ON FITTING EXPONENTIALS BY NONLINEAR LEAST SQUARES

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ABSTRACT

This paper is concerned with the problem of fitting discrete data, or a continuous function, by least squares using exponential functions. We examine the questions of uniqueness and sensitivity of the best least squares solution, and provide analytic and numerical examples showing the possible non-uniqueness, and extreme sensitivity of these solutions.

1. INTRODUCTION

The problem (D) of numerically fitting given discrete data (t_i, y_i), $i = 1,\dots,n$, by a sum of exponentials $y(t) = \sum_{j=1}^{m} a_j e^{b_j t}$ in the best least squares sense, so that we minimize $I = \sum_{i=1}^{n} (y(t_i)-y_i)^2$ over all possible $\underline{a}$ and $\underline{b}$, is well known to be fraught with peril. Various algorithms have been proposed for this special nonlinear least squares problem (see e.g. Evans et al (1980), Osborne (1975), and Ruhe (1980)), and examples of this type have been used to test more general nonlinear least squares algorithms (Golub and Pereyra (1973), Kaufman (1978)). Lanczos (1956, pg. 279) was the first to point out the extreme sensitivity or ill-condition of determining the exponential coefficients, and showed that various parameter values $(\underline{a},\underline{b})$ can give near-optimal residuals. In Section 2, we shall discuss this example and others, with a view to characterizing when such problems are ill-conditioned, and even when the solutions are not unique. This problem (D) is also of interest because of its relationship to the general problem of estimating parameters in differential equations; indeed it is essentially equivalent to the (simplest) case of parameters appearing linearly in the differential equation system (see Varah (1982)).

This problem (D) is closely related to the continuous problem (C) of fitting an exponential sum $y(t) = \sum_{j=1}^{m} a_j e^{b_j t}$ to a given function $f(t)$ so as to minimize $I(\underline{a},\underline{b}) = \frac{1}{2}\int_0^{\infty} (y(t)-f(t))^2 dt$. This problem is more amenable to analysis than (D), and in Section 3 we examine the question of uniqueness, and give some examples of non-unique solutions, extending work of Kammler (1979). Finally in Section 4, we treat the special case where $f(t)$ is itself an exponential sum; in this case one can be more explicit about non-uniqueness, and we give several examples.

2. THE DISCRETE PROBLEM

We specialize at once to the case of two exponentials, for two reasons: first of all, the necessary extensions to three or more exponentials are easily seen, and more importantly, as we shall see, numerical results with two exponentials are dubious enough; those with three or more are almost certainly meaningless.

Thus the problem can be stated easily enough: we have a least squares function

$$I(\underline{a},\underline{b}) = \sum_i (a_1 e^{b_1 t_i} + a_2 e^{b_2 t_i} - y_i)^2 \equiv \sum_i r_i^2 \tag{2.1}$$

with first order minimum conditions

$$\begin{aligned} \frac{\partial I}{\partial a_1} &= 2\sum_i r_i e^{b_1 t_i} = 0\ , & \frac{\partial I}{\partial b_1} &= 2\sum_i r_i t_i a_1 e^{b_1 t_i} = 0 \\ \frac{\partial I}{\partial a_2} &= 2\sum_i r_i e^{b_2 t_i} = 0, & \frac{\partial I}{\partial b_2} &= 2\sum_i r_i t_i a_2 e^{b_2 t_i} = 0 \end{aligned} \tag{2.2}$$

or $J^T\underline{r} = 0$, where J is the Jacobian matrix $J_{ij} = \frac{\partial r_i}{\partial \alpha_j}$, $\underline{\alpha} = (a_1,a_2,b_1,b_2)$. The $\frac{\partial I}{\partial a_j} = 0$ equations can be used to solve for the linear parameters a_1,a_2, and these substituted to give I as a function of b_1,b_2 only, but this is messy.

Some idea of the nature of the critical point(s) arrived at by solving (2.2) can be obtained by evaluating the 4x4 Hessian matrix H,

$$\begin{aligned} H_{kj} = \frac{1}{2}\frac{\partial^2 I}{\partial\alpha_k \partial\alpha_j} &= \sum_i \left(\frac{\partial r_i}{\partial \alpha_k}\right)\left(\frac{\partial r_i}{\partial \alpha_j}\right) + \sum_i r_i \frac{\partial^2 r_i}{\partial\alpha_k \partial\alpha_j} \\ &= J^T J + G \end{aligned} \tag{2.3}$$

where $G_{jk} = \underline{v}^{(j,k)T}\underline{r}$. In fact, most of G is zero at a solution of (2.2), the only nonzero terms being

$$G_{33} = a_1 \sum_i r_i t_i^2 e^{b_1 t_i}, \qquad G_{44} = a_2 \sum_i r_i t_i^2 e^{b_2 t_i}.$$

We should mention here that we <u>assume</u> $b_1 \neq b_2$; if $b_1 = b_2$ (the confluent case) we must adjust I accordingly. We will consider this more explicitly when dealing with the continuous problem in Sections 3 and 4.

Even this simple problem (2.1) is very ill-conditioned. We give some indication of this using two well-known examples, that of Lanczos mentioned earlier, and that of Osborne (1972). The Osborne data, after subtracting out the asymptotic constant 0.3754, are given in Table 1. The Lanczos data (see Lanczos (1956), pg. 273) are generated from three exponentials,

$$.0951e^{-t} + .8607e^{-3t} + 1.5576e^{-5t} \tag{2.4}$$

using $\Delta t = .5$. Unfortunately this gives the additional problem of decaying to zero too fast; there are simply not enough nontrivial data values. We generate data using the same three exponential sum, but using $\Delta t = 0.1$ instead and $n = 33$, the same as the Osborne data; this is given in Table 1 as well.

TABLE 1

t	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7
$y(O_s)$	.4686	.5326	.5566	.5606	.5496	.5326	.5056	.4746
$y(L_a)$	2.5134	1.6684	1.1232	0.7679	.5338	.3776	.2720	.1997

t	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7
$y(O_s)$	.4426	.4086	.3756	.3426	.3096	.2826	.2526	.2276	.2046	.1826
$y(L_a)$	.1493	.1138	.0883	.0697	.0560	.0459	.0378	.0316	.0268	.0229

t	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7
$y(O_s)$	.1626	.1466	.1306	.1146	.1036	.0916	.0816	.0726	.0626	.0556
$y(L_a)$	.0198	.0172	.0151	.0133	.0117	.0104	.0093	.0083	.0074	.0067

t	2.8	2.9	3.0	3.1	3.2
$y(O_s)$	.0486	.0446	.0336	.0356	.0306
$y(L_a)$	.0060	.0054	.0048	.0044	.0039

Both sets of data appear to have unique minima, as in Table 2.

Table 2

	a_1	a_2	b_1	b_2	I	$\lambda_1(H)$	$\lambda_2(H)$
Osborne	1.93	-1.46	-1.29	-2.22	$.55\times10^{-4}$	.00011	.06
Lanczos	.29	2.22	-1.52	-4.47	$.78\times10^{-4}$	.0010	.03

Some idea of the ill-conditioned of these problems can be seen from the size of the Hessian eigenvalues, although this is only very local information, and really a more global view is appropriate. Thus we give as well in Figures 1 and 2 a geometrical picture with a 3-dimensional plot of the function $[I(b_1,b_2)]^{1/2}$, for each b_1, b_2 using the appropriate linear parameters a_1, a_2. Ranges were $-0.4 \geq b_1, b_2 \geq -7.0$ for both. Of course the plots are symmetric about the line $b_1 = b_2$. Notice that the Osborne data gives rise to a rather narrow valley to the minimum and beyond - this results from the fact that one explonential fits the data surprisingly well. The Lanczos data plot is rather different: the valley is broader, in a different direction, and not so easily distinguished. Both surfaces appear to be convex in the region $b_1 > b_2$, with unique minima, although verifying convexity appears to be very difficult, and we have not been able to characterize those data which lead to convex surfaces, or even give sufficient conditions. We shall return to this problem in the continuous case.

To appreciate the ill-condition involved here, we can try to measure the sensitivity of the parameters to changes in the data. For example, suppose the data values are in error by no more than δ (indeed, the Osborne data is only given to 3 decimal places). Then we can tolerate a change in $\sqrt{I}$ of $\varepsilon = \delta\sqrt{N}$. Following Bard (1974), pg. 171, this gives rise to an uncertainty region about the minimum which, assuming I is locally quadratic, is the ellipse $(\delta b)^T H(\delta b) \leq 2\varepsilon^2$, where H is the 2x2 Hessian using only b_1, b_2 as variables (not the 4x4 Hessian used earlier). Thus $\|\delta b\|$ can be as large as $\varepsilon/\sqrt{\lambda_1(H)}$. With $\delta = .001$ in the above cases, this uncertainty region is quite large; we have not computed it precisely but we know it contains the points in Table 3:

TABLE 3

	b_1	b_2	b_1	b_2
Osborne	-1.2	-2.5	-1.4	-1.9
Lanczos	-1.27	-4.33	-1.8	-4.6

Yet these data sets are not in the least pathological; other data sets give comparable results. Indeed, one can devise data sets where the situation is much worse, i.e. with a flatter, yet non-convex surface, merely by forming a different exponential sum in (2.4). We consider one specific example briefly here, and return to it in Section 4 where we discuss the continuous approximation problem. We use the general sum

$$\alpha_1 e^{-t} + \alpha_2 e^{-3t} + \alpha_3 e^{-5t} \qquad (2.5)$$

choosing the special case $\underline{\alpha} = (.1, .4, -.3)$.

The difference in the nature of the surface $I(b_1,b_2)$ can be seen by examining the confluent case $b_1 = b_2$. Along this line the Osborne and Lanczos data appear to give rise to a convex function $I(b_1,b_1)$, with a unique minimum at some finite (negative) value of b_1. This point is in fact a saddle point of the surface, with the surface decreasing in value away from $b_1 = b_2$ until the (apparent) global minimum is reached (see Figures 1 and 2). However the new example is not convex along $b_1 = b_2$.

Algebraically, the confluent case has the form $(c + dt_i)e^{bt_i}$, with

$$I(b) = \sum_1^N [(c+dt_i)e^{bt_i} - y_i]^2.$$

The first order conditions for a critical point are

$$\sum_1^N [(c+dt_i)e^{bt_i} - y_i]t_i^k = 0, \qquad k = 0,1,2.$$

If we define $\begin{cases} s_k = \Sigma t_i^k e^{2bt_i}, & k = 0,1,2,3 \\ z_k = \Sigma y_i t_i^k e^{bt_i}, & k = 0,1,2 \end{cases}$,

and solve for the linear parameters c and d, we get a single equation for b:

$$(s_2^2 - s_1 s_3)z_0 + (s_0 s_3 - s_1 s_2)z_1 = (s_0 s_2 - s_1^2)z_2. \qquad (2.6)$$

This equation is rather nasty, and it appears very difficult in general to give criteria for a unique solution, so as to make $I(b)$ convex. We conjecture that this will imply a unique global minimum for $b_1 \leq b_2$, much as in Figures 1 and 2.

Now consider the special case mentioned earlier. For $\alpha = (.1,.4,-.3)$, we generate 33 data points as with the Lanczos data. Examination of the confluent case reveals 3 critical points, as shown in Table 4.

TABLE 4

$\alpha = .1, .4, -.3$			
b	-.98	-1.34	-2.38
I(b)	$1.68\text{x}10^{-3}$	$1.85\text{x}10^{-3}$	$0.78\text{x}10^{-3}$
nature	min	saddle	saddle

This case has two distinct minima; one as above at $b_1 = b_2 = -.98$, and the other (global) minimum at $b_1 = -1.55$, $b_2 = -10.5$ with $I(b_1,b_2) = .15\text{x}10^{-3}$. The I-function is very flat near both minima, with the 4x4 Hessian having an eigenvalue of $.33\text{x}10^{-5}$ in the latter case. The 3-D plot of the surface $[I(b_1,b_2)]^{1/2}$, for $-.4 \geq b_1 b_2 \geq -10.0$ is given in Figure 3. In the neighbourhood of the local minimum (-.98,-.98), I is very flat: for $-.9 \geq b_1 b_2 \geq -1.5$, $1.68\text{x}10^{-3} \leq I \leq 2.02\text{x}10^{-3}$. Moreover, near the global minimum (-1.55,-10.5), it is also; if we again allow .001 error in each data point, we find the uncertainty region contains (-1.45,-20) and (-1.7,-5.7).

A similar situation occurs for very many data sets; because of this we feel that the fitting of exponentials must be attempted with great care. Moreover, there seems to be little correlation between this sensitivity and monotonicity of the data. In the following sections, we shall discuss the continuous problem in greater analytic detail.

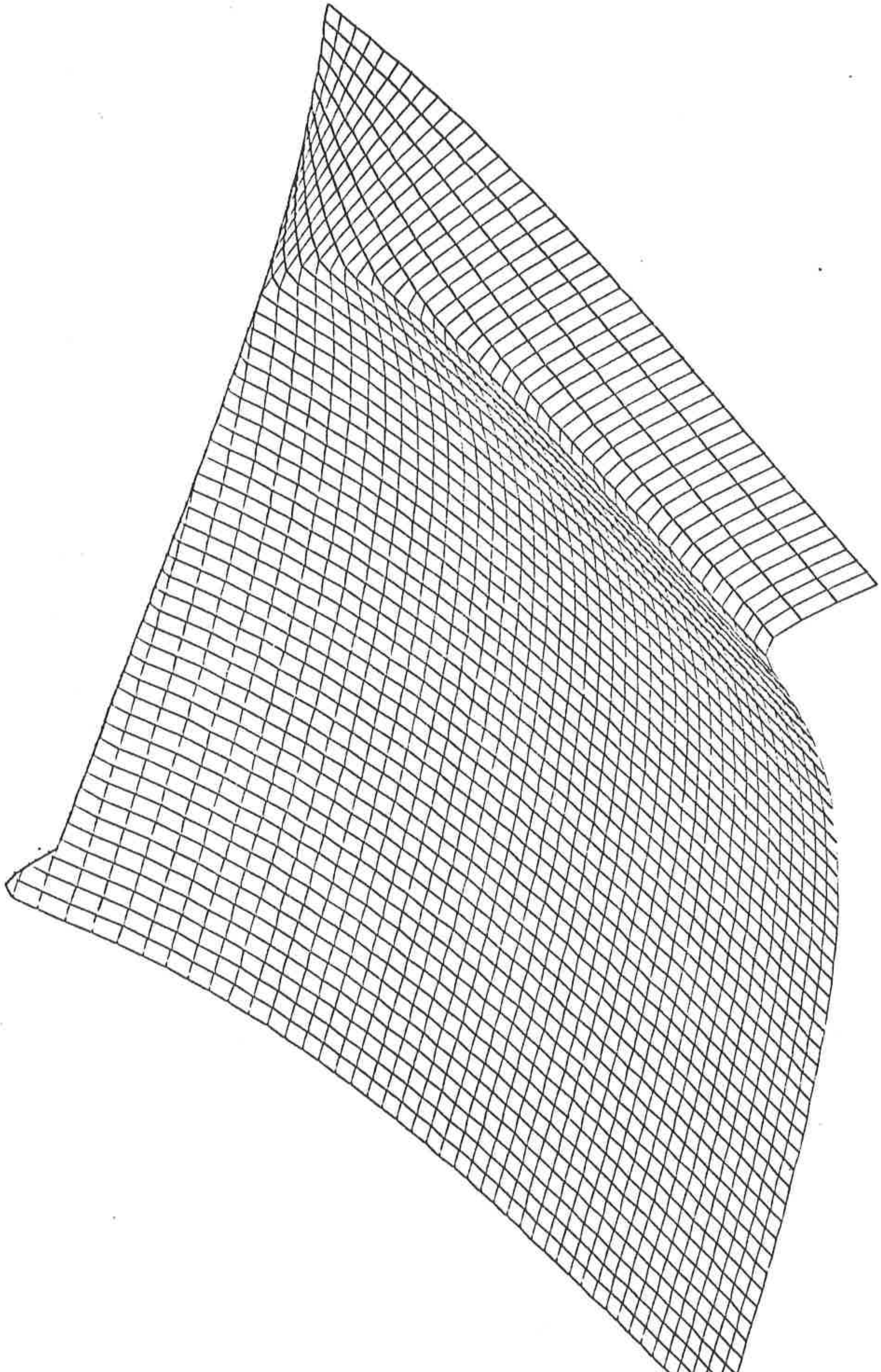


FIGURE 1

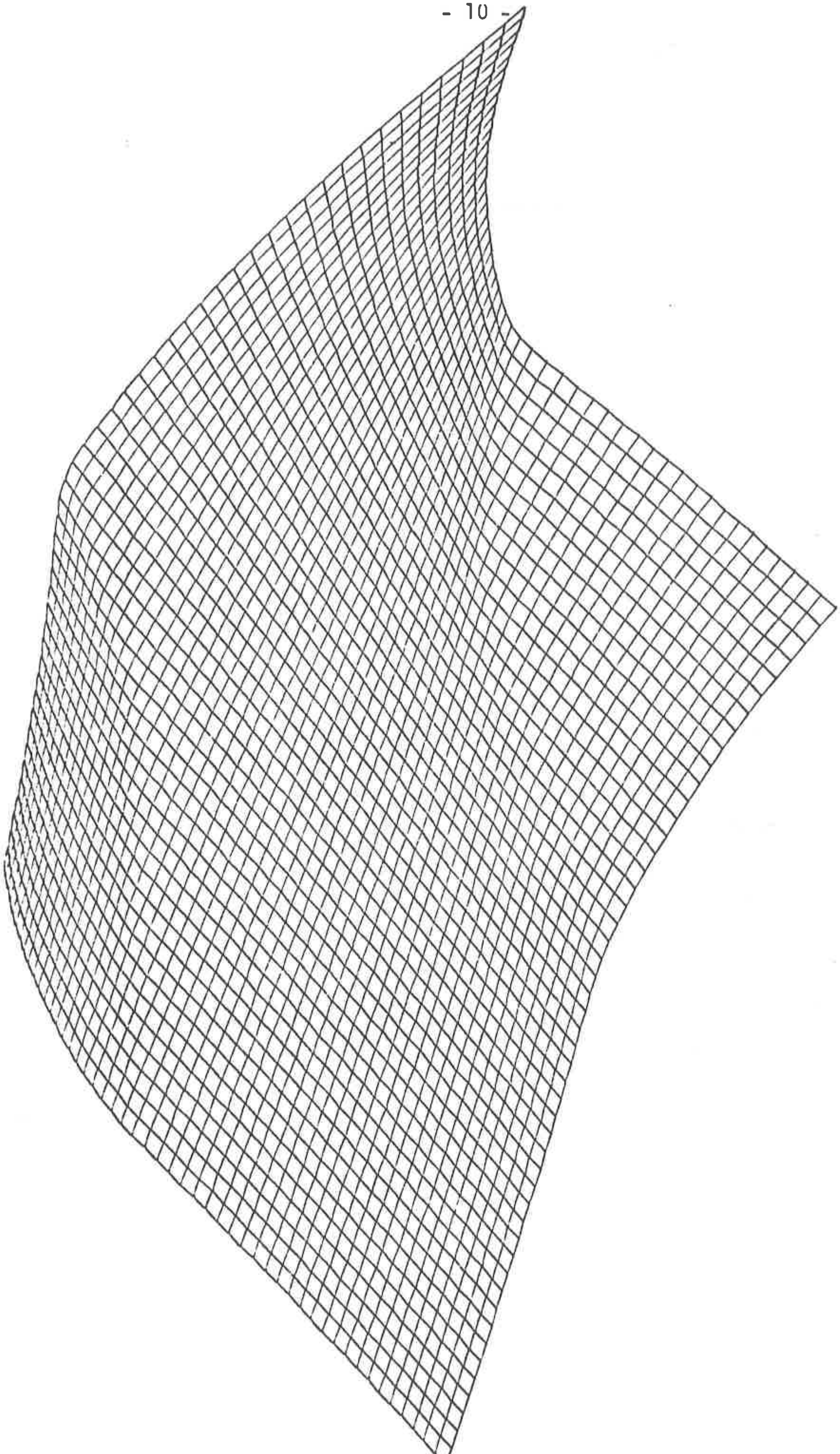


FIGURE 2

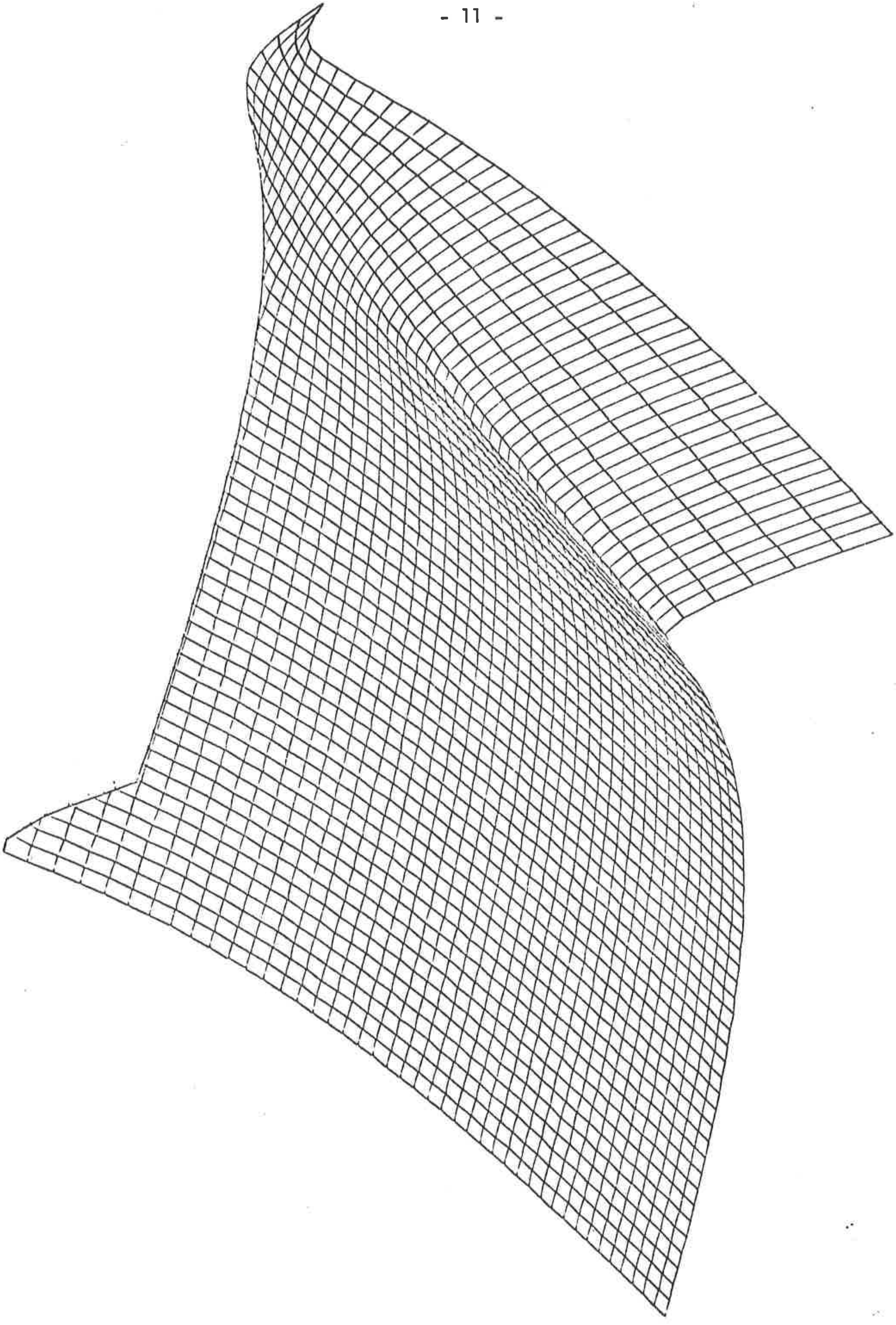


FIGURE 3

3. THE CONTINUOUS PROBLEM

Here we are given a function $f(t)$, $0 \leq t < \infty$, and wish to approximate it by an exponential sum $y(t) = \sum_{j=1}^{m} a_j e^{b_j t}$ so as to minimize

$$I(a,b) = \frac{1}{2} \int_0^\infty (y(t)-f(t))^2 dt. \tag{3.1}$$

We assume the exponentials are decaying, i.e. $b_j < 0$, $j = 1,\ldots,m$. The first-order conditions for a minimum (or more generally for any critical point) are, for $j = 1,\ldots,m$,

$$\frac{\partial I}{\partial a_j} = \int_0^\infty (y-f)e^{b_j t} dt = 0$$

and

$$\frac{\partial I}{\partial b_j} = a_j \int_0^\infty (y-f)te^{b_j t} dt = 0.$$

If we define what are essentially the Laplace transforms of y and f,

$$z(b) = \int_0^\infty y(t)e^{bt}dy = -\sum_{i=1}^{k} \frac{a_i}{b_i+b}$$

and

$$g(b) = \int_0^\infty f(t)e^{bt}dt,$$

then these first-order conditions are equivalent (assuming no $a_j = 0$) to the functions $z(b)$, $z'(b)$ interpolating $g(b)$, $g'(b)$ at the solution points $\{b_j\}$; $j = 1,\ldots,m$;

$$\begin{aligned} z(b_j) &= -\sum_{i=1}^{k} \frac{a_i}{b_i+b_j} = \int_0^\infty f(t)e^{b_j t}dt = g(b_j) \\ z'(b_j) &= \sum_{i=1}^{k} \frac{a_i}{(b_i+b_j)^2} = \int_0^\infty tf(t)e^{b_j t}dt = g'(b_j). \end{aligned} \tag{3.2}$$

These equations are sometimes called the Aigrain/Williams equations (see Kammler (1979)) and of course make the error $(y-f)$ orthogonal to $e^{b_j t}$ and $te^{b_j t}$ over $[0,\infty)$. They are linear in the $\{a_j\}$, but nonlinear in the $\{b_j\}$, so the existence and uniqueness of solutions is not clear, and may vary with the function $f(t)$.

It is of interest to compute the Hessian matrix H of second partial derivatives of I; we get

$$\frac{\partial^2 I}{\partial a_j \partial a_k} = \int_0^\infty e^{b_j t} e^{b_k t} dt = \frac{-1}{b_j+b_k}$$

$$\frac{\partial^2 I}{\partial a_j \partial b_j} = \int_0^\infty (y-f)te^{b_j t}dt + a_j \int_0^\infty te^{2b_j t}dt$$

$$= 0 + \frac{a_j}{(2b_j)^2} \qquad \text{(at a critical point)}$$

$$\frac{\partial^2 I}{\partial a_j \partial b_k} = a_k \int_0^\infty te^{b_j t} e^{b_k t} dt = \frac{a_k}{(b_j+b_k)^2}$$

$$\frac{\partial^2 I}{\partial b_j \partial b_k} = a_j a_k \int_0^\infty t^2 e^{b_j t} e^{b_k t} dt = \frac{-2a_j a_k}{(b_j+b_k)^3}$$

$$\frac{\partial^2 I}{\partial b_j^2} = a_j^2 \int_0^\infty t^2 e^{2b_j t} dt + a_j \int_0^\infty (y-f)t^2 e^{b_j t} dt$$

$$= \frac{-2a_j^2}{(2b_j)^3} + g_j \quad .$$

Thus, as in the discrete case, the Hessian consists of two parts,

$$H = H_0 + G,$$

with H_0 depending explicitly on the $\{a_j, b_j\}$ and G explicitly on f(t). If we order the variables $a_1,\ldots,a_m,b_1,\ldots,b_m$, then H_0 has the form

$$H_0 = \left[\begin{array}{c|c} \dfrac{-1}{b_j+b_k} & \dfrac{a_k}{(b_j+b_k)^2} \\ \hline \dfrac{a_j}{(b_j+b_k)^2} & \dfrac{-2a_ja_k}{(b_j+b_k)^3} \end{array}\right] \qquad j,k = 1,\ldots,m. \qquad (3.3)$$

If we factor out the $\{a_j\}$ by a diagonal congruency transformation, the remaining matrix is the Gram matrix for the functions e^{b_jt}, te^{b_jt}, $j = 1,\ldots,m$. Thus H_0 is positive definite and the nature of a particular critical point depends on G. If the solution y(t) is a good fit, so that the terms g_j are small, H will be very close to H_0, and in this case the sensitivity of the solution parameters will depend effectively on the eigenvalues of H_0.

However, H_0 is <u>very</u> ill-conditioned: for $b_j = j$, the top left block is the Hilbert matrix of order m, and H_0 is in fact much more ill-conditioned than this. Even for $m = 2$, $\lambda_1(H) < 10^{-4}$; for $m = 3$, $\lambda_1(H) < 10^{-7}$, and for $m = 4$, $\lambda_1(H) < 10^{-10}$. In practice, we have found that the Hessian eigenvalues are indeed very close to those of H_0 (at the minimum point), so that the problem is intrinsically very ill-conditioned.

Moreover, the situation is really much worse than this: there is the strong possibility of multiple solutions of (3.2) for a given function f(t), even in very simple cases. We illustrate this by extending an example of Kammler (1979), fitting two exponentials by one, i.e.

$$f(t) = e^{-t} + \alpha e^{\beta t}, \qquad y(t) = ae^{bt}.$$

We assume $\alpha_1\beta$ are given, a,b are to be found, and that b,β are negative. The equation (3.2) are as follows:

$$\frac{\partial I}{\partial a} = 0 \Rightarrow \frac{a}{2b} = \frac{1}{b-1} + \frac{\alpha}{b+\beta} \tag{3.4}$$

$$\frac{\partial I}{\partial b} = 0 \Rightarrow a = 0 \quad \text{or} \quad \frac{a}{4b^2} = \frac{1}{(b-1)^2} + \frac{\alpha}{(b+\beta)^2} \tag{3.5}$$

However, using (3.4) gives

$$I = \frac{a^2}{2b} + \frac{1}{2} - \frac{\alpha^2}{2\beta} - \frac{2\alpha}{\beta-1} \tag{3.6}$$

so I is always smaller if $a \neq 0$, i.e. $a = 0$ never gives a minimum. Using (3.4) to define a, and substituting in (3.5) gives

$$(b+1)(b+\beta)^2 + \alpha(b-\beta)(b-1)^2 = 0 \tag{3.7}$$

which is a cubic for $b = b(\alpha,\beta)$ with one or three real solutions. To see when three real solutions can exist, express I as a function of b alone (using (3.4)):

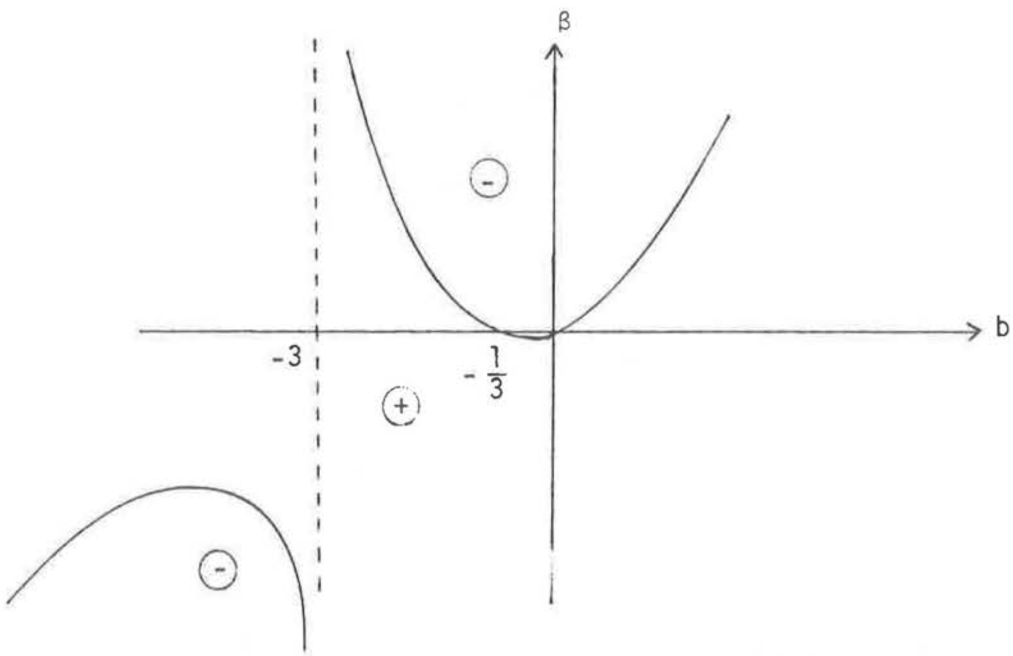
$$I(b) = 2b\left(\frac{1}{b-1} + \frac{\alpha}{b+\beta}\right)^2 + \frac{1}{2} - \frac{\alpha^2}{2\beta} - \frac{2\alpha}{\beta-1}. \tag{3.8}$$

Now $\frac{dI}{db} = 0$ gives a = 0 or (3.7) as above; however at solutions of (3.7)

$$\frac{d^2I}{db^2} = \frac{4(\beta+1)^2 b}{(b-\beta)^2(b-1)^5(b+\beta)} [3b^2+b-b\beta-3\beta]$$

whose <u>sign</u> is completely determined by the quantity in square brackets. A plot of this in the b-β plane is shown in Figure 4.

FIGURE 4



Notice that the only chance for having three real roots is for (b,β) to be in the $(-)$ region (i.e. with $I''(b) < 0$) for one of the roots b, so that a local maximum is achieved. In particular, notice that (from (3.7)) if $\alpha < 0$, $b > \beta > -1$ or $b < \beta < -1$ implying $I''(b) > 0$ so there is a unique minimum in this case. Also note that f(t) is only non-monotone in this case.

Now consider b,β as our free parameters (not α,β) with α given by (3.7). We can restrict our attention to the small $\ominus$ region R near zero and below the $b = 0$ axis; the other $\ominus$ region is obtained by a simple transformation: $b \to 1/b$, $\beta \to 1/\beta$; $\alpha \to -\alpha/\beta$, the other b-roots $\to$ reciprocals, $a \to -a/b$, and $I \to I$. That is, for each (b,β) pair in R, there is a reciprocal pair $(\frac{1}{b}, \frac{1}{\beta})$ with the same solution. However in R, we have <u>three</u> b-solutions; there is one b for which $I''(b) < 0$, i.e. a local maximum. However we must have two other local minima (say x_1,x_2) with $-\infty < x_1 < b < x_2 < 0$, since $I'(b) > 0$ for $b \to 0^-$, $b \to -\infty$. Actually, this holds for interior points of R only; on the boundary, we get a double root (say $x_1 = b$) and even a triple root at the minimum of the b-β curve (i.e. $b = \sqrt{8} - 3$).

Of particular interest are cases where the two local minima x_1,x_2 have identical I-values, so we in fact have a non-unique <u>global</u> minimum. This occurs for a continuum of values (b,β) inside R given by $\beta = -b^2$ (notice this curve leaves R at the minimum $b = \sqrt{8} - 3$). On this curve, the other b-roots x_1,x_2 are given by (for $\sqrt{8} - 3 < b < 0$)

$$x^2 + (b^2+4b+1)x + b^2 = 0$$

or

$$x_{1,2} = \frac{-(b^2+4b+1) \pm (b+1)\sqrt{b^2+6b+1}}{2} .$$

At these x-values, the corresponding a-values from (3.4) are

$$a(x) = 2x\left(\frac{1}{x-1} - \frac{b}{x-b^2}\right) = 2\left(\frac{1}{1-1/x} - \frac{b}{1-b^2/x}\right) .$$

Notice that if $x \to b^2/x$, $a(x) \to a(b^2/x) = 2b(\frac{1}{x-1} - \frac{b}{x-b^2}) = \frac{b}{x} a(x)$, and hence $\frac{a^2(x)}{2x} = \frac{a(x)a(b^2/x)}{2b} = \frac{a^2(b^2/x)}{2(b^2/x)}$. Thus since $x_2 = b^2/x_1$ for the two roots, we have $\frac{a^2(x_1)}{2x_1} = \frac{a^2(x_2)}{2x_2}$ and thus from (3.6), $I(x_1) = I(x_2)$.

Thus we can have multiple solutions and non-unique minima even in this relatively simple case; as Kammler (1979) notes, such problems are extremely ill-conditioned numerically, particularly for b near the triple root.

From now on, we specialize to the case of two exponentials, i.e. $y(t) = a_1 e^{b_1 t} + a_2 e^{b_2 t}$. Then the variational equations are (see (3.2))

$$\left.\begin{aligned} &\frac{-a_1}{2b_1} + \frac{-a_2}{b_1+b_2} = g(b_1) \equiv g_1; \quad \frac{-a_1}{b_1+b_2} + \frac{-a_2}{2b_2} = g(b_2) \equiv g_2 \\ &\frac{a_1}{4b_1^2} + \frac{a_2}{(b_1+b_2)^2} = g'(b_1) \equiv g_1'; \quad \frac{a_1}{(b_1+b_2)^2} + \frac{a_2}{4b_2^2} = g'(b_2) \equiv g_2'. \end{aligned}\right\} \tag{3.9}$$

The first two equations define a_1, a_2 via $B\underline{a} = \underline{g}$, with

$$B = \begin{bmatrix} \frac{-1}{2b_1} & \frac{-1}{b_1+b_2} \\ \frac{-1}{b_1+b_2} & \frac{-1}{2b_2} \end{bmatrix}.$$

Then the remaining two are

$$\left.\begin{aligned} &\left(\frac{1}{2b_1} - \frac{2b_2}{b_1^2-b_2^2}\right)g_1 + \frac{b_2}{b_1(b_1-b_2)}\, g_2 = -g_1' \\ &\frac{-b_1}{b_2(b_1-b_2)}\, g_1 + \left(\frac{1}{2b_2} + \frac{2b_1}{b_1^2-b_2^2}\right) g_2 = -g_2' \end{aligned}\right\} . \tag{3.10}$$

Moreover, the functional

$$I(a(b),b) \equiv \int_0^\infty (y-f)^2 dt = \int_0^\infty f^2 dt - \underline{g}^T B^{-1} \underline{g}$$

which after some manipulation can be expressed as

$$I = \int_0^\infty f^2 dt + 2(b_1+b_2)[(\frac{b_1 g_1 - b_2 g_2}{b_1 - b_2})^2 + b_1 b_2 (\frac{g_1 - g_2}{b_1 - b_2})^2]. \qquad (3.11)$$

This last form is particularly useful, as it holds in the confluent case ($b_1 = b_2$) as well if limits are used. If $b_1 = b_2 = b$, then $y(t) = (ct+d)e^{bt}$, and the variational equations give

$$c = -4b^2(g+2bg'), \qquad d = -4b(g+bg')$$

where $g = g(b)$, $g' = g'(b)$ as before. Then in terms of b only,

$$I = \int_0^\infty f^2 dt + 4bg^2 + 8bgg' + 8b^3(g')^2 \qquad (3.12)$$

which indeed is the limit of (3.11) as $b_2 \rightarrow b_1 = b$. The conditions for a critical point in this case boil down to one equation:

$$I'(b) = 4[g^2 + 6bgg' + 8b^2(g')^2 + 2b^2 gg'' + 4b^3 g'g''] = 0.$$

Because of the symmetry in $I(b_1,b_2)$ across $b_1 = b_2$, any solutions of this equation are critical points of I in the b_1,b_2 plane, and may be local minima, maxima, or saddle points.

In principle, for a given function $f(t)$, equations (3.10) could be used to find solutions and (3.11) could be differentiated to find the Hessian. However this appears to be difficult in any specific practical case, and we prefer to try to understand the problem by plotting the surface $I(b_1,b_2)$.

As an example, consider $f(t) = t^2e^{-t}$. Then

$$g(b) = \frac{2}{(1-b)^3}, \quad g'(b) = \frac{6}{(1-b)^4}, \quad g''(b) = \frac{24}{(1-b)^5}.$$

The variational equations (3.10) are difficult to analyze; however the confluent case $b_1 = b_2 = b$ is somewhat easier:

$$I(b) = \frac{3}{4} + 4b\,\frac{4}{(1-b)^6} + 8b^2\,\frac{12}{(1-b)^7} + 8b^3\,\frac{36}{(1-b)^8}$$

and it is easy to check that $I'(b) = 0$ at three points:

$b_2 = -0.2;$ $\qquad I(b_2) \cong .214 \qquad$ (local minimum)

$b_1 = \frac{-5+\sqrt{12}}{13} \cong -.118;$ $\qquad I(b_1) \cong .202 \qquad$ (saddle point)

$b_3 = \frac{-5-\sqrt{12}}{13} \cong -.651;$ $\qquad I(b_3) \cong .0125 \qquad$ (global minimum)

There appear to be no critical points for $b_1 \neq b_2$, and we plot the surface $[I(b_1,b_2)]^{1/2}$ in Figure 5, with $-.05 \geq b_1b_2 \geq -2.0$.

Other choices of $f(t)$ will give very different surfaces, of course, and in the next section we consider the special case where $f(t)$ is itself an exponential sum.

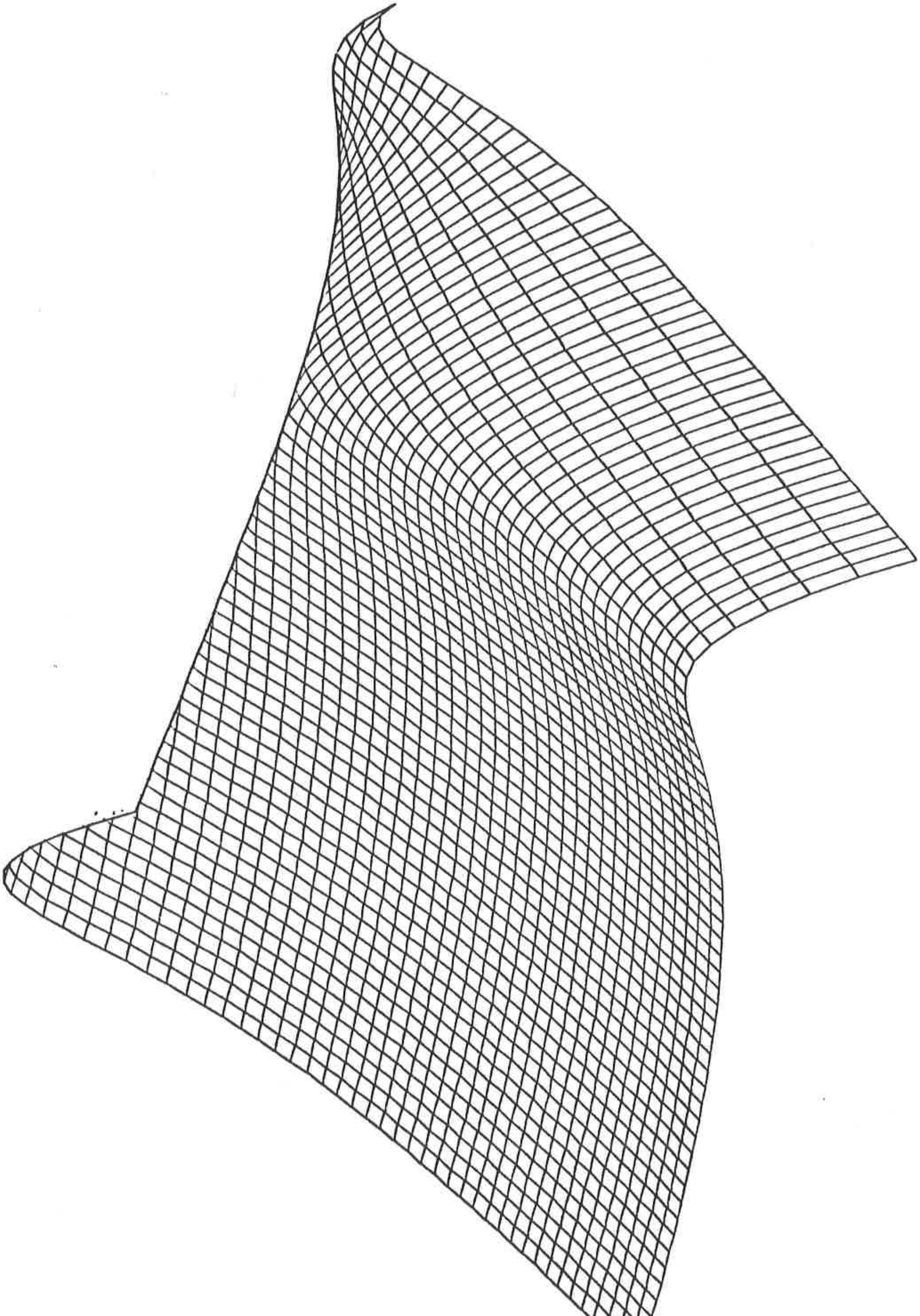


FIGURE 5

4. EXPONENTIAL DATA

Here we consider fitting two exponentials $y(t) = a_1 e^{b_1 t} + a_2 e^{b_2 t}$ to $f(t) = \sum_{j=1}^{n} \alpha_j e^{\beta_j t}$ as we did in the discrete case in Section 2. Thus $g(b) = \sum_1^n \frac{-\alpha_j}{b+\beta_j}$, and the variational equations (3.10) can, after some manipulation, be written

$$\left.\begin{aligned} \sum_{j=1}^{n} \alpha_j \frac{(b_1-\beta_i)(b_2-\beta_i)}{(b_1+\beta_i)^2(b_2+\beta_i)} &= 0 \\ \sum_{j=1}^{n} \alpha_j \frac{(b_1-\beta_i)(b_2-\beta_i)}{(b_1+\beta_i)(b_2+\beta_i)^2} &= 0 \end{aligned}\right\} . \tag{4.1}$$

Clearly, some results about the location of roots (b_1,b_2) can be inferred from (4.1). For example, if the $\alpha_j > 0$ for all j, and $\beta_n < \ldots < \beta_1 < 0$, then at least one of (b_1,b_2) must lie inside (β_n,β_1).

However, it is very difficult to give any more general results about the nature of the solutions (b_1,b_2): even if the β_j are fixed, the nature of the surface $I(b_1,b_2)$ varies enormously with the choice of $\underline{\alpha} = (\alpha_1,\ldots,\alpha_n)$. From (3.11), we can express $I(b_1,b_2)$ as

$$\begin{aligned} I &= \alpha^T C\alpha - g^T B^{-1} g, \qquad c_{ij} = \frac{-1}{\beta_i+\beta_j} \\ &= \alpha^T A\alpha, \end{aligned} \tag{4.2}$$

with $A = DCD$, and D diagonal with $d_i = \frac{(b_1-\beta_i)(b_2-\beta_i)}{(b_1+\beta_i)(b_2+\beta_i)}$. Moreover, we can express the Hessian similarly:

$$H = \begin{pmatrix} \alpha^T \dfrac{\partial^2 A}{\partial b_1^2} \alpha & \alpha^T \dfrac{\partial^2 A}{\partial b_1 \partial b_2} \alpha \\ \alpha^T \dfrac{\partial^2 A}{\partial b_1 \partial b_2} \alpha & \alpha^T \dfrac{\partial^2 A}{\partial b_2^2} \alpha \end{pmatrix}.$$

One can explicitly compute the partial derivatives; indeed,

$$\frac{\partial^2 A}{\partial b_1^2} = 4b_1^3(\bar{D}G\bar{D})$$

where $\bar{D}$ is diagonal, $\bar{d}_i = \dfrac{b_2-\beta_i}{(b_2+\beta_i)(b_1+\beta_i)^3}$, and $g_{ij} = 1 - 3\dfrac{\beta_i\beta_j}{b_1^2} + \dfrac{\beta_i\beta_j}{b_1^2}(\dfrac{\beta_i}{b_1} + \dfrac{\beta_j}{b_1})$. However, to show uniqueness of a minimum point (b_1,b_2) for example, we need convexity of $I(b_1,b_2)$, i.e. H positive definite for all $b_1 < 0$, $b_2 < 0$, for some particular choice of $\underline{\alpha}$ and $\underline{\beta}$. This, seems to be very difficult: the matrix G is unfortunately indefinite over much of the region $b_1 < 0$.

Even the confluent case is intractable, although interesting: one can readily express the function I(b) from (4.2) and its derivatives; for example

$$\frac{dI}{db} = -4\alpha^T \hat{D}\hat{G}\hat{D}\alpha,$$

with D diagonal, $\hat{d}_i = \dfrac{b-\beta_i}{(b+\beta_i)^3}$, and $\hat{g}_{ij} = b^2 - \beta_i\beta_j$. Again, however, the nature of the function varies tremendously with α. For some α, $\frac{dI}{db} = 0$ at only one point (a minimum), and for these it appears that $I(b_1,b_2)$ has a unique minimum as well; for others however, the confluent case admits 3 or more solutions and the full function $I(b_1,b_2)$ can have several minima. As well, $I(b_1,b_2)$ can be very flat over a large range of b_1,b_2. We can illustrate these different aspects with examples, all taken with n = 3 and $\beta_1 = -1$, $\beta_2 = -3$, $\beta_3 = -5$.

<u>Example 1</u>: (the Lanczos data) α = .0951, .8607, 1.5576

Here the confluent case has one minimum, which is a saddle point for the full function $I(b_1,b_2)$. This in turn has a unique minimum for $b_1 \geq b_2$ at (-1.47,-4.42) with $I = .85\text{x}10^{-5}$ and $\lambda_{min}(H) = .0021$. The surface is very similar to that of the discrete problem, given in Figure 2.

<u>Example 2</u>: α = .1, .4, -.3

Here (as in the discrete problem) the confluent case has three critical points, one a local minimum and the other saddle points for the full problem. In addition, the full problem has a minimum for $b_1 > b_2$.

The minima are: (-1.17,-1.17), $I = .99\text{x}10^{-4}$

(-1.54,-11.2), $I = .18\text{x}10^{-4}$, $\lambda_{min}(H) = .48\text{x}10^{-6}$.

Again the surface is similar to that in Figure 3.

Notice also that this surface is very flat: indeed for the whole region $-1 \geq b_1,b_2 \geq -3$, we have

$$.06\text{x}10^{-3} \leq I(b_1,b_2) \leq .25\text{x}10^{-3}.$$

<u>Example 3</u>: α = .14, -.70, .70

Here the confluent case has 5 critical points, listed in Table 5.

TABLE 5

b	-0.20	-0.33	-0.73	-2.11	-7.2
$I(b)$	$.1165\times10^{-2}$	$.1174\times10^{-2}$	$.1124\times10^{-2}$	$.1456\times10^{-2}$	$.078\times10^{-2}$
nature	minimum	saddle	minimum	maximum	minimum

The surface is incredibly flat in this case; over the whole range $-0.1 \geq b_1 b_2 \geq -10.0$, $.078\times10^{-2} \leq I(b_1,b_2) \leq .146\times10^{-2}$. Thus if the surface is scaled like the others (where max $I(b_1,b_2) \cong 1.0$), it would appear totally flat. Scaled up however, it is much more interesting: see Figure 6. The three local minima from the confluent case $b_1 = b_2$ appear to be the only minima; however almost any value of b_1 and b_2 will do just as well. Notice that here $\underline{\alpha}$ is very nearly the eigenvector corresponding to the smallest eigenvalue of A in (4.2).

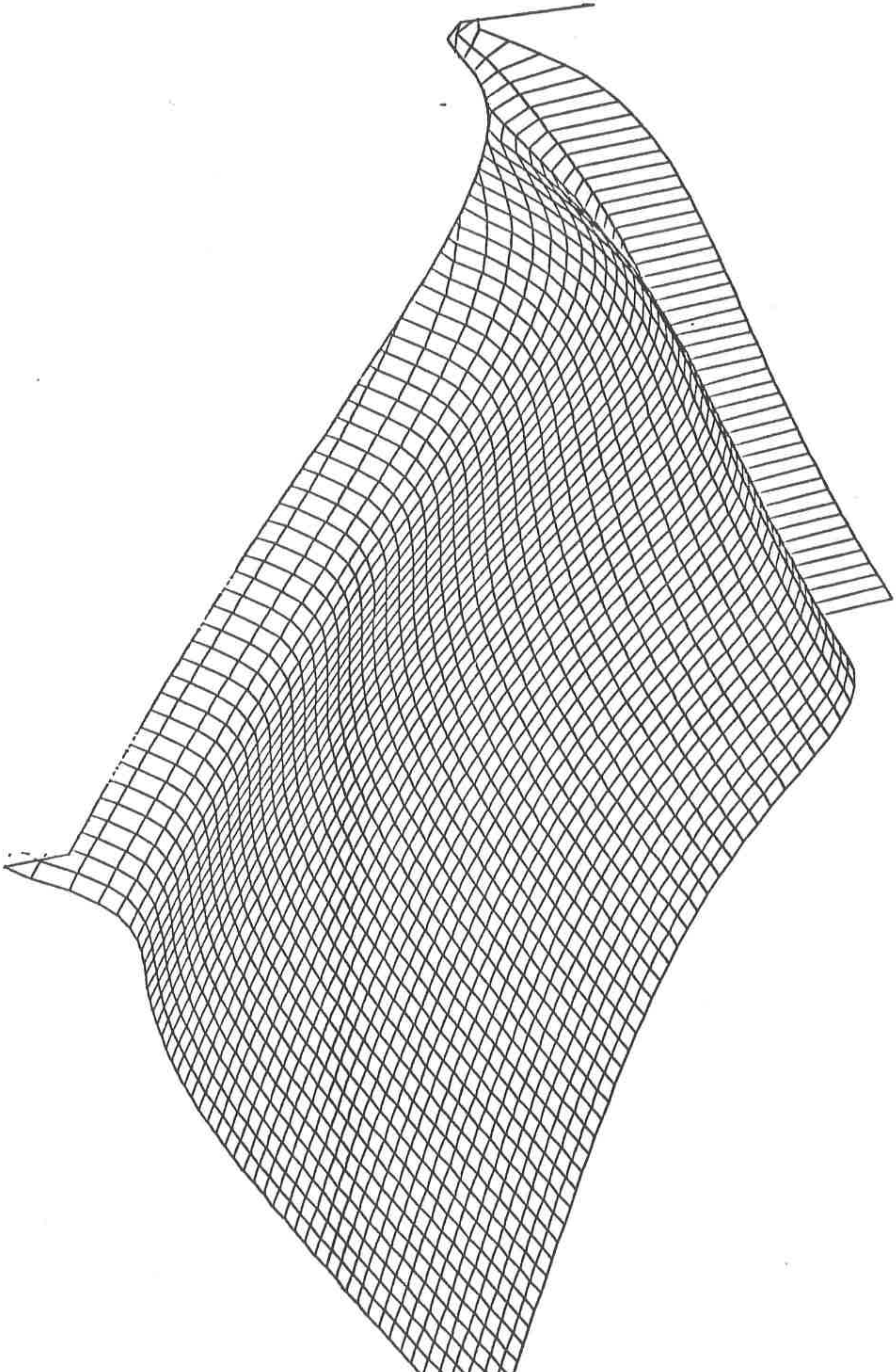


FIGURE 6

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