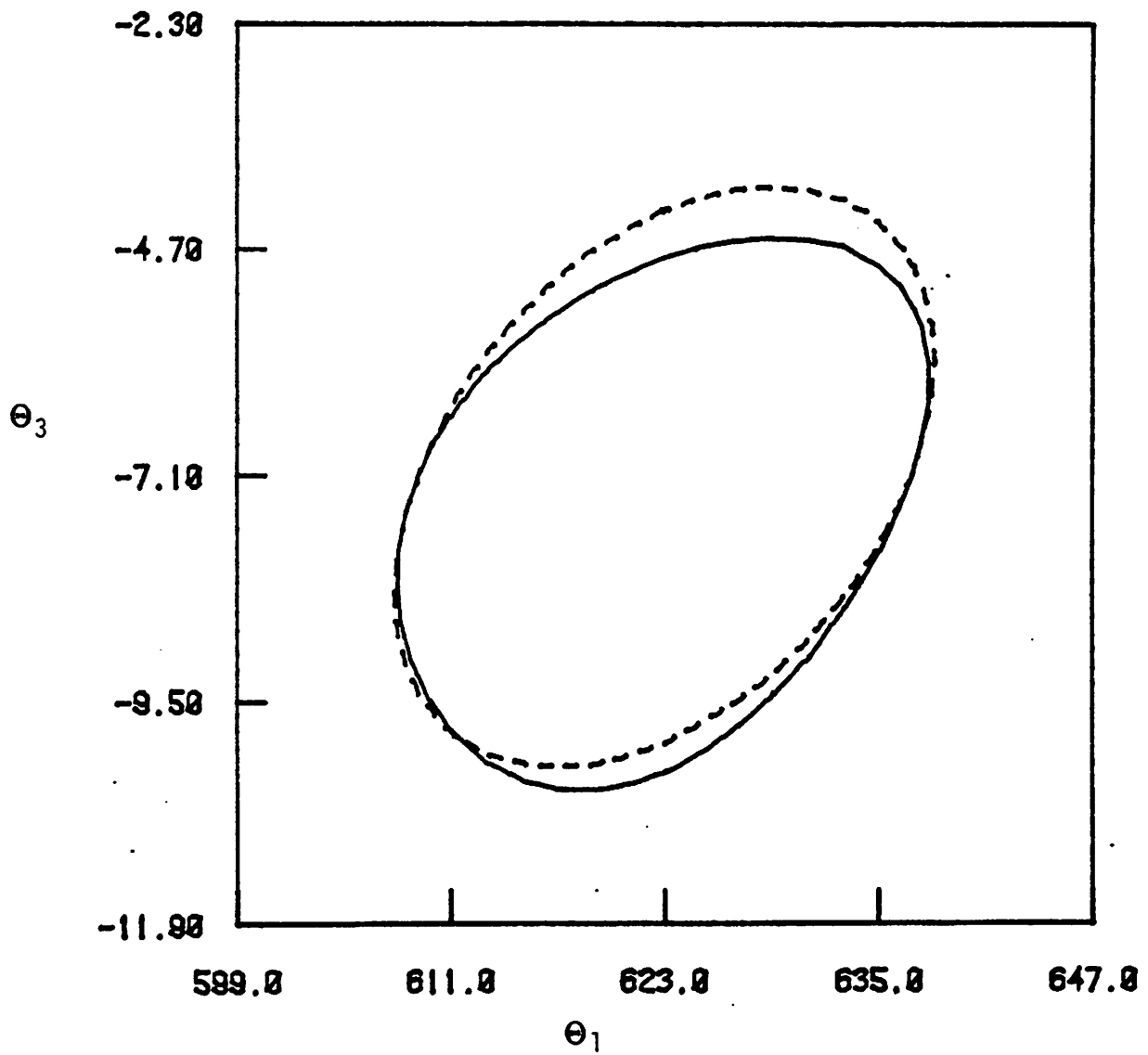


Figure 1. 95% Confidence Regions for (θ_1^*, θ_3^*) . Linear Approximation ---, Exact —.

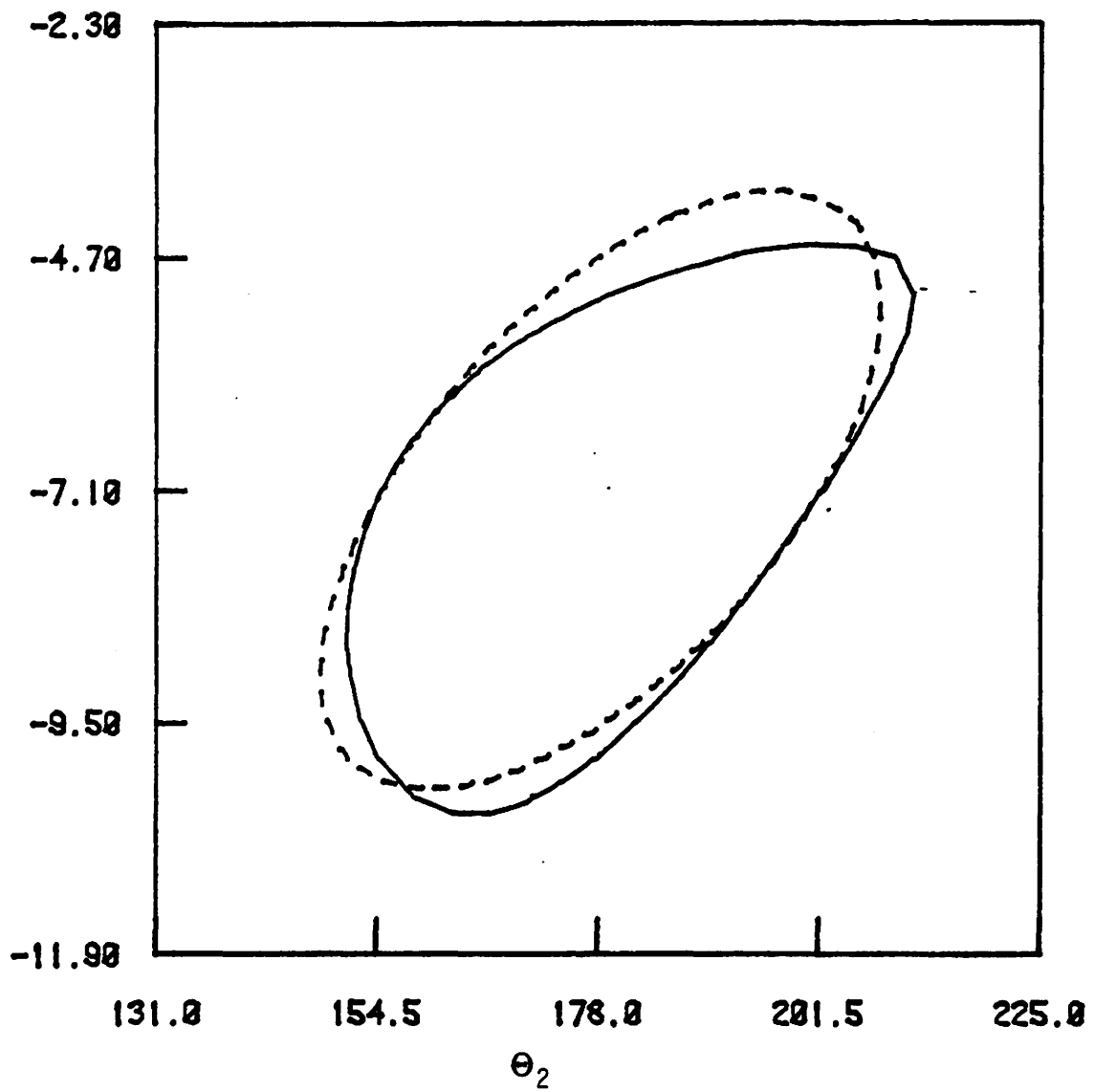


Figure 2. 95% Confidence Regions for (θ_2^*, θ_3^*) . Linear Approximation ---, Exact —.

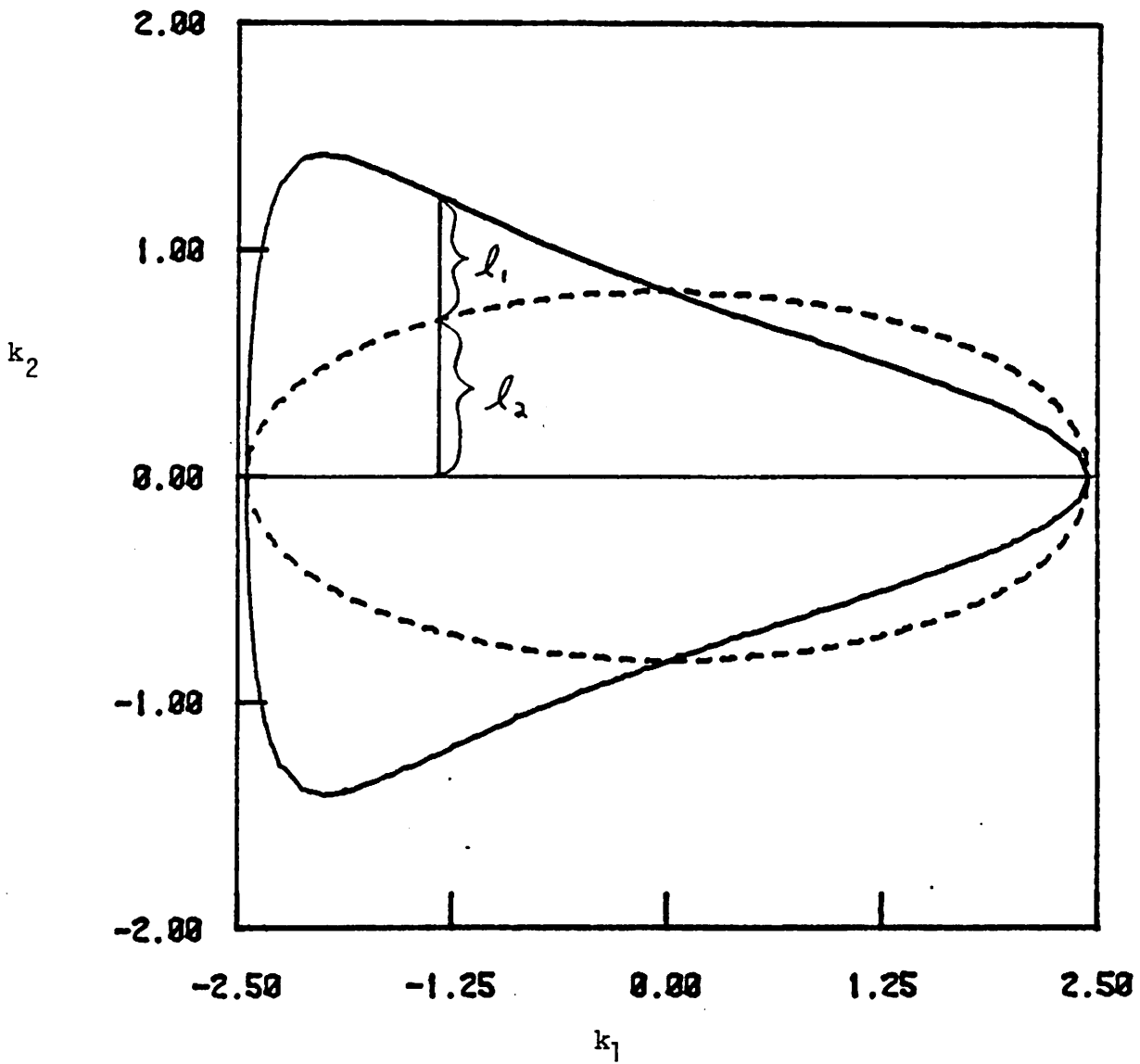


Figure 3. 95% Confidence Regions for (k_1^*, k_2^*) when $(\hat{\theta}_1, \hat{\theta}_2) = (3, 0)$.
 Linear Approximation ---, Exact —.

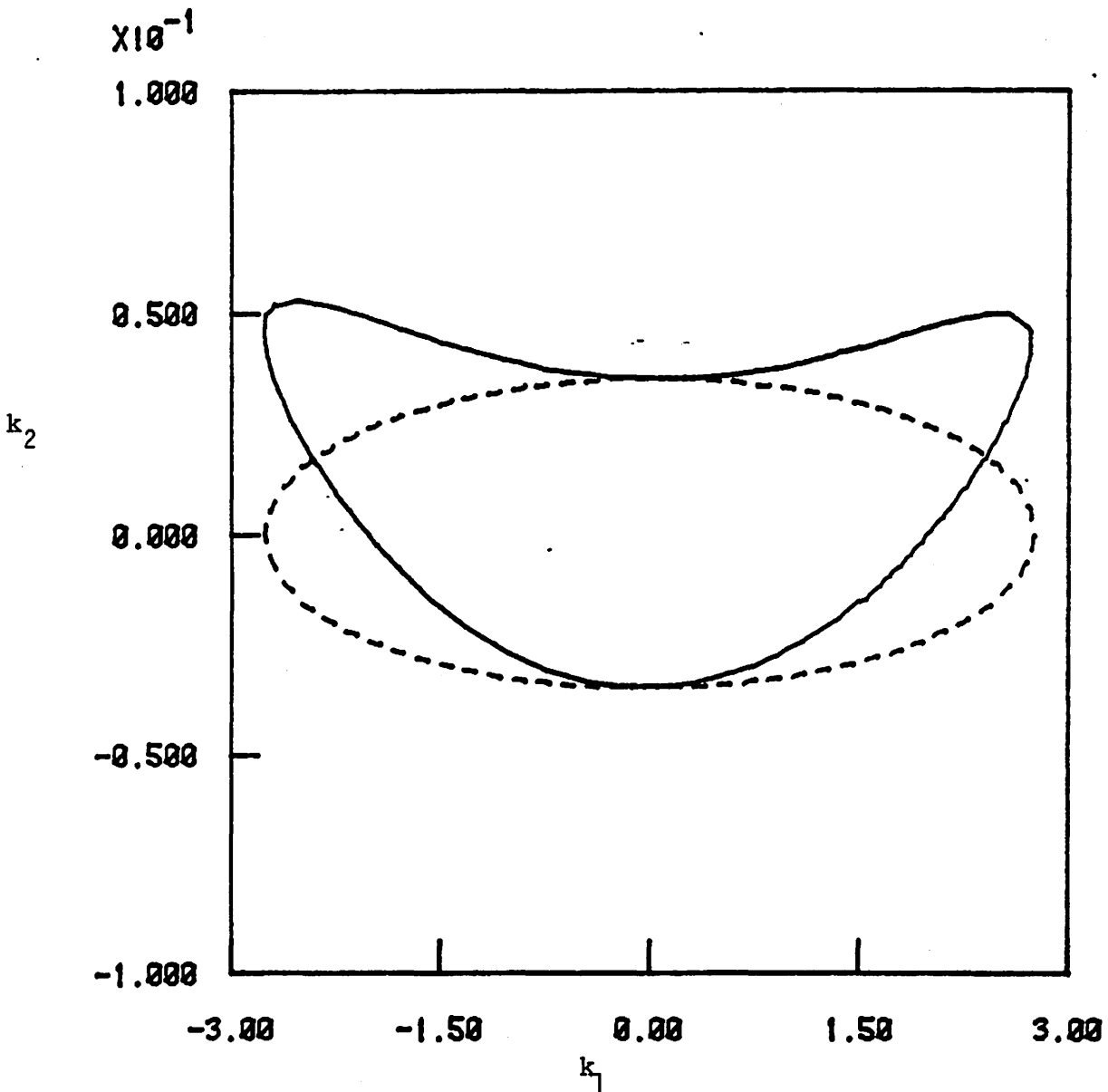


Figure 4. 95% Confidence Regions for (k_1^*, k_2^*) when $(\hat{\theta}_1, \hat{\theta}_2) = (62, 32)$.
 Linear Approximation ---, Exact —.

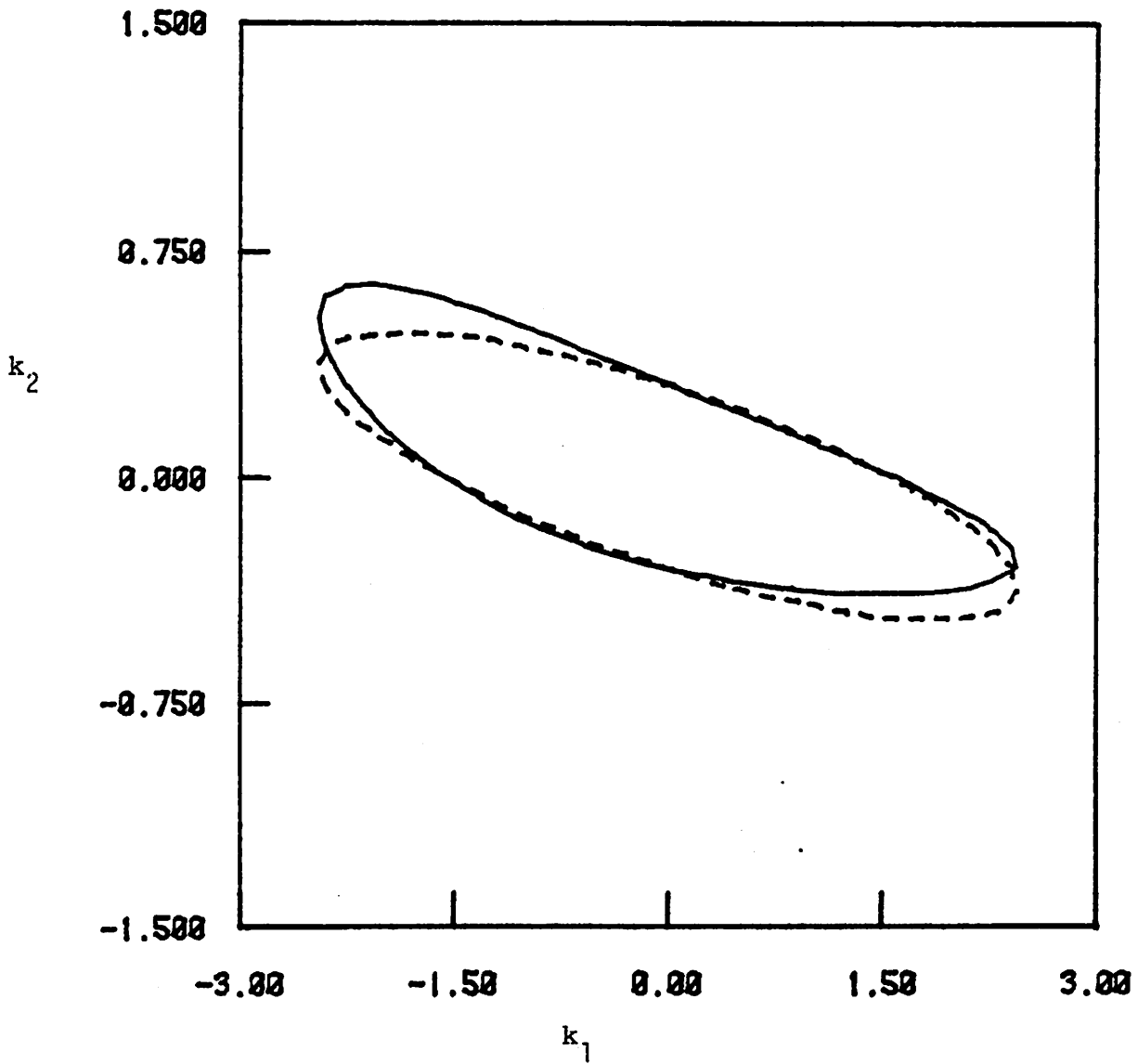


Figure 5.a. 95% Confidence Regions for (k_1^*, k_2^*) when $(\hat{\theta}_1, \hat{\theta}_2) = (8, 1.2)$.
 Linear Approximation ---, Exact —.

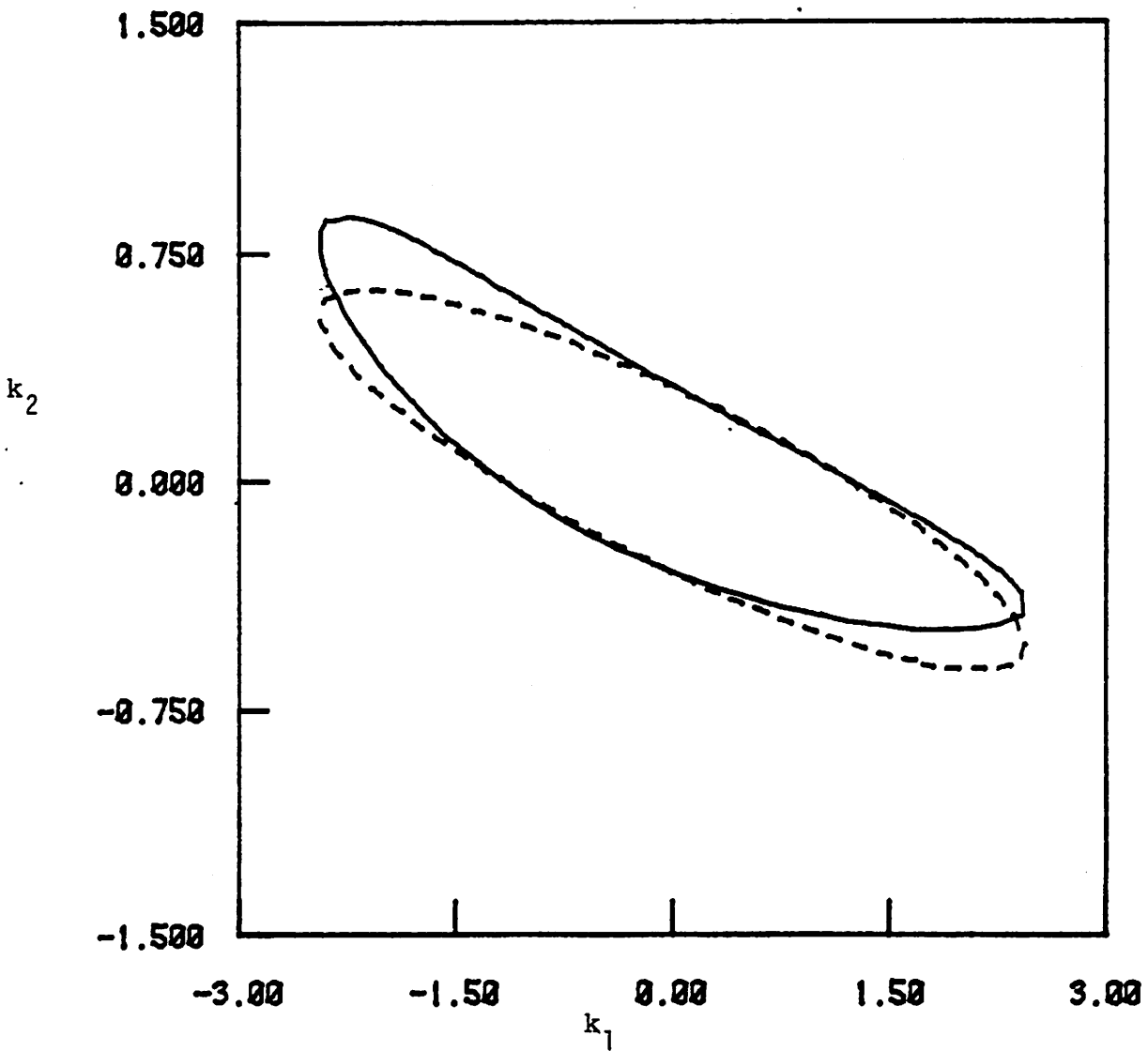


Figure 5.b. 95% Confidence Regions for (k_1^*, k_2^*) when $(\hat{\theta}_1, \hat{\theta}_2) = (8, 1.8)$.
 Linear Approximation ---, Exact —.

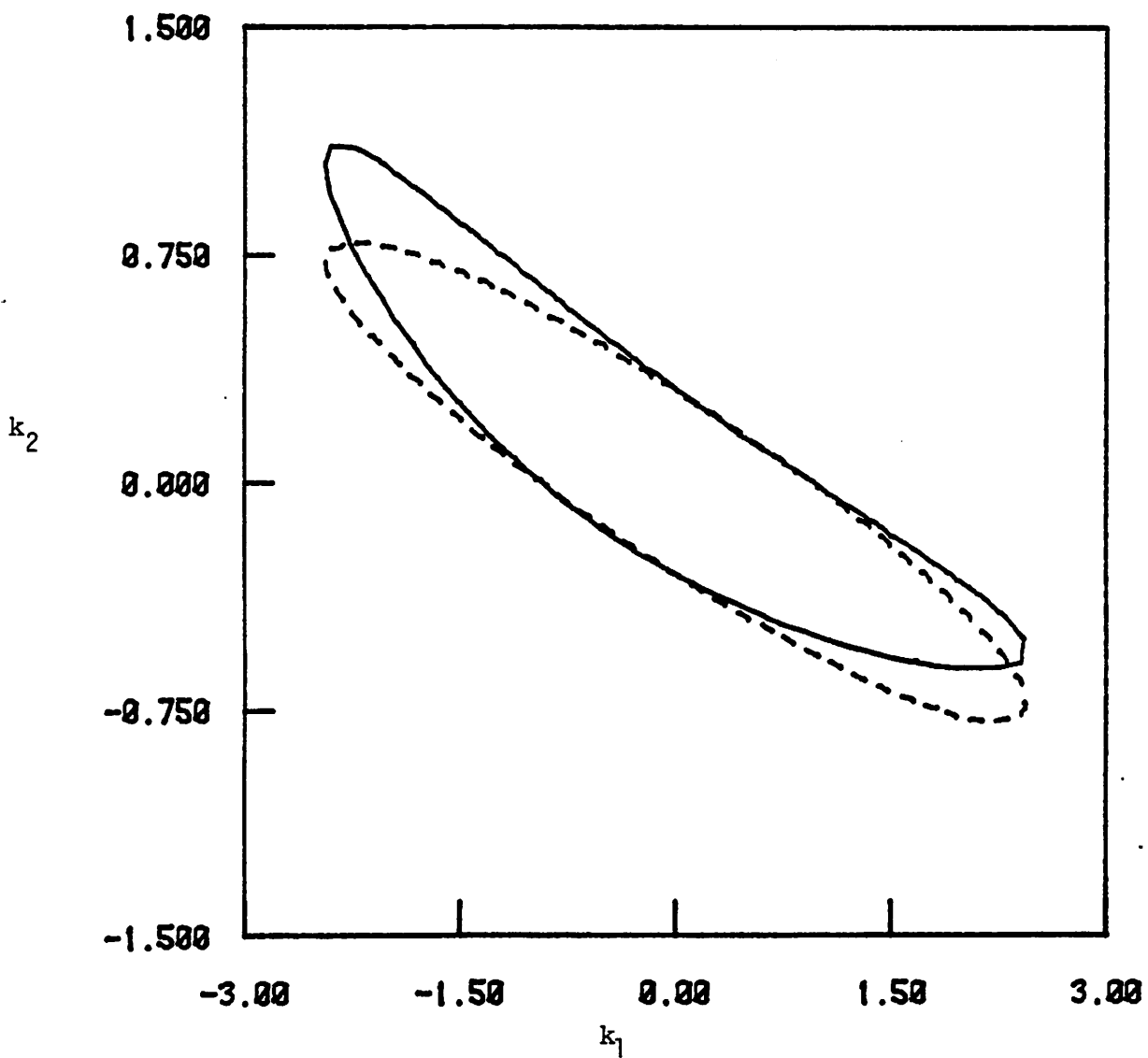


Figure 5.c. 95% Confidence Regions for (k_1^*, k_2^*) when $(\hat{\theta}_1, \hat{\theta}_2) = (8, 2.4)$.
 Linear Approximation ---, Exact —.

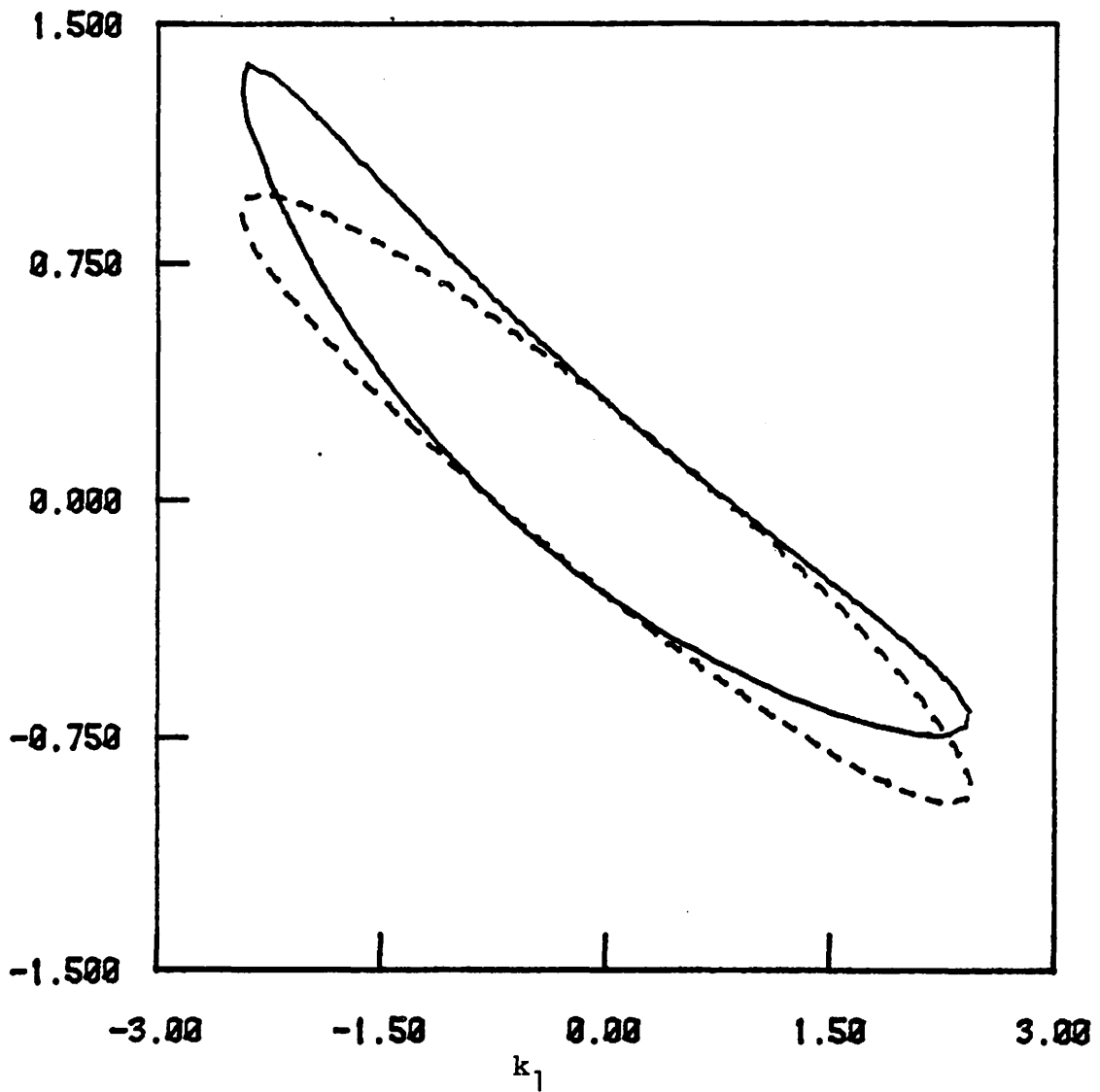


Figure 5.d. 95% Confidence Regions for (k_1^*, k_2^*) when $(\hat{\theta}_1, \hat{\theta}_2) = (8, 3)$.
 Linear Approximation ---, Exact —.