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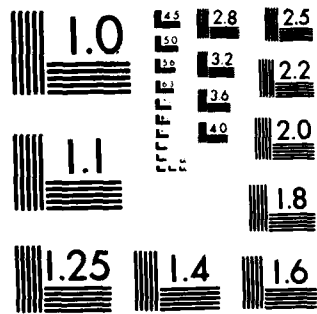
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Some Common-Sense Optimization Techniques for Non-Differentiable Functions of Several Variables

By

B.N. Borah

and

J.F. Chew

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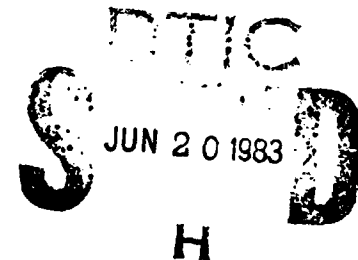
Dr. Bolindra N. Borah, Professor of
Applied Mathematics and Computer
Science

Dr. James F. Chew, Associate Professor
of Mathematics

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- 1 -

SOME COMMON-SENSE OPTIMIZATION TECHNIQUES FOR
NON-DIFFERENTIABLE FUNCTIONS OF SEVERAL VARIABLES

ABSTRACT:

The problem of obtaining global optima of non-differentiable functions of several variables is studied. In general, the functions are multimodal and continuous on a compact domain. Two distinct methods are proposed and to some extent compared: The method of systematic search and the random search technique. The method of uniform saturation [the one variable version of the systematic search method] is based on bisecting the interval (in the one-variable case) repeatedly. Without loss of generality, we may restrict the discussion to the closed unit interval $I = [0,1]$. At the first stage, $n = 1$, bisect the interval I using the point $x = 1/2$. Let $M_1 = \max [f(1/2), f(1)]$. At the second stage, $n = 2$, bisect each of the intervals $[0,1/2]$ and $[1/2,1]$ using the points $x = 1/4$ and $x = 3/4$ respectively. Let $M_2 = [m_1, f(1/4), f(3/4)]$. By the n th stage we would have subdivided the interval I into 2^n subintervals, each of length $(1/2)^n$, wherein the partition points over and above those previous stages are $i(1/2)^n$, $i = 1, 3, \dots, 2^n - 1$. Thus the M_n 's are inductively given by $M_n = \max [M_{n-1}, f(i/2^n); i = 1, 3, \dots, 2^n - 1]$. It is now clear that M_n is monotonic increasing sequence, $M_1 \leq M_2 \leq M_2 \leq \dots$. If we repeat the procedure enough times, we would "saturate" the interval I by evenly spaced points in such a way that the distance between

two neighboring points diminishes geometrically as n -increases. Thus we "zero-in" on a solution of the problem. This method is later modified to the case of functions of two or three variables.

The Random Search Technique used here determines all the optimal points of the non-differentiable continuous functions with many variables defined on compact domain. The procedure begins with evaluating the given function at pre-determined number of points selected randomly over the closed bounded domain. Suppose m points are selected randomly over the domain and the function is evaluated at each of the m points. The minimum functional value and the point at which the minimum occurs (if the problem is one of minimization) are saved. This step is carried out n times, where n is sufficiently large. The resulting n points will cluster around the minima. Suppose there are r cluster points, then there is a possibility that around each cluster point, a local minimum may exist. We develop a single program to find all the cluster groups as well as cluster points using a local optimization routine. Thus the global minimum is obtained by simple comparison. The new method developed here is clearly an improvement with regards to time and accuracy over the methods proposed by Becker and Lago and Price's CRS procedure.



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INTRODUCTION

There are many optimization procedures which enable one to determine the minimum of a unimodal function in n -space. If the function is differentiable in a compact domain, global minima may be obtained through the use of derivatives. However, the problem of global optimization of multimodal function has received comparatively little attention, more so when the function in question is non-differentiable. No efficient method has been developed to tackle global optimization problems.

As a general principle, the accuracy with which a procedure locates optima improves with the number of functional evaluations. In principle, however, one seeks a balance between a degree of certainty and the cost of implementation. A procedure which locates optima with great precision and certainty would be practically worthless if it requires economically unfeasible number of calculations.

There are several methods presently utilized to seek global optima; among them are those suggested by Brooks [1], Becker and Lago [2] and Price's CRS method [3]. The Simple Random Method accepts the optimum function value as global optimum after making a specified number of trials randomly selected from the domain. The stratified Random Search method divides the domain into a number of subdomains of equal size and selects, at random, a trial point from each subdomain and each time keeps the optimal function value. The procedure is repeated a good many times. Some improvement on the simple random search is provided by Becker and Lago. Their

procedure begins with a Simple Random Search over the domain, instead of retaining the single point with the optimal function value, Becker and Lago retain a predetermined number of points with optimal function values in each trial. If the number of trials is sufficiently high, the retained points tend to cluster around some optima. Then a mode seeking algorithm is used to group the points into discrete clusters and to define the boundaries of the subregions each embracing a cluster. The clusters are graded, by searching in each for the retained points with the lowest function value and then rated according to the relative values of the cluster minima. The entire procedure is then repeated using as the initial search region that subdomain, defined by the mode seeking algorithm around the 'best' cluster. The user may choose to examine also the second best cluster, or indeed all clusters, according to the extent of his doubt as to whether or not the global minimum will be found in the subdomain defined by the best cluster.

The controlled Random Search (CRS) suggested by Price is similar to Becker and Lago, but CRS combines the random search and mode-seeking algorithm into a single continuous process. But the problems of inefficiency and economic consideration still remain.

METHOD OF SOLUTIONS

This paper deals with two methods: (I) Systematic Search (The Method of Uniform Saturation), (II) Random Search. In both cases it is assumed that the functions are defined and continuous on a compact domain. They are also assumed to be multimodal functions. In general the systematic search does not provide all the optimal points, the primary emphasis here being location of a global optimum.

Despite several restrictions and difficulties, the Random Search method attempts to obtain all the optima, one optimum point in each mode.

I. SYSTEMATIC SEARCH (The Case of Two or Three Variables)

Suppose $f(x,y)$ is continuous on the closed unit square $S = \{(x,y): 0 \leq x,y \leq 1\}$. Then certainly a subdivision of the interval $[0,1]$ into, say, 50 equal subintervals would have to be considered as a reasonable partition. That is to say, 50 is a reasonably small number. Yet even with 50 partition points on each of the x and y axes, we are faced with $50 \times 50 = 2500$ partition points of the unit square S . For the case of a function $f(x)$ of one variable, we certainly would want to partition the interval $[0,1]$ into MORE than 50 subintervals to get a reasonable assurance that an optimum has been included. Hence we cannot be confident that the global optimum will be among the values at the 2500 partition points of the square S .

The case of a function of three variables is much worse. Here a subdivision of each co-ordinate AXIS into 50 partition points results in $50 \times 50 \times 50 = 125,000$ points of the cube. This is just to get a crude starting point. Hence we see that the number of evaluations becomes prohibitive very rapidly and so, to have any hope whatsoever of handling the multivariable case, we would have to abandon the purely exhaustive scheme (Method of Uniform Saturation) used in the univariable case.

The proposed method is based on two steps. The first step involves consideration of an initial grid on the domain. An initial

point is then obtained based on the grid. The second step starts with the initial point and proceeds by the method of 'crossings'.

Any direct search procedure such as the one presently given would require a large number of evaluations. For a function $f(x,y)$ of two variables on a rectangle, we consider 100 partition points on each of the x and y axes to be reasonable. This gives rise to $100 \times 100 = 10,000$ partition points. We realize that 10,000 evaluations might not be cost-effective and that other more efficient methods might be employable. The fact remains that this procedure is direct, simple to execute and self-contained (not based on other search procedures already in existence).

Several theorems pertaining to functions of two variables are proved and some twenty one illustrative, computational examples are provided. These examples comprise Tables 1, 2 and 3. The computer programs are given in Appendix A.

The One-Variable Case: (The Method of Uniform Saturation)

Consider the non-linear programming (NLP) problem: MAXIMIZE
 $f(x) : a \leq x \leq b$, where $f : I \rightarrow R$ is a continuous real-valued
function defined on the closed interval $I = [a,b]$. Without loss of
generality, we may restrict the discussion to the closed unit in-
terval $I = [0,1]$. At the first stage, $n = 1$, bisect the interval
 I using the point $x = 1/2$. Let $M_1 = \max \{f(1/2), f(1)\}$. At the
second stage, $n = 2$, bisect each of the intervals $[0,1/2]$ and
 $[1/2,1]$ using the points $x = 1/4$ and $x = 3/4$ respectively. Let
 $M_2 = \max \{M_1, f(1/4), f(3/4)\}$. At the third stage, $n = 3$, bisect
each of the intervals $[0,1/4]$, $[1/4,1/2]$, $[1/2,3/4]$, and $[3/4,1]$ us-
ing the points $x = 1/8$, $x = 3/8$, $x = 5/8$, and $x = 7/8$ respectively.
Set $M_3 = \max \{M_2, f(i/8) : i = 1,3,5,7\}$.

By the n 'th stage we would have subdivided the interval I in-
to 2^n subintervals, each of length $(1/2)^n$, wherein the new parti-
tion points over and above those of the previous stages are
 $i(1/2)^n : i = 1,3,\dots,2^n - 1$. Thus the M_n 's are inductively given
by $M_n = \max \{M_{n-1}, f(i/2^n) : i = 1,3,\dots,2^n - 1\}$. It is now clear
that M_n is monotone increasing, viz. $M_1 \leq M_2 \leq M_3 \dots$. If we repeat
the procedure enough times, we would "saturate" the interval I by
evenly spaced points in such a way that the distance between two
neighboring points diminishes geometrically as n increases. Thus
we "zero in" on a solution of the problem. That is, if x_0 SOLVES
the problem, then there is a bisecting point x_k WITHIN ANY PRE-
SCRIBED DISTANCE from x_0 . Thus if $\epsilon > 0$ is preassigned, we are as-
sured of the existence of an x_k for which $|x_k - x_0| < \epsilon$ whenever

n is such that $2^n > 1/\epsilon$. Since the function $f(x)$ is continuous, we know that $f(x_k)$ will be close to $f(x_0)$ whenever x_k is "sufficiently" close to x_0 .

The Two-Variable Case

We next consider a real-valued function $f(x,y)$ which is continuous on the closed unit square $S = \{(x,y) : 0 \leq x,y \leq 1\}$. The non-linear programming (NLP) problem is: MAXIMIZE $f(x,y) : (x,y) \in S$.

Theorem 1 Let $f(x,y)$ be a real-valued function which is continuous on a compact domain D . Then

$$\text{MAXIMUM}_{(x,y) \in D} f(x,y) = \text{MAX}_{x \in D_y} \{ \text{MAX}_{y \in D_x} f(x,y) \}, \text{ where for}$$

each fixed x , $D_x = \{y : (x,y) \in D\}$ and for each fixed y , $D_y = \{x : (x,y) \in D\}$.

Proof Clearly $\text{MAXIMUM}_{(x,y) \in D} f(x,y) \geq \text{MAX}_{x \in D_y} \{ \text{MAX}_{y \in D_x} f(x,y) \}$. Suppose

that the inequality is strict:

$$\text{MAXIMUM}_{(x,y) \in D} f(x,y) > \text{MAX}_{x \in D_y} \{ \text{MAX}_{y \in D_x} f(x,y) \}. \text{ Say}$$

$$\text{MAXIMUM}_{(x,y) \in D} f(x,y) = f(x_0, y_0)$$

$$\begin{aligned} \text{then } f(x_0, y_0) &> \text{MAX}_{x \in D_y} \{ \text{MAX}_{y \in D_x} f(x,y) \} \\ &\geq \text{MAX}_{y \in D_x} f(x_0, y) \\ &\geq f(x_0, y_0), \text{ a} \end{aligned}$$

contradiction.

As a corollary, we have:

If $f(x,y)$ is continuous on the closed unit square S , then

$$\begin{aligned} \text{MAXIMUM}_{(x,y) \in S} f(x,y) &= \text{MAX}_{0 \leq x \leq 1} \{ \text{MAX}_{0 \leq y \leq 1} f(x,y) \} = \\ &\text{MAX}_{0 \leq y \leq 1} \{ \text{MAX}_{0 \leq x \leq 1} f(x,y) \}. \end{aligned}$$

We point out that the assumption of continuity cannot be weakened to separate continuity as the following example shows.

Example 1

$$f(x,y) = \begin{cases} xy/(x^4 + y^4) & \text{if } (x,y) \in S - (0,0) \\ 0 & \text{if } (x,y) = (0,0) \end{cases}$$

Theorem 2 Let $f(x,y)$ be continuous on the unit square S . For each $a \in [0,1]$, define $h(a) = \text{MAXIMUM}_{0 \leq y \leq 1} f(a,y)$. Then the function $h: [0,1] \rightarrow \mathbb{R}$ is continuous.

Proof

Let $a \in [0,1]$ and let $\epsilon > 0$ be given. Uniform continuity of $f(x,y)$ implies the existence of $\delta = \delta(\epsilon) > 0$ such that $|f(a,y) - f(x,y)| < \epsilon$ whenever $|x - a| < \delta$. Take x such that $|x - a| < \delta$ and let the maximum of $f(a,y)$ over y occur at \bar{y} and let the maximum of $f(x,y)$ over y occur at $\bar{\bar{y}}$. That is, $h(a) = \text{MAXIMUM}_{0 \leq y \leq 1} f(a,y) = f(a, \bar{y})$ and $h(x) = \text{MAXIMUM}_{0 \leq y \leq 1} f(x,y) = f(x, \bar{\bar{y}})$.

Then $|f(a, \bar{y}) - f(x, \bar{y})| < \epsilon$ and $|f(a, \bar{\bar{y}}) - f(x, \bar{\bar{y}})| < \epsilon$
 $f(a, \bar{y}) < f(x, \bar{y}) + \epsilon \leq f(x, \bar{\bar{y}}) + \epsilon$ and $f(a, \bar{\bar{y}}) - f(x, \bar{\bar{y}}) > -\epsilon$
 $f(a, \bar{y}) - f(x, \bar{\bar{y}}) < \epsilon$ and $f(a, \bar{y}) - f(x, \bar{\bar{y}}) > -\epsilon$.

Thus $|f(a, \bar{y}) - f(x, \bar{\bar{y}})| < \epsilon$ whenever $|x - a| < \delta$ or
 $|h(a) - h(x)| < \epsilon$ whenever $|x - a| < \delta$. This shows
 $h: [0,1] \rightarrow \mathbb{R}$ is uniformly continuous on $[0,1]$.

The example cited earlier shows that the assumption of continuity on $f(x,y)$ in Theorem 2 cannot be relaxed to separate continuity.

Example 2

$$f(x,y) = \begin{cases} xy/(x^4 + y^4) & \text{if } (x,y) \in S - \{(0,0)\} \\ 0 & \text{if } (x,y) = (0,0). \end{cases}$$

It is easily verified that here the function $h(a) = \underset{0 < y < 1}{\text{MAXIMUM}} f(a,y)$

is given by:

$$h(a) = \begin{cases} \frac{3}{4(\sqrt[3]{3} a^2)} & \text{if } 0 < a \leq 1 \\ 0 & \text{if } 0 = a. \end{cases} \quad \text{That is, } h(a) \text{ is } \underline{\text{not}}$$

continuous at $a = 0$.

The next theorem appeared as Problem E 2854 and its solution in the April 1982 issue of the American Mathematical Monthly.

Theorem 3 Let $f(x,y)$ be a real-valued continuous function on the unit square $S = \{(x,y) : 0 \leq x,y \leq 1\}$. Additionally, suppose that for each $a \in [0,1]$, the maximum of $f(a,y)$ over y occurs at ONLY ONE value of y , say $\underset{0 < y < 1}{\text{MAXIMUM}} f(a,y) = f(a,y^*(a))$. Then the assignment $a \mapsto y^*(a)$ defines a continuous function $y^* : [0,1] \rightarrow [0,1]$.

Proof

The proof is by contradiction. Suppose y^* is not continuous at some $a \in [0,1]$. Let $\{a_n\}$ be a sequence in $[0,1]$ convergent to a such that $b_n = y^*(a_n)$ fails to converge to $y(a)$. Since $\{b_n\}$ is a sequence in a compact space, we may assume, without loss of generality,

that $\{b_n\}$ converges to some number $b \in [0,1]$ (otherwise we select a convergent subsequence). Let $f(a, y^*(a)) - f(a, b) = \epsilon$. Since $f(a, y^*(a)) = \text{MAXIMUM}_{0 \leq y \leq 1} f(a, y)$ we see that $f(a, y^*(a)) \geq f(a, b)$; i.e.,

$\epsilon \geq 0$. The uniqueness of the maximum implies that $\epsilon > 0$. For if $\epsilon = 0$ then $f(a, y^*(a)) = f(a, b)$ or BOTH $y^*(a)$ AND b maximize $f(a, y)$ and $y^*(a) = b$, violating the assumed uniqueness of the maximum.

We have:

$$\begin{aligned} |f(a, y^*(a)) - f(a, b)| &\leq |f(a, y^*(a)) - f(a_n, b_n)| + |f(a_n, b_n) - f(a, b)| \\ &= |h(a) - h(a_n)| + |f(a_n, b_n) - f(a, b)| \end{aligned}$$

where h is as defined in Theorem 2.

Theorem 2 together with the fact that $a_n \rightarrow a$ implies that $|h(a) - h(a_n)| < 1/2\epsilon$ whenever n is sufficiently large. Also, continuity of $f(x, y)$ together with the convergences $a_n \rightarrow a$ and $b_n \rightarrow b$ implies $|f(a_n, b_n) - f(a, b)| < 1/2\epsilon$ whenever n is sufficiently large. Thus taking n so large that BOTH $1/2\epsilon$ -inequalities hold simultaneously we obtain the following contradiction:

$$\begin{aligned} |f(a, y^*(a)) - f(a, b)| &< 1/2\epsilon + 1/2\epsilon \\ &\epsilon < \epsilon. \end{aligned}$$

We acknowledge our gratitude to Dr. Charles Giel (formerly of A&T State University) for the proof of Theorem 3 above.

In a private communication, Professor R. A. Struble of North Carolina State University, gave the following solution to Problem E 2854 and hence an independent proof of Theorem 3.

Alternate Proof of Theorem 3 (Direct Proof)

Let $a \in [0,1]$ be given and let $\{a_n\}$ be a sequence in $[0,1]$ such that $a_n \rightarrow a$. We show $y^*(a_n) \rightarrow y^*(a)$. The sequence $\{y^*(a_n)\}$ is in the

compact space $[0,1]$ and hence we may assume that $\{y^*(a_n)\}$ is convergent to some number $b \in [0,1]$ (otherwise we select a convergent subsequence). Continuity of $f(x,y)$ implies that $f(a_n, y^*(a_n)) \rightarrow f(a,b)$ and $f(a_n, y^*(a)) \rightarrow f(a, y^*(a))$. From the definition by y^* , it follows $f(a, y^*(a_n)) \geq f(a_n, y^*(a))$. Thus $\lim f(a_n, y^*(a_n)) \geq \lim f(a_n, y^*(a))$ or $f(a,b) \geq f(a, y^*(a))$. The last inequality says b maximizes $f(a,y)$ over y so that uniqueness of the maximum now implies $b = y^*(a)$; i.e., $y^*(a_n) \rightarrow y^*(a)$.

The proof of Theorem 3 published in the American Mathematical Monthly is shorter than either of the proofs given here; however the published proof relies on a compact graph theorem and, in our opinion is less instructive. Problem E 2854 asks if Theorem 3 may be generalized as follows. Suppose the requirement of the uniqueness of the maximum is no longer imposed and the function $y^* : [0,1] \rightarrow [0,1]$ is modified so that $y^*(a) = \text{MIN} \{y : y \text{ maximizes } f(a,y)\}$. Does the assignment $a \mapsto y^*(a)$ define a continuous function $y^* : [0,1] \rightarrow [0,1]$? The answer is NO! The following counterexample is given in the American Mathematical Monthly.

Example 3

$$f(x,y) = (x-1/2)(y-1/2). \text{ Here } y^*(a) = \begin{cases} 0 & : a \leq 1/2 \\ 1 & : a > 1/2 \end{cases}$$

Professor J. G. Mauldron of Amherst College points out that the function of Example 3 is unsatisfactory because it fails to satisfy the uniqueness property miserably at $a = 1/2$ in the sense that the set $\{y : y \text{ maximizes } f(1/2,y)\} = [0,1]$ and offers the following example instead.

Example 4

$$f(x,y) = (x-y)^2. \text{ Here } y^*(a) = \begin{cases} 1 & : a < 1/2 \\ 0 & : a \geq 1/2. \end{cases}$$

For the function $f(x,y)$ of Example 4, the departure from the uniqueness condition is MINIMAL in the sense that the $\{y:y \text{ maximizes } f(a,y)\}$ is a singleton for $a \neq 1/2$, while the set $\{y:y \text{ maximizes } f(1/2,y)\} = \{0,1\}$.

Professor Mauldron offers the following example to illustrate that the continuity requirement on $f(x,y)$ in Theorem 3 cannot be relaxed to separate continuity.

Example 5

$$f(x,y) = \begin{cases} y & \text{if } x = 0 \\ 8y(x-y)/x^2 & \text{if } x \neq 0 \end{cases}$$

The function $f(x,y)$ satisfies the uniqueness condition but is only separately continuous. The induced function $y^*(a)$ is discontinuous at $a = 0$:

$$y^*(a) = \begin{cases} 1 & \text{if } a = 0 \\ 1/2a & \text{if } 0 < a \leq 1 \end{cases}$$

Looking at Examples 3 and 4, one may be tempted to conjecture that $y^* : [0,1] \rightarrow [0,1]$ enjoys the property of one-sided continuity.

Professor Richard Tucker of A&T State University gives the following counter-example.

Example 6

$$F(x,y) = \begin{cases} f(x,y) : 0 \leq x \leq 1/2, 0 \leq y \leq 1 \\ f(1-x,y) : 1/2 < x \leq 1, 0 \leq y \leq 1 \end{cases}$$

where $f(x,y)$ is as in Example 4 or $f(x,y) = |x - y|$.

$$\text{Here } y^*(a) = \begin{cases} 1 : 0 \leq a < 1/2 \\ 0 : a = 1/2 \\ 1 : 1/2 < a \leq 1. \end{cases}$$

COMPUTATIONAL EXAMPLES

Aaron Chew wrote the BASIC programs for use on Texas Instruments 99/4A personal computer with Extended Basic module and Peripheral Expansion System. We express our deep appreciation to Aaron for his programming assistance.

The TWO-VARIABLE PROGRAM is based on the following procedure. Let $f(x,y)$ be defined on the closed rectangle $R = \{(x,y) : a \leq x \leq b; c \leq y \leq d\}$. First use an Initial Grid on the rectangle obtained by putting evenly spaced points on the sides of the rectangle lying on the co-ordinate axes:

$$a = x_0 < x_1 < x_2 < \dots < x_M = b; c = y_0 < y_1 < y_2 < \dots < y_M = d$$

where $x_i = a + i \frac{(b-a)}{M}$ and $y_j = c + j \frac{(d-c)}{M}$. The procedure first produces an initial approximation (\bar{x}, \bar{y}) based on the points (x_i, y_j) of the initial grid. The Main Program then uses (\bar{x}, \bar{y}) as STARTING POINT and proceeds as follows. Fix $x = \bar{x}$ and minimize $f(\bar{x}, y)$ over $y \in [c, d]$ using evenly spaced partition of the type used in the one-variable case; namely, evenly spaced points $(1/2)^N$ apart. Say $\text{MIN}_y f(\bar{x}, y)$ occurs at $y = \bar{y}_1$. Next minimize $f(x, \bar{y}_1)$ over $x \in [a, b]$, again using points that are $(1/2)^N$ apart. Say $\text{MIN}_x f(x, \bar{y}_1)$ occurs at $x = \bar{x}_2$. Refer to (\bar{x}_2, \bar{y}_2) as the second CROSSING. Repeat as often as desired.

II. RANDOM SEARCH

The domain of the function is closed and bounded and it will always be possible to select the initial starting points at the boundary. All the examples discussed here are of functions whose domains are of the shape of hypercubes, $a_i \leq x_i \leq b_i$. Therefore, starting points may be taken as a_i , $i = 1, 2, 3, \dots$. The next point may be taken as $a_i + \epsilon$, where $\epsilon = (b_i - a_i)/N$, if one decides to use N points to obtain the first minimum. It is not really important which formula is used to generate points over the domain, as long as those domains are searched repeatedly without duplication. We evaluate at the first N points just generated and store the minimum and the coordinates of the minimizing point. We repeat the procedure M times. Therefore, in all M minimum values are saved together with the coordinates of the minimizing points. All the generated points have to be tested whether they belong to the domain before they can be used. The essential features of the algorithm are indicated in the flow-diagram (Figure 1).

The M stored points should cluster around the minima. An illustration of this concept is shown in Figure 2. The main task of this procedure is to locate all the cluster groups. We have achieved only partial success in reaching this objective because of a problem described below:

If some of minima lie very near to each other, this procedure cannot separate the clusters, because the radius of the hypersphere which embrace these cluster points should be very small and therefore many points still remain outside of any hypersphere. These points which are outside give false cluster groups and thereby increase the function evaluations later tremendously. Let us take the

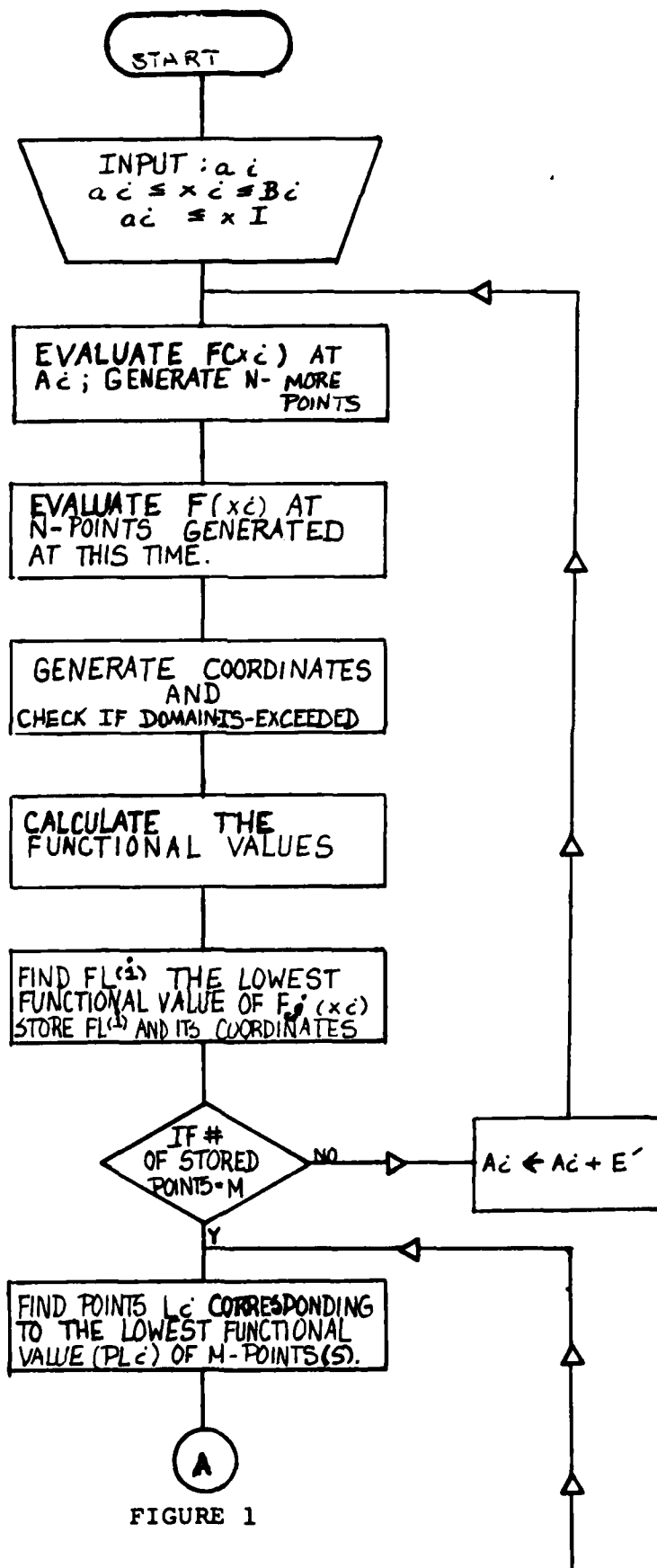


FIGURE 1

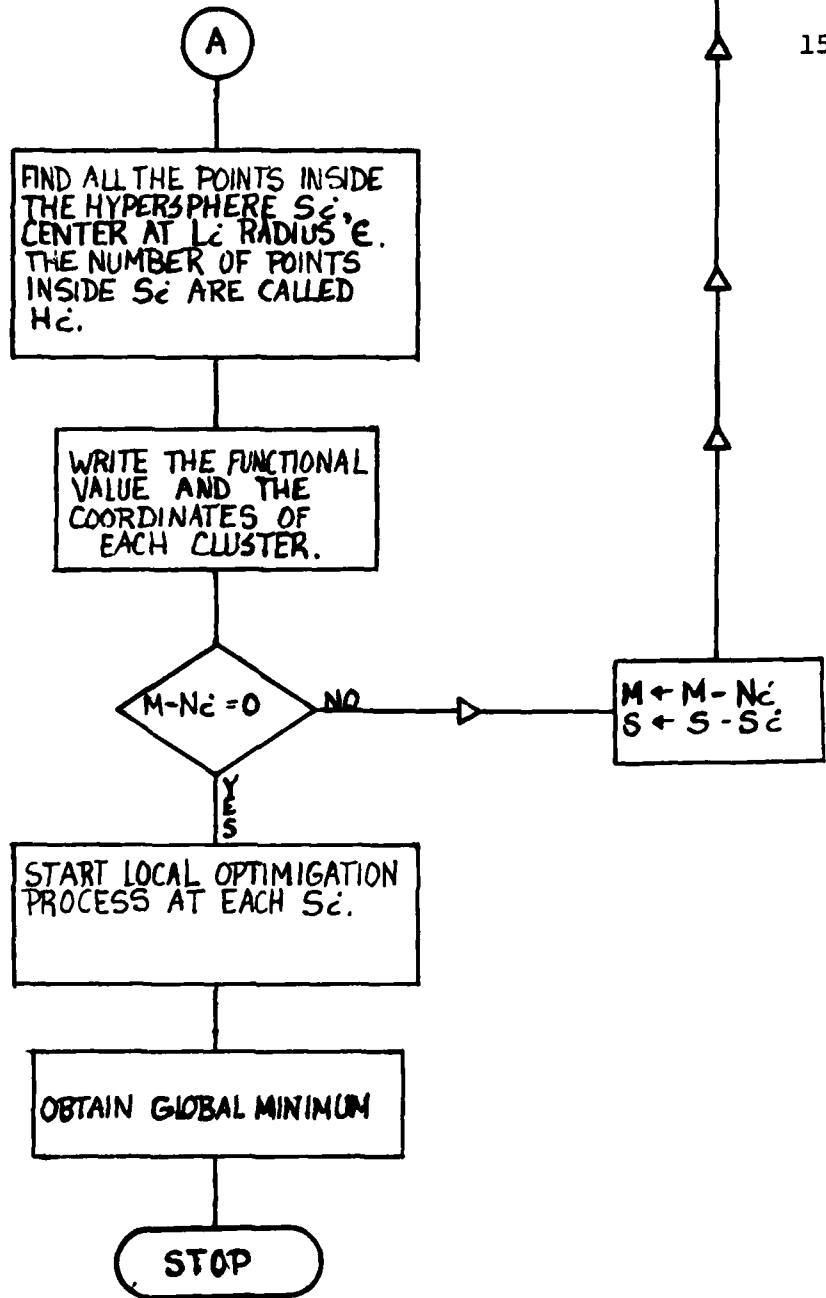


FIGURE 1

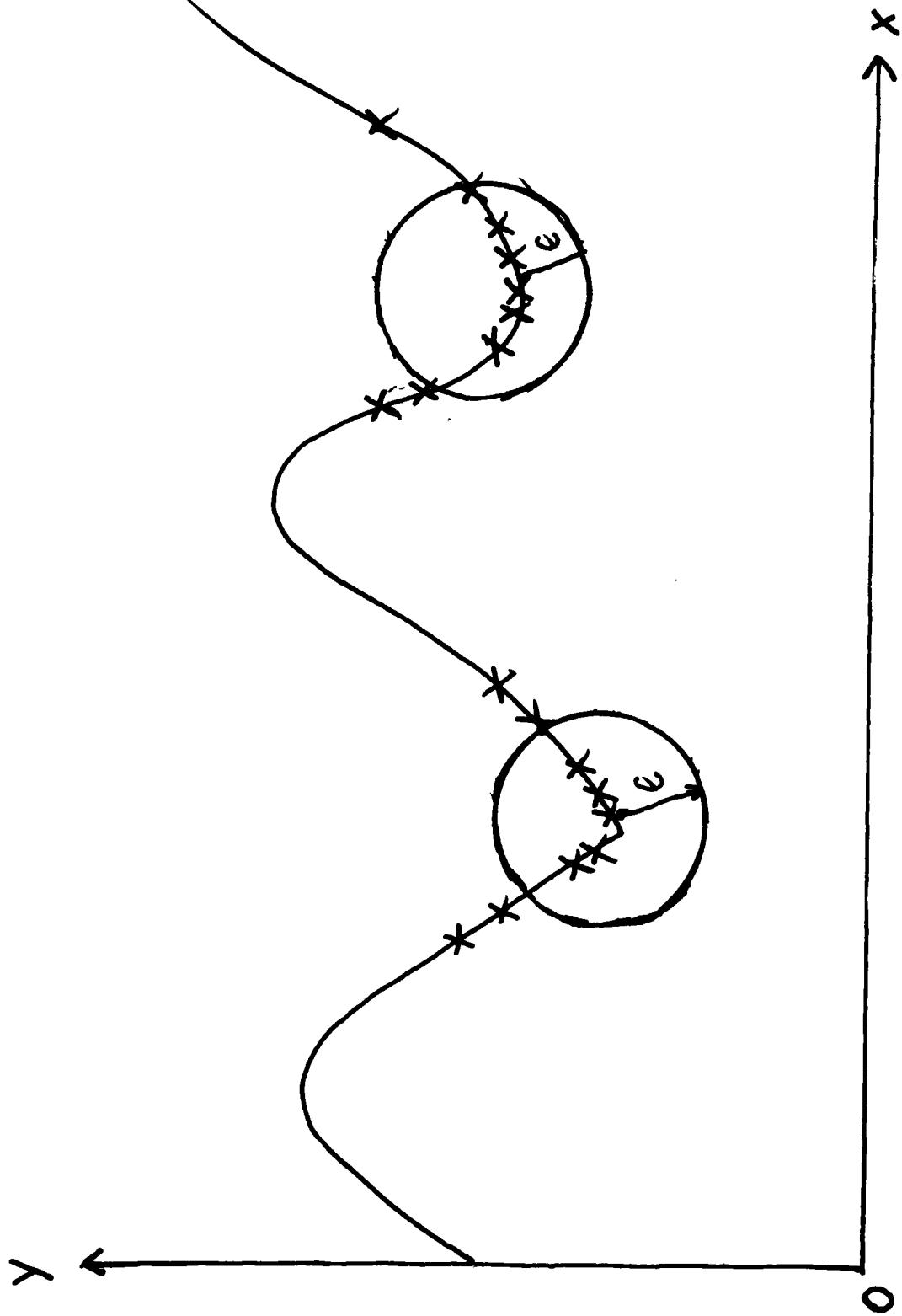


FIGURE 2

following function as example: $f(x_1, x_2) = (|x_1| - 1)^2 + (|x_2| - 2)^2$
 $-4 \leq x_1, x_2 \leq 4.$

There are four minima with function value $f = 0$ and coordinates $(-1, -2), (-1, 2), (1, -2), (1, 2)$. All these clusters lie quite far apart and our procedure can obtain all of them very quickly. However, if $f(x_1, x_2) = (|x_1| - 0.1)^2 + (|x_2| - 0.5)^2$ this procedure will lead to one minimum point only since all four points $(0.1, 0.5), (0.1, -0.5), (-0.1, 0.5)$ and $(-0.1, -0.5)$ are lying on a very small rectangle.

After separating the cluster the next biggest task is to find the actual minimum in each cluster group. Any local optimizing method may be used. However, Nelder and Mead Simplex Search method is the most efficient one for non-differentiable functions. We have used Nelder and Mead Simplex Search method [4] in our program. The Nelder and Mead Simplex Search requires $m + 1$ points for m -dimensional space and they may not lie on the same hyperplane. Therefore, each cluster group, or the hyperspheres which embrace the cluster groups must include at least $m + 1$ points to start the initial simplex. So, not only is the counting of points necessary in each cluster but also sometimes the points must be regenerated if the points fall short.

The checking of collinearity is another important task in Simplex Search method. If the simplex repeats itself for a specific number of times, this has to be modified to prevent from collapsing the simplex. One way to solve this problem is to replace a point from the collapsing simplex by a point which lies on the orthogonal direction to the hyperplane.

The Choice of the Number of Retained Points:

The number of retained points may depend on the size of the domain and as well as the number of variables. Suppose we start with fifty points; fifty functional evaluations are performed and one point with lowest functional value is retained. If one wants to retain 50 points, 2500 function evaluations are required. Therefore, the number of function evaluations is very high where as storage requirement is comparatively less.

Constraints:

All the global optimization problems may be regarded as constrained in the sense that the search is confined within the initially prescribed domain. If any point falls out of this domain, that point has to be discarded. When additional constraints are imposed, then, depending on the number and complexity of these constraints, a sufficiently large number of points has to be selected to insure that a reasonable proportion of points from the totality of trial points be included.

The program is written in FORTRAN IV and several examples are discussed. Since we are using Simplex Search Method, the number of dimensions must be more than one. The program is attached in Appendix B.

Example 1

The function to be minimized is

$$f(x,y,z) = (x - y + z)^2 + (-x + y + z)^2 \\ + (x + y - z)^2, \\ - 1 \leq x, y, z \leq 1$$

It is easy to show that f is a strictly convex quadratic function with an unique minimum at $(0,0,0)$ and $f = 0$.

After 2732 iterations, we have

$$f = 0$$

$$x = 0$$

$$y = 0$$

$$z = 0$$

Actual values: $f = 0, x = 0, y = 0, z = 0$

The method of systematic search takes 12096 iterations to arrive at this result.

In this connection it must be pointed out that in using the systematic search method, we have tried to adhere to standardized values for the number of initial grid points and the number of crossings. Since the function is NON-NEGATIVE and the actual optimal point is $(0,0,0)$, the method of bisection would yield the answer on the very first bisection (27 evaluations at most!). Hence the computer operator would STOP the computer after ONLY 27 evaluations because he sees that f already attains 0 [and can never be improved] after 27 evaluations.

Example 2

This example is used to compare the result obtained by the method systematic search (discussed in this paper, Example 19, Table 3) and the actual values. The function is

$$f(x,y,z) = |x-1| + |y-1.5| + |6z-1|.$$

$$0 \leq x, y \leq 3, 0 \leq z \leq 1.5.$$

Actual solution:

$$\text{Min}(f(x,y,z)) = 0$$

$$x = 1, y = 1.5, z = 0.1666\dots$$

By the Systematic Search Method:

$$\text{Min}(f(x,y,z) = 0.00390625$$

$$x = 1, y = 1.5, z = 0.16605625$$

Number of evaluations: 18752

By the Random Search Method:

$$\text{Min}(f(x,y,z) = 0.000001326$$

$$x = 1, y = 1.5, z = 0.166667$$

Number of evaluations: 3008

Example 3

As another example, let us take the following function which was chosen by both Becker and Lago and Price's CRS algorithm (with additional constraint):

$$f(x_1, x_2, x_3) = 9 - 8x_1 - 6x_2 - 4x_3 + 2x_1^2 + 2x_2^2 \\ + x_3^2 + 2x_1x_2 + 2x_1x_3$$

$$0 \leq x_1x_2 \leq 3, 0 \leq x_3 \leq 1.5.$$

The actual solution is

$f = 0, x_1 = 1, x_2 = 1, x_3 = 1$. The Random Search method achieves this solution in 2686 evaluations where $f = -0.1192 \times 10^{-06}$

$$x_1 = 1, x_2 = 0.9999, x_3 = 1$$

The method of systematic search takes 14144 evaluations.

Example 4

As a final example, we like to consider the following function to obtain all the four minima. Becker and Lago and Price also discussed a similar function. Their function was

$$f(x_1, x_2) = (|x_1| - 5)^2 + (|x_2| - 5)^2.$$

Price obtained all the four minima around $0(10^{-6})$ after 5000

evaluations but not obtained the coordinates. We take

$$f(x_1, x_2, x_3) = (|x_1| - 5)^2 + (|x_2| - 5)^2 + (x_3 - 1)^2$$

$$-10 \leq x_1, x_2, x_3 \leq 10.$$

All the four minima are obtained after 4010 evaluations:

Function Value	Coordinates		
	x_1	x_2	x_3
0.8298×10^{-10}			
0.244×10^{-9}	5.0	5.0	1.0
0.1591×10^{-9}	-5.0	-5.0	1.0
0.1699×10^{-9}	-5.0	5.0	1.0
	5.0	-5.0	1.0

Actual minimum is of course 0 at all these four points.

The computer printout of the unified program is enclosed in the Appendix B.

Conclusion:

The Random Search Method described in this paper is not really a Random Search. Besides the initial point - generation technique, everything later becomes more systematic than random. The method seems to be very efficient for problems wherever the Nelder and Mead Simplex Search method applies. It suffers a serious setback if some of the minima are very 'close' to each other. How close is very 'close'? This is an open question. One may use different local optimization techniques to avoid this situation. The problem of collapsing simplex may be handled as suggested in this paper.

Examining the program, one discovers that the storage requirement is not as great as it first appears. All the initial points

generated need not be saved. We need only to save the number of retained points which actually form clusters.

The work on the Method of Systematic Search has generated some mathematical theory and, it appears that more theoretical developments may be possible. Some of the advantages of the systematic search method are:

- (1) it is applicable to functions of a single variable
- (2) it is direct
- (3) it is easy to execute (the problems of simplicial collapse, etc. do not appear)
- (4) it is independent of other search procedures already in existence
- (5) it goes after the global optimum without first calculating local optima
- (6) it is not sensitive to 'nearness' of the local optima to each other

The method suffers from the standpoint of being computationally uneconomical in that the number of evaluations increases geometrically with an increase in the number of variables. Also the method of systematic search does not, in general, obtain all the local minima. This, in turn, may lead to some doubt as to where the actual global minimum occurs.

This is a serious problem attributed to all procedures which find global minimum without calculating derivatives such as the method of Becker and Lago and Price's Controlled Random Search Procedure. However, the method of Random Search appears to overcome this problem.

Summary of Most Important Results:

(a) The following three theorems have been established:

- (1) Theorem 1: Let $f(x,y)$ be a real valued function which is

Continuous on a compact domain D . Then

$$\text{Max}_{(x,y) \in D} f(x,y) = \text{Max}_{x \in D_y} \left\{ \text{Max}_{y \in D_x} f(x,y) \right\} \text{ where for each fixed } x,$$

$D_x = \{y: (x,y) \in D\}$ and for each fixed y , $D_y = \{x: (x,y) \in D\}$.

(2) Theorem 2: Let $f(x,y)$ be continuous on the unit square S . For each $a \in [0,1]$, define $h(a) = \text{Max}_{0 < y < 1} f(a,y)$. Then the function $h: [0,1] \rightarrow \mathbb{R}$ is continuous.

(3) Theorem 3*: Let $f(x,y)$ be a real valued continuous function on the unit square $S = \{(x,y): 0 \leq x,y \leq 1\}$. Additionally suppose that for each $a \in [0,1]$, the maximum of $f(a,y)$ over y occurs at only one value of y , say $\text{Max} f(a,y) = f(a,y^*(a))$. Then the assignment $a \mapsto y^*(a)$ defines a continuous function $y^*: [0,1] \rightarrow [0,1]$.

(b) A complete program to find the various cluster groups of a multimodal non-differentiable continuous function defined on a compact domain and to pinpoint the minimum value of the function at each cluster group using local optimizing technique is written.

List of All Participating Personnel:

1. Dr. Bolindra N. Borah, Professor, Department of Mathematics and Computer Science, N. C. A&T State University (Co-Principal Investigator).
2. Dr. James F. Chew, Associate Professor, Department of Mathematics and Computer Science, N. C. A&T State University (Co-Principal Investigator).
3. Mr. Duane D. Holmes, Student Assistant, Senior, Mathematics, N. C. A&T State University.

*This theorem appeared as problem E2854 and its solution in the April 1982 issue of the American Mathematical monthly.

4. Mr. Chester Terry, Student Assistant, Senior, Mechanical Engineering, N. C. A&T State University.
5. Mr. Pomorantz D. Sutton, Student Assistant, Junior, Computer Science, N. C. A&T State University.

5. Bibliography:

1. Brooks, S. H., A Discussion of Random Methods for Seeking Maxima Operation Research, Vol. 6, pp. 244-251, (1958).
2. Becker, R. W., and Lago, G. V., A Global Optimization Algorithm, Proceeding of the Eighth Allerton Conference on Circuits and System Theory, (1970).
3. Price, W. L., A Controlled Random Search Procedure for Global Optimization, Computer Journal, Vol. 20, No. 4 (1977).
4. Nelder, J. A., and Mead, R., A Simplex Method for Function Minimization, The Computer Journal, Vol. 7, pp. 308-313 (1965).

NOTE: We could not obtain the paper from J. J. Bryan, S. J. Dwyer and G. V. Lago (1969), so no reference is mentioned in this work.

#	function (f)	DOMAIN	COMPUTED SOLUTION	ACTUAL SOLUTION
1	MIN $(100(x-x^2)^2 + (6.4(x-.5)^2 - x -.6)^2)$	$0 \leq x \leq .5$	f = .6428737641 x = .05078125 N = 10; 512 evaluations	x between .0507 & .0508
2	MAX $(1 - x^2 + \sin x)$	$0 \leq x \leq .5$	f = 1.232465575 x = .4501953125 N = 10; 512 evaluations	x between .450 & .451
3	MAX $(-3x^3 + 3x^2 + x)$	$0 \leq x \leq 2$	f = 1.1840949 x = .8046875 N = 10; 2048 evaluations	f = 1.1840949 x = $\frac{1 + \sqrt{2}}{3} \approx .8047378541$
4	MAX $(x \cos x)$	$0 \leq x \leq 1.6$	f = .561096 x = .8609375 N = 10; 1639 evaluations	
5	MAX $(e^{-x} \cos (x + 1/4\pi))$	$4 \leq x \leq 9$	f = .0063522 x = 4.712890625 N = 10; 5120 evaluations	f = .0063522 x = $\frac{3\pi}{2} \approx 4.712389$
6	MAX $(2 - 3x - 1)$	$0 \leq x \leq 1$	f = 1.9902343 x = .3330078125 N = 10; 1024 evaluations	f = 2 x = $1/3 = .333 \dots$
7	MAX $\frac{2x^2}{(x+1)(x-2)}$	$-1/2 \leq x \leq 1$	f = 0 x = 0 N = 10; 1536 evaluations	f = 0 x = 0

TABLE 1

#	function (f)	DOMAIN	COMPUTED SOLUTION	ACTUAL SOLUTION
8	MAX $(-2x^2)/(x+1)(x-2)$	$-10 \leq x \leq -2$	f = -1.777777778 x = -4 N = 10; 8192 evaluations	f = -16/9 = -1.777... x = -4
9	MAX $(x^2 + 3x + 2)/(x+3)(x-1)$	$-2 \leq x \leq -1$	f = .0669873 x = -1.5361322813 N = 10; 1024 evaluations	f = .669873 x = -5 + 2√3 = -1.5358984
10	MIN $100(y-x^2)^2 + (6.4(y-5)^2 - x - .6)^2$	$0 \leq x, y \leq 1$ $y \leq x$ $x + y \leq 1$	f = .0000693987 x = .34 y = .115234375; M = 50; N = 9 CROSS = 3; 4036 evaluations	f = 0 x = .3414 y = .116554
11	MIN $100(y-x^2)^2 + (6.4(y-5)^2 - x - .6)^2$	$0 \leq x, y \leq 1$ $x \leq y$ $x + y \leq 1$	f = .642941 x = .05 = y; M = 60; N = 9 CROSS = 3; 5136 evaluations	f(.05075) = .6429119 x = y between .0507 & .0508
12	MIN $1 + \sin^2 x + \sin^2 y - .1 e^{-(x^2 + y^2)}$	$-1/2 \leq x, y \leq 1/2$	f = .9 x = 0 = y; M = 50; N = 9 CROSS = 3; 4036 evaluations	f = .9 x = 0 = y
13	MAX $(x+y)/(x^2 + y^2 + 1)$	$0 \leq x, y \leq 1$ $0 \leq x, y \leq 1$	f = .707106 x = .70703125 = y; M = 50; N = 9 CROSS = 3; 4036 evaluations	f = $\frac{1}{\sqrt{2}} \approx .7071068$ x = $\frac{1}{\sqrt{2}} \approx .7071068 \approx y$
14	MAX $\sin(\pi x) + \sin(\pi y) + \sin(\pi(x+y))$		f = 2.598065347 x = .333984372 y = .33203125; M = 50; N = 9 CROSS = 3; 4036 evaluations	f = 2.5980762 x = 1/3 = .333... y = 1/3 = .333...

TABLE 2

#	function (f)	DOMAIN	COMPUTED SOLUTION	ACTUAL SOLUTION
15	MAX $(9y - 32x - y^3 - x^4)$	$-3 \leq x \leq 0$ $0 \leq y \leq 2$	f = 58.39230413 x = -2 y = 1.732; M = 50; N = 9 CROSS = 3; 9668 evaluations	f = 58.392305 x = -2 y = $\sqrt{3} \approx 1.7320508$
16	MAX $(x-y + (x-1 - y ^2))$	$-2 \leq x \leq 2$ $-1 \leq y \leq 3$	f = 17 x = -2 y = -1; M = 60; N = 9 CROSS = 3; 11,788 evaluations	
17	MAX $(xy)/(x^2 + y^2)$	$1 \leq x \leq 2$ $0 \leq y \leq 1$	f = .5 x = 1 = y; M = 60; N = 9 CROSS = 3; 5136 evaluations	
18	MIN $(9-8x-6y-4z+2x^2+2y^2+z^2+2xy+2xz)$	$0 \leq x,y,z \leq 1.5$ $x+y+2z \leq 3$	f = .1125 x = 1.35; M = 20; N = 9 y = .75; CROSS = 3 z = .45; 11,114 evaluations	f = 1/9 = .111... x = 4/3 = 1.333... y = 7/9 = .777... z = 4/9 = .444...
19	MIN $(x-1 + y-1.5 + 6z-1)$	$0 \leq x,y \leq 3$ $0 \leq z \leq 1.5$ $x+y+2z \leq 3$	f = .00390625 x = 1 ; M = 20; N = 9 y = 1.5; CROSS = 3 z = .16605625; 18752 evaluations	f = 0 x = 1 y = 1.5 z = 1/6 = .1666...
20	MIN $(9-8x-6y-4z+2x^2+2y^2+z^2+2xy+2xz)$	$0 \leq x,y,z \leq 1.5$	f = .0000953674 x = 1.013671875; M = 20; N = 9 y = .9921875 ; CROSS = 3 z = .986328125 ; 11,114 evaluations	f = 0 x = 1 y = 1 z = 1
21	MIN $((x-y+z)^2 + (-x+y+z)^2 + (x+y-z)^2)$	$-1 \leq x,y,z \leq 1$	f = 0 ; M = 20; N = 9 x = y = z = 0 ; CROSS = 1 12096 evaluations	f = 0 x = y = z = 0

6. Appendixes:

APPENDIX A

PROGRAM ONE (VARIABLE) (See Example #1)

```
1  CONS = 1.E 20
10  INPUT "N" : N
20  INPUT "START & END POINT" : B,E
30  FOR X = B TO E STEP .5 ^ N
40  A = 100*(X -X ^ 2) ^ 2 + [6.4*(X-.5) ^ 2 - X - .6] ^ 2 :: GOSUB 100
50  NEXT X
55  GOTO 110
100 IF A < CONS THEN CONS = A :: X0 = X :: PRINT "ANSWER"; CONS ::
    PRINT "X"; X0 :: PRINT :: RETURN ELSE RETURN
110 END
```

PROGRAM TWO (VARIABLE) (See Example #10)

```

X = ROW ; Y = COLUMN

5      INPUT "INIT GRID?" : IG :: CONS = 1. E + 100
15     INPUT "CROSSING" : LOOP :: INPUT "N" : CUTTER :: INPUT
      "ROW BEGINNING" : RB :: INPUT "ROW END" : RE :: INPUT
      "COLUMN BEGINNING" : CB :: INPUT "COLUMN END" : CE
20     R1 = RB :: GOSUB 80
30     FOR L123 = 1 TO LOOP
35     FOR COL = CB TO CE STEP .5 ^ CUTTER :: ANSWER = 100*
      ((COL-R1 ^ 2) ^ 2) + (6.4* ((COL - .5) ^ 2) - R1 - .6) ^ 2 ::
      GOSUB 65 :: NEXT COL
45     FOR ROW = RB TO RE STEP .5 ^ CUTTER :: ANSWER = 100*
      ((C1 - ROW ^ 2) ^ 2) + (6.4* ((C1 - .5) ^ 2 - ROW - .6) ^ 2 ::
      GOSUB 70 :: NEXT ROW
55     NEXT L123
60     GOTO 100
65     IF ANSWER < CONS AND R1 ≥ COL AND COL + R1 ≤ 1 THEN
      CONS = ANS :: C1 = COL :: PRINT "ANSWER" ; CONS ::
      PRINT "ROW" ; R1 :: PRINT "COLUMN" ; C1
66     RETURN
70     IF ANSWER < CONS AND ROW ≥ C1 AND C1 + ROW ≤ 1 THEN CONS =
      ANSWER :: R1 = ROW :: PRINT "ANSWER" : CONS :: PRINT
      "ROW" ; R1 :: PRINT "COLUMN" ; C1
71     RETURN

```

PROGRAM TWO (VARIABLE) (Continued)

```
75     IF ANSWER < CONS AND ROW ≥ COL AND ROW + COL ≤ 1 THEN
        CONS = ANSWER ::
R1 = ROW  : : C1 = COL :: PRINT "ANSWER" ; CONS :: PRINT "ROW" ;
        R1 :: PRINT "COLUMN" ; C1
76     RETURN
80     FOR COL = CB TO STEP (CE-CB)/IG
85     FOR ROW = RB TO RE STEP (RE-RB)/IG :: ANSWER = 100*
        ((COL-ROW ^ 2) ^ 2) + (6.4* ((COL - .5) ^ 2 - ROW - .6) ^ 2
        :: GOSUB 75 :: NEXT ROW
90     NEXT COL
95     RETURN
100    END
```


PROGRAM THREE (VARIABLE) (See Example #19)

X = DEPTH; Y = COLUMN ; Z = ROW

```
1   CONS = 1.E 10
10  CALL CLEAR
20  INPUT "INITIAL GRID" : IG
30  INPUT "ROW START & END" : RB,RE
40  INPUT "COLUMN START & END" ; CB,CE
50  INPUT "DEPTH START & END" : DB,DE :: INPUT "LOOP":L
60  INPUT "N" : N
70  FOR DEPTH = DB TO DE STEP (DE-DB)/IG
80  FOR COL = CB TO CE STEP (CE-CB)/IG
90  FOR ROW = RB TO RE STEP (RE-RB)/IG :: A = ABS(DEPTH-1) +
    ABS(COL - 1.5) + ABS(6* ROW - 1) :: GOSUB 500 :: NEXT ROW
100 NEXT COL :: NEXT DEPTH
105 PRINT "OUT OF SUBPROGRAM"
106 FOR L1 = 1 TO L
110 FOR DEPTH = DB TO DE STEP .5^N :: A = ABS(DEPTH - 1) +
    ABS(COLO - 1.5) + ABS(6* ROWO - 1) :: GOSUB 600 :: NEXT DEPTH
120 FOR COL = CB TO CE STEP .5^N :: A = ABS(DEPTHO - 1) +
    ABS(COL - 1.5) + ABS(6* ROWO - 1) :: GOSUB 700 :: NEXT COL
130 FOR ROW = RB TO RE STEP .5^N :: A = ABS(DEPTHO - 1) +
    ABS(COLO - 1.5) + ABS(6* ROW - 1) :: GOSUB 800 :: NEXT ROW
134 PRINT L1
135 NEXT L1
140 END
```

PROGRAM THREE (VARIABLE) (Continued)

```
500  IF < CONS AND DEPTH + COL + 2* ROW ≤ 3 THEN DEPTH = DEPTH
      :: ROWO = ROW :: COLO = COL :: CONS = A :: GOSUB 1000 ::
      RETURN ELSE RETURN

600  IF A < CONS AND DEPTH + COLO + 2* ROWO ≤ 3 THEN CONS = A ::
      DEPTH = DEPTH :: GOSUB 1000 :: RETURN ELSE RETURN

700  IF A < CONS AND DEPTH + COL + 2* ROWO ≤ 3 THEN COLO = COL
      :: CONS = A GOSUB 1000 :: RETURN ELSE RETURN

800  IF A < CONS AND DEPTH + COLO + 2* ROW ≤ 3 THEN CONS = A ::
      ROWO = ROW :: GOSUB 1000 :: RETURN ELSE RETURN

1000 PRINT "ANSWER"; CONS: "DEPTH";DEPTH:"COLUMN";COLO:"ROW";ROWO
      :: PRINT :: RETURN
```

APPENDIX B

COMPUTER PRINT OUT : RANDOM SEARCH

```

P
00100 C FIND ABSOLUTE MINIMUM OF NON-DIFFERENTABLE BOUNDED
00200 C FUNCTION WITH OR WITHOUT CONSTRAINT
00300 C DIMENSION A(3,50,50),FMAX(50),CMAX(50,3),F(50,50),CF(50,
3),
00400 1 MAX(50,50),X(50),Y(50),YMAX(50,50),CYMAX(50,50,3),FMAX1(
50),
00500 2 F(3),CMAX1(50,3),CFAX(50,3),CL1(50,50),FCL(50),CFCL(50,3
),
00600 3 CMAX2(50,3),FMAX2(50),CL(50,50,3),D(6),
00700 4 E(3)
00800 N=20
00900 I1=6
01000 I2=3
01100 OPEN(UNIT=20,FILE='IN1.DAT')
01200 OPEN(UNIT=21,FILE='RES.OUT')
01300 IUI=20
01400 IU=5
01500 C READ DOMAIN PARAMETER
01600 C READ(IUI,*)(D(I),I=1,6)
*P
01700
01800 5 FORMAT(6F5.1)
01900 RAD=4
02000 KOUNT=0
02100
02200 C INITIALIZE THE ARRAY
02300 N=50
02400 DO 7 K=1,I2,1
02500 7 A(K,1,1)=D(K)
02600 C CALCULATE EPSILON VALUES
02700 C
02800 DO 8 I=1,I2,1
02900 8 E(I)=(D(I+3)-D(I))/50.0
03000 C
03100 C GENERATE COORDINATES
03200 C
*P
03300 DO 40 J=1,N,1
03400 DO 30 I=1,N,1
03500 DO 9 K=1,I2,1
03600 9 A(K,I,J)=A(K,1,1)*(-1)**(I*J*K)+I*E(K)*(-1)**I+J*E(K)*(-
1)
03700 1 **J+K*E(K)*(-1)**K
03800 C
03900 C CHECK IF EXCEEDS DOMAIN
04000 C
04100 DO 25 K=1,I2,1
04200 IF(A(K,I,J).LE.D(K)) A(K,I,J)=D(K+3)-J*E(K)
04300 IF(A(K,I,J).GE.D(K+3)) A(K,I,J)=D(K)+J*E(K)
04400 25 CONTINUE
04500 C
04600 C CALCULATE THE FUNCTIONAL VALUES
04700 C
04800 N1=J
*

```

```

P
04900      K1=I
05000      F(I,J)=CAL(A,K1,N1)
05100      KOUNT=KOUNT+1
05200      C      WRITE(IU,26)(A(K,I,J),K=1,I2),F(I,J)
05300      26      FORMAT(4X,3(E10.4,4X),4X,E10.4/)
05400      30      CONTINUE
05500      C
05600      C      CALL SUBROUTINES TO FIND MIN OF THE 50 POINTS JUST EVALA
TED.
05700      C
05800      K=J
05900      I3=I2
06000      CALL FMAXI(A,F,FMAX,CMAX,K,N,I3)
06100      C
06200      C      CALCULATION TO START NEXT SET OF POINTS
06300      C
06400      AJ=J
*P
06500      AJ=AJ/50.
06600      DO 35 K=1,I2,1
06700      35      A(K,1,1)=A(K,1,J)+AJ*(-1)**J
06800      40      CONTINUE
06900      C
07000      C      OUTPUT MINIMUM VALUE & COORDINATES
07100      C
07200      WRITE(IU,45)
07300      45      FORMAT(//,5X,'VALUE OF THE FUNCTION',5X,'FIRST COORDINAT
E',5X,'SECOND
07400      1COORDINATE',5X,'THIRD COORDINATE',/)
07500      DO 50 I=1,N,1
07600      50      WRITE(IU,55) FMAX(I),(CMAX(I,K),K=1,I2)
07700      55      FORMAT(5X,E11.5,5X,E11.5,5X,E11.5,5X,E11.5)
07800      C
07900      C      CALL PLOTTING ROUTINE
08000      C
*P
08100      DO 200 J=1,4,1
08200      JJ=J
08300      CALL MAX2(CMAX,FMAX,FMAX2,CMAX2,N,JJ,I2)
08400      GO TO (60,62,64,67)J
08500      60      WRITE(IU,61)J
08600      61      FORMAT(10X,' GROUP',I3)
08700      WRITE(IU,65) FMAX2(J),(CMAX2(J,K),K=1,I2)
08800      65      FORMAT(5X,E12.4,E12.4,E12.4,E12.4,/)
08900      GO TO 80
09000      62      WRITE(IU,61)J
09100      WRITE(IU,65)FMAX2(J),(CMAX2(J,K),K=1,I2)
09200      GO TO 80
09300      64      WRITE(IU,61) J
09400      WRITE(IU,65) FMAX2(J),(CMAX2(J,K),K=1,I2)
09500      GO TO 80
09600      67      WRITE(IU,61)J
*

```

```

P
09700      WRITE(IU,65)FMAX2(J),(CMAX2(J,K),K=1,I2)
09800      80      K=0
09900      DO 84 I=1,N,1
10000      IF(FMAX(I).EQ.9.1E+10)GO TO 84
10100      DIST=0.0
10200      DO 81 KI=1,I2,1
10300      P(KI)=CMAX2(J,KI)-CMAX(I,KI)
10400      81      DIST=DIST+(P(KI)**2)
10500      Q=SQRT(DIST)
10600      IF(Q.GE.RAD) GO TO 84
10700      K=K+1
10800      FCL(K)=FMAX(I)
10900      DO 82 KI=1,I2,1
11000      82      CFCL(K,KI)=CMAX(I,KI)
11100      FMAX(I)=9.1E+10
11200      DO 83 KI=1,I2,1
*P
11300      83      CMAX(I,KI)=9.1E+10
11400      84      CONTINUE
11500      K=K+1
11600      FCL(K)=FMAX2(J)
11700      DO 85 KI=1,I2,1
11800      85      CFCL(K,KI)=CMAX2(J,KI)
11900      FMAX2(J)=9.1E+10
12000      IF(K .EQ. 0.) GO TO 220
12100      GO TO(101,111,121,131)J
12200      101     K1=K
12300      DO 106 I=1,K1,1
12400      CL1(J,I)=FCL(I)
12500      FCL(I)=0.
12600      DO 105 KI=1,I2,1
12700      CL(J,I,KI)=CFCL(I,KI)
12800      105     CFCL(I,KI)=0.
*P
12900      106     CONTINUE
13000      GO TO 200
13100      111     K2=K
13200      DO 116 I=1,K2,1
13300      CL1(J,I)=FCL(I)
13400      FCL(I)=0.
13500      DO 115 KI=1,I2,1
13600
13700      CL(J,I,KI)=CFCL(I,KI)
13800      115     CFCL(I,KI)=0.
13900      116     CONTINUE
14000      GO TO 200
14100      121     K3=K
14200      DO 126 I=1,K3,1
14300      CL1(J,I)=FCL(I)
14400      FCL(I)=0.
*
```

```

P
14500      DO 125 KI=1,I2,1
14600      CL(J,I,KI)=CFCL(I,KI)
14700      125  CFCL(I,KI)=0.
14800      126  CONTINUE
14900      GO TO 200
15000      131  K4=K
15100      DO 136 I=1,K4,1
15200      CL1(J,I)=FCL(I)
15300      FCL(I)=0.
15400      DO 135 KI=1,I2,1
15500      CL(J,I,KI)=CFCL(I,KI)
15600      135  CFCL(I,KI)=0.
15700      136  CONTINUE
15800      200  CONTINUE
15900      C
16000      C      WRITE THE FUNCTION-VALUE AND THE COORDINATES OF THE WHOL
E CLUSTER
*P
16100      C
16200      220  IF(K1.EQ.0) GOTO 225
16300      WRITE(IU,222) K1
16400      222  FORMAT(10X,' CLUSTER ',I3)
16500      DO 224 I=1,K1,1
16600      224  WRITE(IU,*) CL1(1,I),(CL(1,I,KI),KI=1,I2)
16700      225  IF(K2.EQ.0) GOTO 230
16800      WRITE(IU,226)K2
16900      226  FORMAT(10X,'CLUSTER ',I3)
17000      DO 228 I=1,K2,1
17100      228  WRITE(IU,*) CL1(2,I),(CL(2,I,KI),KI=1,I2)
17200      230  IF(K3.EQ.0) GO TO 235
17300      WRITE(IU,232)K3
17400      232  FORMAT(10X,'CLUSTER ',I3)
17500      DO 234 I=1,K3,1
17600      234  WRITE(IU,*) CL1(3,I),(CL(3,I,KI),KI=1,I2)
*P
17700      235  IF(K4.EQ.0) GO TO 240
17800      WRITE(IU,236) K4
17900      236  FORMAT(19X,'CLUSTER ',I3)
18000      DO 238 I=1,K4,1
18100      238  WRITE(IU,*) CL1(4,I),(CL(4,I,KI),KI=1,I2)
18200      240  WRITE(IU,250)
18300      250  FORMAT(5X,'MAX FUNCT ',5X,'COORD TE-1',5X,'COORD TE-2',
5X,
18400      1  'COORD TE-3',//)
18500      KK=0
18600      DO 350 J=1,4,1
18700      GO TO (302,306,310,314)J
18800      302  IF(K1.EQ.0) GO TO 350
18900      J1=K1
19000      I=J
19100      ICOUNT=0
19200      303  CALL SMPLEX(CL1,CL,CYMAX,YMAX,D,I,J1,I2,ICOUNT)
*
```

```

P
19300      WRITE(IU,305) ICOUNT
19400      305  FORMAT(2X,'GROUP ITERATION',2X,I4)
19500      KK=KK+ICOUNT
19600      WRITE(IU,304) YMAX(J,1),(CYMAX(J,1,KI),KI=1,I2)
19700      304  FORMAT(5X,E10.4,3(6X,E10.4),//)
19800      GO TO 350
19900      306  IF(K2.EQ.0) GO TO 350
20000      J1=K2
20100      I=J
20200      GO TO 303
20300      310  IF(K3.EQ.0) GO TO 350
20400      J1=K3
20500      I=J
20600      GO TO 303
20700      314  IF(K4.EQ.0) GO TO 350
20800      J1=K4
*P
20900      I=J
21000      GO TO 303
21100      350  CONTINUE
21200      KNT=KK+KOUNT
21300      WRITE(IU,355) KNT
21400      355  FORMAT(10X,'TOTAL ITERATION',2X,I5)
21500      CLOSE(UNIT=20,FILE='IN1.DAT')
21600      CLOSE(UNIT=21,FILE='RES.OUT')
21700      STOP
21800      END
21900      SUBROUTINE MAX2(CMAX3,FMAX3,FAX2,CFAX2,M,L,II)
22000      DIMENSION FAX2(50),CMAX3(50,3),FMAX3(50),CFAX2(50,3),TEM
(3)
22100      II=3
22200      DO 10 I=1,M,1
22300      IF(FMAX3(I).GE.FMAX3(1)) GO TO 10
22400      TEMP=FMAX3(1)
*P
22500      FMAX3(1)=FMAX3(I)
22600      FMAX3(I)=TEMP
22700      DO 5 K=1,3,1
22800      TEM(K)=CMAX3(1,K)
22900      CMAX3(1,K)=CMAX3(I,K)
23000      CMAX3(I,K)=TEM(K)
23100      5  CONTINUE
23200      10  CONTINUE
23300      C
23400      C  STORE THE CURRENT LOWER VALUE
23500      C
23600      FAX2(L)=FMAX3(1)
23700      FMAX3(1)=9.1E+10
23800      DO 12 K=1,3,1
23900      CFAX2(L,K)=CMAX3(1,K)
24000      12  CMAX3(1,K)=9.1E+10
*
```



```

P
24100      RETURN
24200      END
24300      SUBROUTINE FMAX1(B,H,FMAX1,CMAX1,L,N1,L3)
24400      DIMENSION B(3,50,50),H(50,50),FMAX1(50),CMAX1(50,3),TEM(
3)
24500      L3=3
24600      DO 10 I=1,N1,1
24700      IF(H(I,L).GE.H(1,L)) GO TO 10
24800      TEMP=H(1,L)
24900      H(1,L)=H(I,L)
25000      H(I,L)=TEMP
25100      DO 5 KK=1,L3,1
25200      TEM(KK)=B(KK,1,L)
25300      B(KK,1,L)=B(KK,I,L)
25400      B(KK,I,L)=TEM(KK)
25500      CONTINUE
25600      *P
25700      C      STORE THE CURRENT LOWEST VALUE AND COORDINATES
25800      C
25900      FMAX1(L)=H(1,L)
26000      DO 12 KK=1,L3,1
26100      CMAX1(L,KK)=B(KK,1,L)
26200      RETURN
26300      END
26400      C
26500      C      LOCAL OPTIMIZATION USING NELDER AND MEADS SMPLEX METHOD
26600      CC
26700      SUBROUTINE SMPLEX(ACL1,CACL1,CZMAX,ZMAX,DD,L,M,I4,KOUT)
26800      DIMENSION ACL1(50,50),CACL1(50,50,3),CZMAX(50,50,3),ZMAX
(50,50),
26900      1  TEMPO(50),DD(6),SUM2(3),X2(4,4),SUM(3)
27000      DIMENSION BST(4,4),CBST(4,4,3),CR(4,3),CP(4,3),PING(4,3)
,
27100      1  FCR(4),FPMG(4),FCW(4),FEX(4),CW(4,3)
27200      DIMENSION X1(4)
27300      *P
27400      DIMENSION EX(4,3)
27500      RADD=0.00004
27600      I4=3
27700      ITER=0.
27800      N2=I4+1
27900      IU=5
28000      DO 3 I=1,N2,1
28100      BST(L,I)=+.91E+10
28200      DO 3 K=1,I4,1
28300      CBST(L,I,K)=(+1)**K*0.91E+11
28400      WRITE(IU,*)BST(L,1),BST(L,2),BST(L,3),BST(L,4)
28500      C
28600      C      FIND THE LOWEST POINT AND THE COORDINATES BST(L,1)
28700      C
28800      WRITE(IU,5) M
28900      5  FORMAT(10X,'THE NUMBER IS ',I4)
*
```

```

P
28900      DO 10 I=1,M,1
29000      IF(ACL1(L,I).EQ.0.91E+10) GOTO 10
29100      IF(BST(L,1).LE.ACL1(L,I)) GO TO 10
29200      TEMP=BST(L,1)
29300      BST(L,1)=ACL1(L,I)
29400      ACL1(L,I)=TEMP
29500      DO 8 K=1,I4,1
29600      TEMPO(K)=CBST(L,1,K)
29700      CBST(L,1,K)=CACL1(L,I,K)
29800      CACL1(L,I,K)=TEMPO(K)
29900      CONTINUE
30000      WRITE(IU,*)BST(L,1)
30100      C
30200      C      FIND THE SECOND BEST
30300      C
30400      DO 20 I=1,M,1
*P
30500      IF(ACL1(L,I).EQ.BST(L,1)) GO TO 20
30600      IF(ACL1(L,I).EQ.0.91E+10) GOTO 20
30700      IF(BST(L,2).LE.ACL1(L,I))GO TO 20
30800      TEMP=BST(L,2)
30900      BST(L,2)=ACL1(L,I)
31000      ACL1(L,I)=TEMP
31100      DO 16 K=1,I4,1
31200      TEMPO(K)=CBST(L,2,K)
31300      CBST(L,2,K)=CACL1(L,I,K)
31400      CACL1(L,I,K)=TEMPO(K)
31500      16
31600      20      CONTINUE
31700      WRITE(IU,*) BST(L,2)
31800      C
31900      C      FIND THE THIRD LOWEST POINT
32000      C
*P
32100      DO 26 I=1,M,1
32200      IF(ACL1(L,I).EQ.BST(L,1)) GO TO 26
32300      IF(ACL1(L,I).EQ.BST(L,2)) GO TO 26
32400      IF(ACL1(L,I).EQ.0.91E+10) GOTO 26
32500      IF(BST(L,3).LT.ACL1(L,I)) GO TO 26
32600      TEMP=BST(L,3)
32700      BST(L,3)=ACL1(L,I)
32800      ACL1(L,I)=TEMP
32900      DO 25 K=1,I4,1
33000      TEMPO(K)=CBST(L,3,K)
33100      CBST(L,3,K)=CACL1(L,I,K)
33200      CACL1(L,I,K)=TEMPO(K)
33300      CONTINUE
33400      WRITE(IU,*) BST(L,3)
33500      C
33600      C      FIND THE FOURTH LOWEST POINT AT THIS TIME
*
```

```

P
33700      C
33800      DO 29 I=1,M,1
33900      IF(ACL1(L,I).EQ.BST(L,1)) GO TO 29
34000      IF(ACL1(L,I).EQ.BST(L,2)) GO TO 29
34100      IF(ACL1(L,I).EQ.BST(L,3)) GO TO 29
34200      IF(ACL1(L,I).GE.BST(L,4)) GO TO 29
34300      IF(ACL1(L,I) .EQ. 0.91E+10) GOTO 29
34400      TEMP=BST(L,4)
34500
34600      BST(L,4)=ACL1(L,I)
34700      ACL1(L,I)=TEMP
34800      DO 28 K=1,I4,1
34900      TEMPO(K)=CBST(L,4,K)
35000      CBST(L,4,K)=CACL1(L,I,K)
35100      28 CACL1(L,I,K)=TEMPO(K)
35200      29 CONTINUE
*P
35300      WRITE(IU,*) BST(L,4)
35400      C
35500      C THE SIMPLEX FORMED BY BST(L,1),BST(L,2),BST(L,3)
35600      C BST(L,4) WHICH
35700
35800      C IS THE BIGGEST ONE SHOULD BE REMOVED
35900      WRITE(IU,30) BST(L,1),BST(L,2),BST(L,3),BST(L,4)
36000      30 FORMAT(2X,F10.4,2X,F10.4,2X,F10.4,2X,F10.4)
36100      C
36200      C SEE IF THE EXIT CRITERIA IS SATISFIED
36300      C
36400
36500      31 DO 35 K=1,I4,1
36600      SUM(K)=0.
36700      DO 35 I=1,N2,1
36800      35 SUM(K)=SUM(K)+CBST(L,I,K)
*P
36900      DO 36 k=1,I4,1
37000      36 X1(K)=SUM(K)/4.
37100      DIF=0.
37200      DO 40 I=1,N2,1
37300      DO 39 K2=1,I4,1
37400      X2(I,K2)=CBST(L,I,K2)-X1(K2)
37500      39 dif=dif+x2(i,K2)**2
37600      40 CONTINUE
37700      DIFB=SQRT(DIF)
37800      ITER=ITER+1
37900      IF(DIFB.LE.RADD) GO TO 500
38000      WRITE(IU,43) DIFB
38100      43 FORMAT(4X,'DIFFERENCE= ',E12.5)
38200      C REMOVE THE HIGHEST FROM THE SIMPLEX
38300      C THE HIGHEST POINT IS THE BST(L,4)
38400      C THE MEDIAN OF THE POINTS BST(L,1),BST(L,2),BST(L,3)
*
```

```

P
38500      DO 48 K=1,I4,1
38600      SUM2(K)=0.
38700      N3=N2-1
38800      DO 46 I=1,N3,1
38900      46  SUM2(K)=SUM2(K)+CBST(L,I,K)
39000      48  CP(L,K)=SUM2(K)/3.
39100      C
39200      C      FIND THE IMAGE OF BST(L,4) THROUGH CP
39300      C
39400      DO 50 K=1,I4,1
39500      50  PIMG(L,K)=2.*CP(L,K)-CBST(L,4,K)
39600      C
39700      C      CHECK IF EXCEEDS THE DOMAIN OF THE FUNCTION
39800      C
39900      DO 52 K=1,I4,1
40000      IF(PIMG(L,K).LT.DD(K)) PIMG(L,K)=DD(K)
*P
40100      52  IF(PIMG(L,K).GT.DD(K+3)) PIMG(L,K)=DD(K+3)
40200      C
40300      C      EVALUATE THE FUCTION AT THESE POINTS
40400      C
40500      L3=L
40600      M1=I4
40700      FPMG(L)=XFCT(PIMG,M1,L3)
40800      KOUT=KOUT+1
40900      write(iu,54) fpmg(l)
41000      54  FORMAT(4X,'FPMG=',E12.4)
41100      IF(FPMG(L).LT.BST(L,1)) GO TO 200
41200      IF(FPMG(L).LT.BST(L,2)) GO TO 100
41300      IF(FPMG(L).GT.BST(L,4)) GO TO 60
41400      DO 56 K=1,I4,1
41500      56  CR(L,K)=(3*CP(L,K)-CBST(L,4,K))/2.
41600      C
*P
41700      C      CHECK IF EXCEEDS DOMAIN
41800      C
41900      DO 58 K=1,K4,1
42000      IF(CR(L,K).LT.DD(K)) CR(L,K)=DD(K)
42100      58  IF(CR(L,K).GT.DD(K+3)) CR(L,K)=DD(K+3)
42200      C
42300      C
42400      C      EVALURATE THE FUNCTION
42500      C
42600      M1=I4
42700      L3=L
42800      FCR(L)=XFCT(CR,M1,L3)
42900      KOUT=KOUT+1
43000      BST(L,4)=FCR(L)
43100      DO 59 K=1,I4,1
43200      59  CBST(L,4,K)=CR(L,K)
*
```

```

P
43300      GO TO 400
43400      60      DO 65 K=1,I4,1
43500      65      CW(L,K)=(CP(L,K)+CBST(L,4,K))/2.
43600      C
43700      C      SEE IF EXCEEDS DOMAIN
43800      C
43900      DO 70 K=1,I4,1
44000      IF(CW(L,K) .LT. DD(K)) CW(L,K)=DD(K)
44100      70      IF(CW(L,K) .GT. DD(K+3)) CW(L,K)=DD(K+3)
44200
44300      M1=I4
44400      L3=L
44500      FCW(L)=XFCT(CW,M1,L3)
44600      KOUT=KOUT+1
44700      BST(L,4)=FCW(L)
44800      DO 75 K=1,I4,1
*P
44900      75      CBST(L,4,K)=CW(L,K)
45000      GO TO 400
45100      100     BST(L,4)=FPMG(L)
45200      DO 110 K=1,I4,1
45300      110     CBST(L,4,K)=PIMG(L,K)
45400      GO TO 400
45500
45600      200     DO 220 K=1,I4,1
45700      220     EX(L,K)=3.0*CP(L,K)-2.0*CBST(L,4,K)
45800      C
45900      C      SEE IF EXCEEDS DOMAIN
46000      C
46100      DO 250 K5=1,I4,1
46200      IF(EX(L,K5) .LT. DD(K5)) EX(L,K5)=DD(K5+3)
46300      250     IF(EX(L,K5) .GT. DD(K5+3)) EX(L,K5)=DD(K5+3)
46400
*P
46500      M1=I4
46600      L3=L
46700      FEX(L)=XFCT(EX,M1,L3)
46800      KOUT=KOUT+1
46900      IF(FEX(L) .LT. BST(L,1)) GO TO 310
47000      WRITE(IU,255) FEX(L)
47100      255     FORMAT(10X,'FEX=',E10.4)
47200      GO TO 100
47300      310     BST(L,4)=FEX(L)
47400      DO 320 K=1,I4,1
47500      320     CBST(L,4,K)=EX(L,K)
47600      400     DO 410 I=1,N2,1
47700      IF(BST(L,1) .LT. BST(L,I)) GO TO 410
47800      TEMP=BST(L,1)
47900      BST(L,1)=BST(L,I)
48000      BST(L,I)=TEMP
*
```

```

P
48100      DO 405 K=1,I4,1
48200      TEMPO(K)=CBST(L,1,K)
48300      CBST(L,1,K)=CBST(L,I,K)
48400      405  CBST(L,I,K)=TEMPO(K)
48500      410  CONTINUE
48600      DO 450 I=2,N2,1
48700      IF(BST(L,2).LT.BST(L,I)) GO TO 450
48800      TEMP=BST(L,2)
48900      BST(L,2)=BST(L,I)
49000      BST(L,I)=TEMP
49100      DO 420 K=1,I4,1
49200      TEMPO(K)=CBST(L,2,K)
49300      CBST(L,2,K)=CBST(L,I,K)
49400      420  CBST(L,I,K)=TEMPO(K)
49500      450  CONTINUE
49600      IF(BST(L,3).LT.BST(L,4)) GO TO 460
*P
49700      TEMP=BST(L,3)
49800      BST(L,3)=BST(L,4)
49900      BST(L,4)=TEMP
50000      DO 455 K=1,I4,1
50100      TEMPO(K)=CBST(L,3,K)
50200      CBST(L,3,K)=CBST(L,4,K)
50300      455  CBST(L,4,K)=TEMPO(K)
50400      460  IF(ITER.LT.10.)GOTO 31
50500      ITER=0.
50600      BST(L,4)=(BST(L,1)+BST(L,2)+BST(L,3)+BST(L,4))/4.
50700      GO TO 400
50800      500  ZMAX(L,1)=BST(L,1)
50900      DO 505 K=1,I4,1
51000      505  CZMAX(L,1,K)=CBST(L,1,K)
51100      WRITE(IU,510) ZMAX(L,1),(CZMAX(L,1,K),K=1,I4)
51200      510  FORMAT(10X,E10.4,3(E10.4,4X),/)
*P
51300      RETURN
51400      END
51500      FUNCTION XFCT(C,II,IP)
51600      DIMENSION C(4,3)
51700      II=3
51800      XFCT=9.0-8.0*C(IP,1)-6.0*C(IP,2)-4.0*C(I
51900      1 P,3)+2.0*C(IP,1)**2+2.0*C(IP,2)**2+C(IP,3)**2
52000      2 +C(IP,1)*C(IP,2)*2.0+2.0*C(IP,1)*C(IP,3)
52100      RETURN
52200      END
52300      FUNCTION CAL(C1,L3,N3)
52400      DIMENSION C1(3,50,50)
52500      CAL=9.0-8.0*C1(1,L3,N3)-6.0*C1(2,L3,N3)-4.0*C1(3,L3,N3)+
52600      1 2.0*C1(1,L3,N3)**2+2.0*C1(2,L3,N3)**2+C1(3,L3,N3)**2
52700      2 +2.0*C1(1,L3,N3)*C1(2,L3,N3)+2.0*C1(1,L3,N3)*C1(3,L3,N3)
52800      RETURN
*
```