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AN ALGORITHM FOR FINDING THE GLOBAL MAXIMUM OF A MULTIMODAL, MULTIVARIATE FUNCTION

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This algorithm for global optimization uses an arbitrary starting point, requires no derivatives, uses comparatively few function evaluations and is not side-tracked by nearby relative optima. The algorithm builds a gradually closer piecewise-differentiable approximation to the objective function. The computer program exhibits a (theoretically expected) strong tendency to cluster around relative optima close to the global. Results of testing with several standard functions are given.

Key words: Global Maximum.

1. Introduction

The maximization method proposed in this paper is a sequential search, that, unlike gradient methods and other sequential techniques, can estimate arbitrarily closely the value and the location of the global maximum of a multimodal function of several variables. It needs no 'favorable' starting point to avoid converging to a non-global relative maximum. In all but the worst cases it can find a close estimate with many fewer sample points than a grid search. The method is a generalization of an algorithm of S.A. Pijavskii [3] and, independently, of B. Shubert [4] for a function of one variable.

In the next section we give some definitions and the simplified sampling rule, which is enough to show convergence, for example, but which needs to be made specific in order to perform computations. The specifics and their justifications are presented in Section 3. In Section 4, convergence and optimality of the method are proved and in the last section computer timings and accuracy for several functions of two variables is discussed.

2. The sampling rule

We will denote by R^N, Euclidean N-space with the usual norm, $\|x-\bar{x}\| = \sqrt{\sum_{i=1}^{N}(x^i-\bar{x}^i)^2}$, where $x=(x^1, x^2, \ldots, x^N)$. R^{N+1} will be, for this paper, the cartesian product, $R^N \times (z\text{-axis})$, i.e., $R^{N+1} = \{(x^1, x^2, \ldots, x^N, z) | x^i, z \in R\}$.

Let f be a real-valued function defined on an N-cube, $I^N = \{x | A_i \leq x^i \leq B_i\}$, in R^N and satisfying the strict Lipschitz condition that, for all $x, \bar{x} \in I^N$,

$$|f(x) - f(\bar{x})| < K \|x - \bar{x}\|,$$

where K is a real, positive constant. We wish to solve the maximization problem:

$$\text{Max } f \quad \text{subject to } x \in I^N.$$

The problem has a solution since f satisfies the Lipschitz condition.

We now define the sampling sequence, $x_0, x_1, \ldots, x_n, \ldots$. Let x_0 be an arbitrary point in I^N. We define F_0, the approximating function, by

$$F_0(x) = K \|x - x_0\| + f(x_0),$$

and its maximum,

$$M_0 = \max_{x \in I^N} F_0(x).$$

The next point, x_1, is chosen so that

$$F_0(x_1) = M_0.$$

(Any such point will do.) Continuing in this way, having chosen x_n, we define

$$F_n(x) = \min_{j=0,\ldots,n} \{K \|x - x_j\| + f(x_j)\}, \qquad M_n = \max F_n(x),$$

and choose x_{n+1} so that $F_n(x_{n+1}) = M_n$.

The graph of F_0 in R^{N+1} is an N-dimensional cone with vertex, $(x_0, f(x_0))$, bounded by I^N, with axis of symmetry parallel to the z-axis and such that sections orthogonal to this axis are spheres. For the remainder of this paper, a *cone* will be assumed to have these properties. (For $N = 2$, it is a right circular cone with slope K.)

The graph of F_n is made up of several intersecting cones which approximate the graph of f; we will call the graph of F_n the approximating surface at step n. It is intuitively clear (at least for $N = 2$) that at each successive step F_n is a better approximation of f and consequently the sequence M_n converges to the maximum. This will be made precise in Section 4.

In using this sampling rule for computations, one must find the maximum of F_n at step n. For $N = 1$, this is easy [4]. For $N > 1$, this amounts to finding the peaks of the approximating surface, which are cone intersections, and, of those, the one which is highest. In the next section a painless way of finding the relative maxima of F_n is shown.

3. Computational refinements

We wish to make finding M_n, the approximate maximum at step n, computationally precise. We will prove that finding the points of relative maximum of the approximating surface means finding the points of intersection of the cones making up the

surface. Furthermore, this can be done by solving a set of N linear equations and a quadratic equation (Theorem 3.1).

Let $v_i = (v_i^1, v_i^2, \ldots, v_i^N, h_i)$, be any point in I^N, then

$$\pi(v_i) = (v_i^1, v_i^2, \ldots, v_i^N, 0)$$

is the projection of v_i to R^N.

Let $C_i = \{(x, z) | z = K\|x - \pi(v_i)\| + h_i\}$.

Let $C = \{C_i | i = 1, \ldots, m\}$ be any finite collection of cones with the property that no vertex is on or above the surface of any other cone in C.

The vertices v_i, $i = 1, \ldots, m$ will be called $N-1$ *coplanar* if their projections to R^N are contained in a plane of dimension $\leq N-1$.

Let F be a function on R^N, defined by

$$F(x) = \min_{i \leq m} \{K\|\pi(v_i) - x\| + h_i\}.$$

Proposition 3.1. *If the vertices, v_i, are $N-1$ coplanar then $\bigcap C_i$ cannot contain a point of relative maximum of F.*

Proof. Suppose $\bigcap C_i$ is non-empty, and suppose the cone vertices are $N-1$ coplanar. Then the projections, $\{\pi(v_i)\}$, are contained in an $N-1$ plane, $Q \subset R^N$. The cone vertices are contained in the N plane, $Q' = Q \times (z\text{-axis})$.

Let $p' \bigcap_{i \leq M} C_i$, $p = \pi(p')$. Let $D(\varepsilon, p) \subset R^N$ be an arbitrarily small N-disk centered at p with radius $\varepsilon > 0$. Let R be the line in R^N through p orthogonal to Q. See Fig. 1. Then there exists a point $q \in D(\varepsilon, p) \cap R$ such that $\|q - \pi(v_i)\| > \|p - \pi(v_i)\|$ for all $i = 1, \ldots, M$. Thus, for all i,

$$K\|q - \pi(v_i)\| + h_i \geq K\|p - \pi(v_i)\| + h_i \geq F(p).$$

Therefore,

$$F(q) = \min_{i \leq m}\{K\|q - \pi(v_i)\| + h_i\} \geq F(p).$$

See Fig. 1. Since ε can be arbitrarily small, this proves that p is not a relative maximum of F. A similar argument shows p is not a relative minimum, thus not a critical point. For our purposes we need only the proposition as stated.

Proposition 3.2. *Suppose two N-cones are defined by $z = K\|x - v\| + h$ and $z = K\|x - \bar{v}\| + \bar{h}$, then the cone intersection is contained in the plane defined by*

$$\sum_{i=1}^{N} 2(\bar{v}^i - v^i)x^i - 2\frac{(\bar{h} - h)}{K^2} z + \frac{\bar{h}^2 - h^2}{K^2} - \sum_{i=1}^{N} [(\bar{v}^i)^2 - (v^i)^2] = 0.$$

Proof. The derivation of this plane equation consists of some tedious algebraic manipulations. One would think it already exists in some analytic geometry text; but since I could find no such reference, I include a sketch of the derivation here.

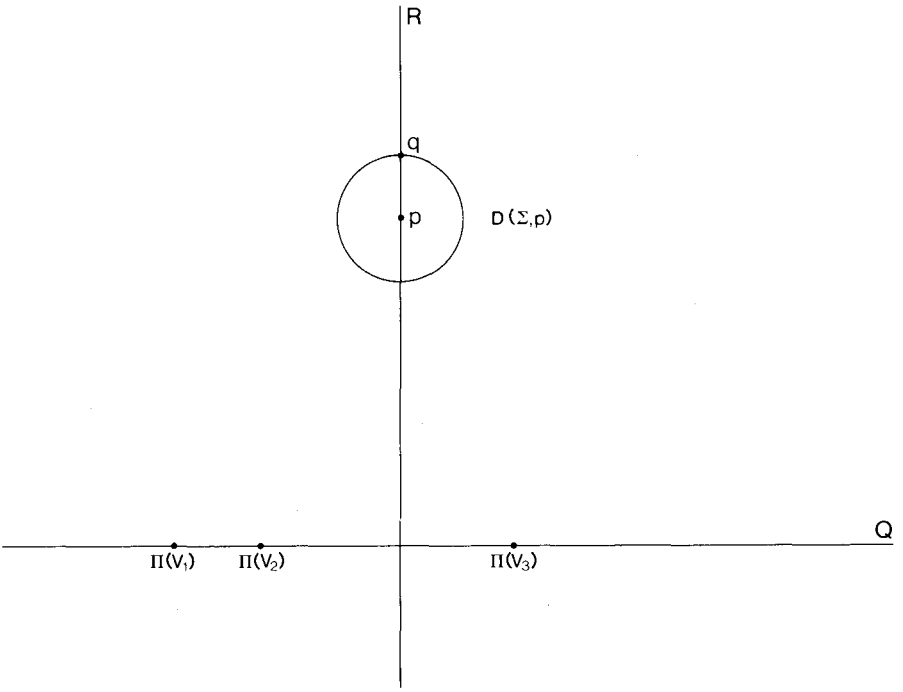

Fig. 1.

The coordinates x^i, $i=1,\ldots,N$ of the intersection of the two given cones, hereafter C_1 and C_2, are determined by the equation

$$K\|x-v\|+h=K\|x-\bar{v}\|+\bar{h},$$

$$K\sqrt{\sum_i (x^i-v^i)^2}+h=K\sqrt{\sum_i (x^i-\bar{v}^i)^2}+\bar{h},$$

$$\sum_i (x^i-v^i)^2-\sum_i (x^i-\bar{v}^i)^2-\frac{(\bar{h}-h)^2}{K^2}=2\frac{(\bar{h}-h)}{K}\sqrt{\sum_i (x^i-\bar{v}^i)^2},$$

$$\vdots$$

$$\sum_i \left[4(\bar{v}^i-v^i)^2-\frac{4(\bar{h}-h)^2}{K^2}\right](x^i)^2$$

$$+8\sum_{i\neq j}\sum (\bar{v}^i-v^i)x^i(\bar{v}^j-v^j)x^j+\text{linear terms in } x^i+\text{constant term}=0. \tag{1}$$

The general plane equation, for the plane, P, is

$$\sum_i c_i x^i+cz+d=0.$$

The coordinates, x^i, of the intersection of a plane and C_1 are given by:

$$-\frac{d-\sum_i c_i x^i}{c} = K\|x-v\|+h,$$

$$\vdots$$

$$\sum_i (c_i^2 - c^2K^2)(x^i)^2 + 2\left(\sum\sum_{i\neq j} c_i x^i c_j x^j\right) + \sum_i 2v^i c^2 K^2 x^i$$

$$+2(d+ch)\left(\sum_i c_i x^i\right) - \sum_i c^2K^2(v^i)^2 + d^2 + 2cdh + c^2h^2 = 0. \tag{2}$$

Comparing the squared terms gives

$$c_i^2 - c^2K^2 = 4(\bar{v}^i - v^i)^2 - 4\frac{(\bar{h}-h)^2}{K^2},$$

$$(c_i+cK)(c_i-cK) = \left[2(\bar{v}^i - v^i) + \frac{2(\bar{h}-h)}{K}\right]\left[2(\bar{v}^i - v^i) - 2\frac{(\bar{h}-h)}{K}\right]$$

and we obtain a possible solution:

$$c_i = 2(\bar{v}^i - v^i), \qquad c = -2\frac{(\bar{h}-h)}{K^2} \tag{3}$$

which checks for the mixed terms in both representations of the intersection, equations (1) and (2). The constant,

$$d = \frac{\bar{h}^2 - h^2}{K^2} - \sum_i [(\bar{v}^i)^2 - (v^i)^2], \tag{4}$$

was obtained from comparing the linear and constant terms of $C_1 \cap P$ with those of $C_2 \cap P$, assuming the above values for c_i and c. These values for c_i, and c, and d also check for the linear and constant terms of equations (1) and (2).

Proposition 3.3. *Given the collection, C, defined above, with $m = N+1$, let P_i be the plane of cone intersection, $C_{N+1} \cap C_i$, $i = 1, \ldots, N$. If $\bigcap_i P_i$ has dimension >1 or if* $\dim \bigcap_i P_i = 1$ *and the line of intersection is parallel to R^N, then the cone vertices, v_i, are $N-1$ coplanar.*

Proof. If $\bigcap_i P_i$ contains a line disjoint from R^N (i.e. points on the line are equidistant from R^N), then parallel translation in each P_i gives lines R_i in $Q_i = P_i \cap R^N$. Let L_i be the line segment connecting the projected vertices, $\pi(v_{N+1})$, $\pi(v_i)$. Considering L_i to be a vector with j-th component, $v_{N+1}^j - v_i^j$, then from the plane parameters of (3) and (4) in Proposition 3.2, the plane Q_i has equation $\sum (v_{N+1}^i - v^i)x^i + d/2 = 0$, with normal vector, L_i. Thus Q_i is orthogonal to L_i (hereafter $Q_i \perp L_i$). Thus we have $R_i \perp L_i$. If the vertices, $\{v_i\}$, are not $N-1$ coplanar, then the members of $L = \{L_i | i = 1, \ldots, N\}$, as vectors, form a basis of an N-plane with origin at $\pi(v_{N+1})$. But then it cannot be that $R_i \perp L_i$, all $i \leq N$. For the parallel translations in R^N of

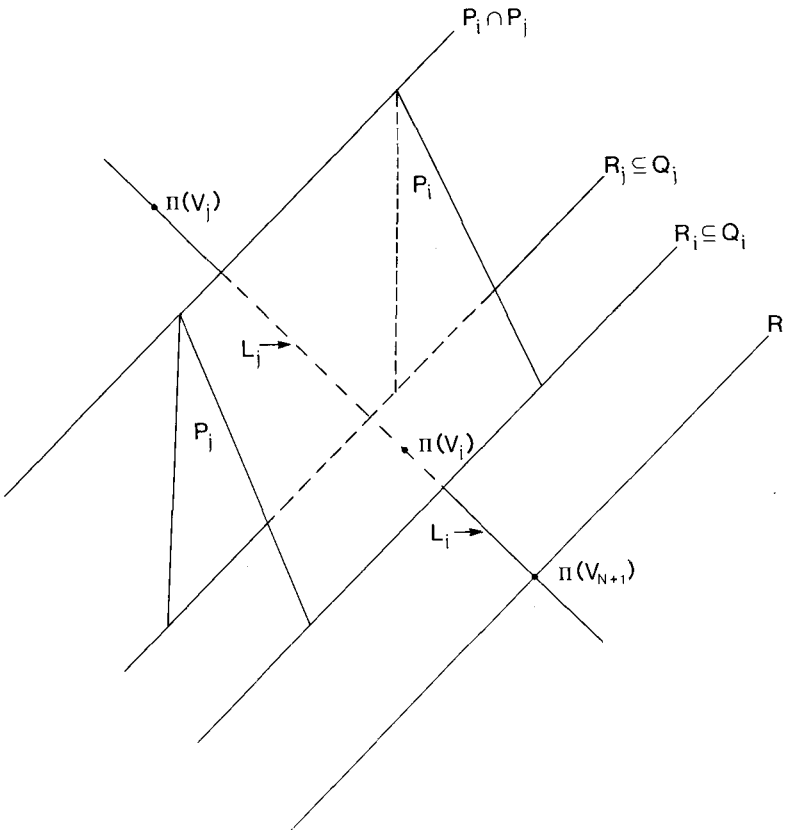

Fig. 2.

R_i to $\pi(v_{N+1})$ must be the same line, R, since the R_i are all parallel. But then $R \perp L_i$, all i, contradicting the assumption that L formed a basis for an N-plane. Thus $\{v_i | i = 1, \ldots, N+1\}$ must be $N-1$ coplanar. See Fig. 2.

Thus, the proposition is proved for the case $\bigcap_i P_i$ is a line parallel to R^N. If $\dim \bigcap_i P_i > 1$, then $\bigcap_i P_i$ contains a line disjoint from R^N and the proof is complete.

Theorem 3.1. *Any point of relative maximum of F_n is a solution to a set of N linear equations and a quadratic equation. It is the unique solution which has larger z-value.*

Proof. By Proposition 3.1, if p is a relative maximum of F_n, then p is in the intersection of at least $N+1$ cones, since the vertices of N or fewer cones are a priori $N-1$ coplanar. By Proposition 3.2, p is in the intersection of N planes. By Proposition 3.3, that intersection is a line which intersects R^N. Thus p is the intersection of that line and a cone, with vertex (v, h), and defined by the positive root of

$$\frac{(z-h)^2}{K^2} = \sum_j (x^j - v^j)^2.$$

We may now rewrite the algorithm in a precise way, which can be used for computer implementation.

The jth iteration of the algorithm consists of the following steps which culminate, as described in Section 1, in selecting a new sample point, $\bar{x}_{j+1}$, and estimate, $f(\bar{x}_{j+1})$, and deciding to stop or reiterate.

Suppose we have the sample point, $\bar{x}_j \in I^N$ ($\bar{x}_0$ in I^N chosen arbitrarily) such that $F_{j-1}(\bar{x}_j) = M_{j-1}$, the global maximum of F_{j-1}. A new sample point, $\bar{x}_{j+1}$, will be chosen from among the points of relative maxima of F_j, which are those of F_{j-1} minus the point $(\bar{x}_j, M_{j-1})$ plus intersections of the jth cone, C_j, at $(\bar{x}_j, f(\bar{x}_j))$ with the cones $C_0, C_1, \ldots, C_{j-1}$. According to Theorem 3.1, we find these intersections, denoted P_{ij}, by first storing plane coefficients, c_i, d, of $\sum_{i=1}^{N} c_i x^i + c_{N+1} z + d = 0$ for each of j cone intersections.

Select N planes at a time from among these j planes and the boundary planes, defined by $x^i = A_i$ and $x^i = B_i$, $i = 1, \ldots, N$, then obtain a solution space to the resulting system of N linear equations in $N+1$ variables. This solution space is invalid for our purposes if it has dimension >1 (the coefficient matrix has rank $< N-1$) or if it is a line disjoint from R^N (the parametric equations for the solution line include $z =$ constant). Thus an allowable parametric linear solution is of the form:

$$\begin{array}{lll} x^1 + a_1 z = b_1, & & x^{k_1} + a_1 x^k = b_1, \\ \quad\vdots & \text{or} & \quad\vdots \\ x^N + a_N z = b_N, & & x^{k_{N-1}} + a_{N-1} x^k = b_{N-1}, \\ & & z \quad + a_N \quad x^k = b_N, \end{array}$$

where $1 \leq k \leq N$ and $\{k_1, \ldots, k_{N-1}\}$ is some arrangement of the superscripts $\{1, \ldots, N\} - \{k\}$.

The second form can be converted to the first and then the variables x^i, $i = 1, \ldots, N$, are substituted into the equation for the cone, C_j, which is then solved for z. This yields two points which are the intersection of the line with the upper and lower halves of the cone defined by $(z - f(\bar{x}_j))^2 = K^2(\|x - \bar{x}_j\|^2)$. We choose the point with larger z-value. This gives us a point, $P_{ij} = (x_{ij}, z_{ij})$, which might or might not be on the approximating surface. If $z_{ij} > K\|x_{ij} - x_k\| + f(x_k)$ for any $k = 0, \ldots, j-1$, then this cone intersection is above the current approximating surface and need not be stored.

Next, from the set of points,

$$P = P_{ik}, \quad k = 0, \ldots, j, \quad i = 1, \ldots, i_k,$$

the one with maximum z_{ik} is chosen. The corresponding point, x_{ik}, is $\bar{x}_{j+1}$. We take an estimate, $f(\bar{x}_{j+1})$, and set $z_{ik} = f(\bar{x}_{j+1})$. The set, P, is thus the collection of all critical points of F_{j+1}.

The stopping rule for this procedure is based on the convergence theorem of Section 4. Let

$$\phi_n = \max\{f(\bar{x}_k) \mid k = 0, \ldots, n\},$$

then Theorem 4.1 implies that $M_n - \phi_n \geq 0$ converges to 0. Thus if $M_j - \phi_j < \varepsilon$, ε the previously chosen allowed error, then the procedure is terminated. The estimate for the maximum of f is $\phi_{j+1} = \max\{f(\bar{x}_{j+1}), \phi_j\}$ which occurs at some $\bar{x}_{k_0}$. The actual maximum is located somewhere in the *region of uncertainty*,

$$\left\{x | F_{j+1}(x) \geq \phi_{j+1} = \overline{I^N - \bigcup_{i=0,j+1} D(r_i, \pi(v_i))}\right\},$$

where v_i is the vertex of C_i and $r_i = (\phi_{j+1} - f(\bar{x}_i))/K \geq 0$.

4. Effectiveness of the algorithm

It can be shown that the method of Section 2 converges to the maximum of f and that the method is a minimax among sequential search rules with regard to estimate error.

Theorem 4.1. *Let ϕ be the global maximum of f, Φ the set of points in I^N at which the maximum is attained, x_n, M_n defined as in Section 2, then*

$$\lim_{n\to\infty} f(x_n) = \phi,$$

$\{M_0, M_1, \ldots, M_n, \ldots\}$ is non-increasing and converges to ϕ, and

$$\lim_{n\to\infty} \inf_{x\in\Phi} \|x - x_n\| = 0.$$

Proof. First, $M_0, M_1, \ldots, M_n, \ldots$ is non-increasing by construction: M_i is chosen as max F_i and graph F_{i+1} consists of erecting a cone at $(x_i, f(x_i))$ on the surface of graph f, thus approximating graph f even closer; thus $M_{i+1} = \max F_{i+1} \leq M_i$. The following is similar to Shubert's [4], but with some changes and is included for the sake of completeness. Given $\{x_i\}$ as above, let $X = \{x | x = x_i, \text{ some } i\}$ (x_i may be duplicated in $\{x_i\}$ but not in X).

Case 1: X is infinite. Thus there exists a limit point, $y \in I^N$, of X, by compactness of I^N. Suppose $f(y)$ is not the maximum, i.e., there is ε such that

$$f(y) < M - \varepsilon \quad \text{where} \quad M = \lim_{n\to\infty} M_n.$$

Let $x_{n_1}, x_{n_2}, \ldots$ be a sequence in X which converges to y and let $k_\varepsilon > 0$ such that $k > k_\varepsilon \Rightarrow \|x_{n_k} - y\| < \varepsilon/2K$. Then, for all $k > k_\varepsilon$,

$$f(x_{n_k}) \leq K\|x_{n_k} - y\| + f(y) < \frac{\varepsilon}{2} + f(y) < M - \frac{\varepsilon}{2}.$$

Thus, for all $k > k_\varepsilon$, if $n \geq n_k$ and $\|x - x_{n_k}\| \leq \varepsilon/2K$, then $F_n(x) < M$.

But $M_n > M$ for all n, so that for $n > n_k$, x_n cannot be in the disk $\{x | \|x - x_{n_k}\| \leq \varepsilon/2K\}$, contradicting the assumption that y is a limit point of X. Thus for all $\varepsilon > 0$, $f(y) > M - \varepsilon$, and since $f(x) \leq M$ for all $x \in I^N$, then $f(y) = M$ for all limit points, y, of $\{x_n\}$.

Since $f(x_n) \leq \phi \leq M$, then $\lim_{n\to\infty} f(x_n) = \phi$, and $\lim_{n\to\infty} M_n = \phi$. The third conclusion follows from the assumption that X is infinite.

Case 2: X is finite. If for some $i > j$, $x_i = x_j$, then, by definition,

$$M_i \leq M_{i-1} = F_{i-1}(x_j) = f(x_j) = f(x_i),$$

thus

$$M_i = f(x_i).$$

So, the next choice, x_{i+1}, must be x_i or some other x_k, where $F_i(x_k) = f(x_i)$. In any case, for all $m > i$,

$$M_m = M_i = f(x_i) \leq M.$$

Since M_n is non-increasing, we have $M_m = M$ and for $m \geq k \geq i$,

$$M = M_m = F_m(x^k) = f(x^k) \leq M,$$

so $f(x_k) = M$ all $k \geq i$.

Thus follows the first and second conclusion. The third follows by assumption of a finite number of values in $\{x_n\}$.

The rate of this convergence is worst for a constant function [4]; for such a function our search rule amounts to a grid search. However, for non-constant functions which we are considering, the rate of convergence is faster. If $f(x_{k+1}) > f(x_k)$ then points generated by $C'_{k+1} \cap C_k$ will be closer to x_{k+1} than to x_k, so that our method clusters around high points [see Section 5]. A grid search or random search ignores the relation $f(x_{k+1}) > f(x_k)$. A gradient search uses this information and for domains of higher dimension most likely converges faster than our method, but need only converge to the global minimum for unimodal functions.

The proof that the algorithm is minimax [4] or optimal in one step [5] in the class, S, of all sequential sampling rules with respect to the estimate error, $\phi - \phi_n$, is similar to Shubert's. However, there are inherent differences which necessitate a proof here.

Let $s_0, s_1, \ldots, s_{n-1}$ denote a sampling sequence (the points at which a function, f, has been evaluated). Let s_i^* denote the sequence generated by our algorithm, denoted s^*. Let $L(K)$ be the set of functions, f, satisfying the global Lipschitz condition with Lipschitz constant, K. Assume each f is defined on the cube I^N, where $0 \leq x^i \leq 1$.

We will show that, at the nth iteration, s^* minimizes the worst possible estimate error for functions in $L(K)$.

Theorem 4.2. *Let* $e_n(f, s) = \text{global maximum of } f - \max\{f(s_i) \mid i = 1, \ldots, n\} = \phi(f) - \phi_n(f, s)$; *then*

$$\inf_{s\in S} \sup_{f\in L(K)} e_n(f, s) = \sup_{f\in L(K)} e_n(f, s^*).$$

Proof. Let $F_k(x) = \min_{j=0,\ldots,k}\{f(s_j) + K\|x - s_j\|\}$, $M_k = \max_{x\in I^n} F_k(x)$, and $y_k = \max f(s_i)$, $i = 1, \ldots, k$. The set $\{\bar{x}_k^j \mid j = 0, 1, \ldots, n_k\}$ denotes the collection of points

at which $F_k(\bar{x}_k^j) = M_k$. Let $D_k = D_{r^0,\bar{x}_k^0}$ a neighborhood of $\bar{x}_k^0$ such that $F_k(x) > y_k$, for all $x \in D_k$. (Any of the $\bar{x}_k^j$ are candidates for s_{k+1}^*; $\bar{x}_k^0$ was chosen arbitrarily.)

At the nth iteration, if $s_n \notin D_{n-1}$; then, since $F_{n-1}(x)$ is an upper bound for values of $f(x)$, $f \in L(K)$, and, given the choices up to now, we have:

$$\sup_f e_n(f, s) = \sup(M_{n-1} - y_n) = M_{n-1} - y_{n-1},$$

attained by f such that $f(s_n) = y_{n-1}$. Call the subset of $L(K)$ consisting of such functions, $\tilde{L}(K)$.

On the other hand, if $s_n \in D_{n-1}$ then the maximum error for $f \in \tilde{L}(K)$ is $\max\{M'_{n-1} - y_{n-1}, P_{s_n} - y_{n-1}\}$ where $M'_{n-1} = \max_{x \notin D_{n-1}} F_{n-1}(x)$ and $P_{s_n} = \max_{x \in D_{n-1}} F_n(x)$ [see Fig. 3]. P_{s_n} is the height of the highest corner formed by intersections of the cone at s_n with graph (F_{n-1}) in D_{n-1}. Since $M'_{n-1} \leq M_{n-1}$ and $P_{s_n} \leq M_{n-1}$, then $\sup_{f \in \tilde{L}(K)} e_n(f, s)$ is minimized by choosing $s_n \in D_{n-1}$, including the choice $s_n^* = \bar{x}_n^0$. More specifically, if $M'_{n-1} \leq P_{\bar{x}_n^0}$, then $s_n = \bar{x}_n^0$ minimizes P_{s_n}. If $M'_{n-1} > P_{\bar{x}_n^0}$, then any s_n in a small enough neighborhood of $\bar{x}_n^0$ minimizes $\sup_f e_n(f, s)$.

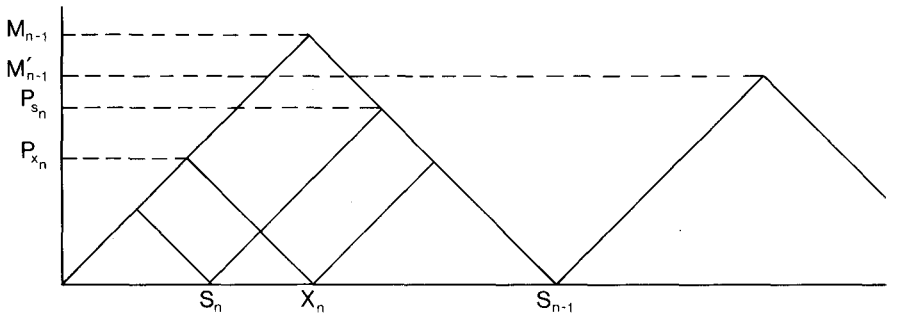

Fig. 3.

Many optimization methods have been developed which minimize the largest interval of uncertainty [2, 6]. In our case this becomes meaningless. For let Φ be the set in I^n on which f attains its maximum, Φ_n, the region of uncertainty at step n (see Section 3), and m $(\Phi_n - \Phi)$ be Lebesgue measure of the difference. Let $m_n(f, s) = m(\Phi_n - \Phi)$ for some function, f, and sequential search, s. Then

$$\inf_s \sup_f m_n(f, s) = \mathrm{vol}(I^N)$$

is achieved for functions such that $f(x_i) = f(x_0)$, $i \leq n$, and such that $\phi = \max f(x)$ is attained at most at a countable number of points. Thus any sequential search rule is minimax with respect to this measure of effectiveness.

5. A numerical example

The algorithm was implemented for the case $N = 2$ in a computer program written for the DEC 2060. We give here details in timing and accuracy for several functions

that were tried. The cases, $N>2$, will be handled by a similar program currently being tested. The program being developed must consider intersecting only 'close' cones to avoid increasing CPU time for each iteration.

The function of two variables,

$$f(x, y) = 4xy \sin 4\pi y,$$

has a global maximum of $f(1.0, 0.6250) = 2.5$ in the region $0 \leq x \leq 1$, $0 \leq y \leq 1$.

The Lipschitz constant, K, was approximated by finding upper bounds, B_1, B_2, for $\partial f/\partial x$ and $\partial f/\partial y$ and letting $K = \sqrt{B_1 + B_2}$. In general, assuming a rectilinear region, $I^N = \{x | a_i \leq x^i \leq b_i\}$, and upper bounds, B_i, on the first partial derivatives, $|\partial f_i/\partial x|$, in I^N, we can choose $K = \sqrt{\sum B_i^2}$ because of the following:

$$\begin{aligned} |\Delta f| &\sim \left| \sum \left(\frac{\partial f_i}{\partial x} \right)_{x_0} \Delta x^i \right| \qquad \text{(the truncated Taylor expansion at } x_0 \in I^N) \\ &< \sum B_i |x^i| \\ &\leq \sqrt{\sum B_i^2} \sqrt{\sum (\Delta x^i)^2}, \quad \text{by the Schwarz inequality.} \end{aligned}$$

The selection of K influences execution time so it should be estimated as closely as possible. The program stops in a few iterations when K is too small (since x_j is found such that $F(x_j) < f(x_j)$), thus K can be adjusted until a suitable upper bound is found.

For example, gross estimates of

$$\frac{\partial f}{\partial x} = 4y \sin 4\pi y \leq 4 \quad \text{and} \quad \frac{\partial f}{\partial y} = 4x \sin 4\pi y + 16\pi xy \cos 4\pi y \leq 4 + 31$$

give $K = 39$. For this value of K and for another test value, $K = 28$, the program determined an answer, with an error of 0.5 in Table 5.2. In Table 5.1, a better estimate, $K = 25$, is used, clearly giving better computer times.

Table 5.1 shows the number of iterations, J, required to end the program and the CPU time (in units equal to the time to evaluate the function SQRIN 1000 times [1]) for different functions:

Table 5.1

	Max. (scaled) computer	Max. (scaled) actual	K	J (iteration)	S TIME (0.57 sec.)
FUNCT	(1.00, 0.6250, 1.0000)	(1.000, 0.6250, 1.0)	8.4	100	37
FUNCT 2	(0.1173, 0.9836, 0.99753)	(0.1427, 0.9757, 1.0)	2.9	100	49
-GOLDPR	(0.4841, 0.2433, 0.99997)	(0.5000, 0.2500, 1.0)	4.0	25	4
-RCOS	(0.5415, 0.1593, 0.99985)	(0.5428, 0.1350, 1.0)	10.0	100	35
	(0.1298, 0.7933, 0.99904)	(0.1239, 0.8017, 1.0)	32.1	100	42
	(0.9920, 0.2495, 0.97380)	(0.9617, 0.0150, 1.0)	60.0	100	37

Table 5.2

K	J	S TIME
25	112	44
28	177	119
39	400	833

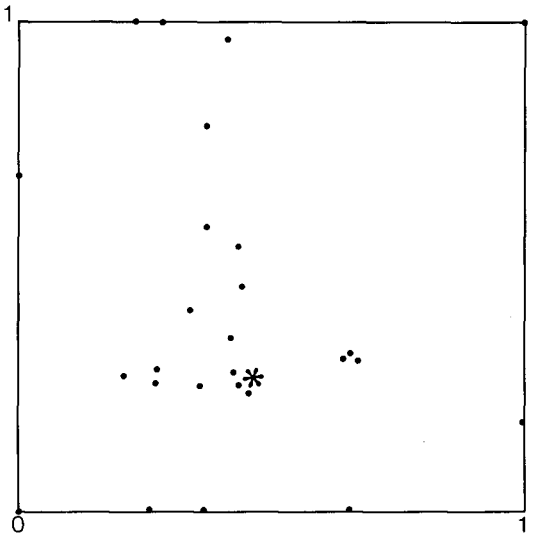

Fig. 4. $\{x^i | i \leq 42\}$ for GOLDPR, * = maximum.

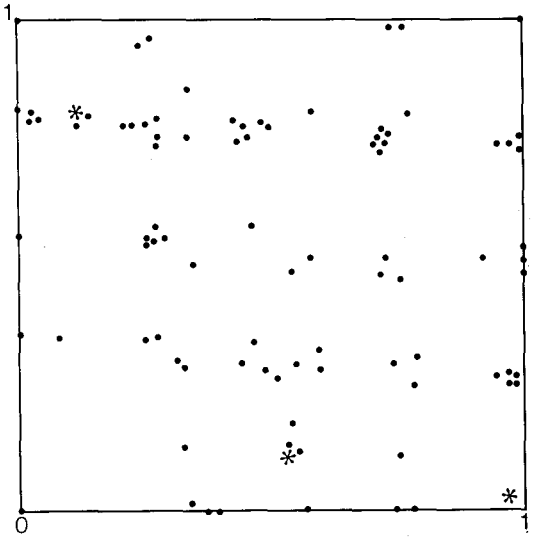

Fig. 5. $\{x^i | i \leq 100\}$ for RCOS, * = maximum.

FUNCT $= 4x_1x_2 \sin 4\pi x_2$, discussed above; FUNCT 2 $= \sin(2x_1+1) + 2\sin(3x_2+2)$; GOLDPR and RCOS are from [1]. The variables and function values were scaled to be in the range $[0, 1]$ and $[-1, 1]$ respectively. It appears that a fast local gradient—or other—search method, following the relatively slower global search would lead to closer approximation of the solution in some cases. Tests of −RCOS showed clustering around all three global maxima. Stopping the program at different iterations allowed each maximum to be selected separately.

Figures 4 and 5 show the sampling sequence chosen by the computer program for two functions, GOLDPR and RCOS, exhibiting pronounced clustering around the global maxima.

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