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Some experiments in global optimization

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SOME EXPERIMENTS IN

GLOBAL OPTIMIZATION

by

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ABSTRACT:

When applied to a problem which has more than one local optimal solution, most nonlinear programming algorithms will terminate with the first local solution found. Several methods have been suggested for extending the search to find the global optimum of such a nonlinear program. In this report we present the results of some numerical experiments designed to compare the performance of various strategies for finding the global solution.

I. INTRODUCTION

It is frequently the case in applied optimization studies that an algorithm which is known to converge to a global optimal solution under certain conditions (such as convexity) will be applied to a problem which does not satisfy these conditions. In particular, optimization problems which are suspected of having several local optima in addition to the global optimum are often solved using algorithms which will stop and indicate a solution whenever any local optimum is reached. In such cases a useful strategy is to repeat the solution process several times starting from different initial points to avoid accepting a solution which is only a local optimum. This is probably the most frequently suggested strategy for avoiding local solutions.

There are also other strategies for avoiding the local solutions in favor of the global optimum. This paper describes some numerical experiments which were done to compare the performance of several strategies for organizing such a global optimization.

II. The Problem

In order to develop and test strategies for avoiding local solutions it is necessary to specify a class of optimization problems to be considered. This paper will concentrate on the "essentially unconstrained" nonlinear programming problem

$$\begin{aligned} &\text{minimize} \quad f(x) \\ &\text{subject to} \quad x \in S \subseteq E^n \end{aligned} \tag{1}$$

where the local and global optimal solutions to (1) are known to occur in the interior of the set S. In such a problem the feasible region S determines a domain to be searched for solutions, but the boundaries of S do not determine the solutions. In this sense problem (1) can be considered "essentially unconstrained."

Problems of this type arise frequently as the "unconstrained" subproblems in interior penalty function algorithms such as the Sequential Unconstrained Minimization Technique of Fiacco and McCormick [3]. In the SUMT method, if the original nonlinear program is not a convex program, then the subproblem (1) may have local solutions which are distinct from the global solution.

For problems like (1) a local optimal solution can be obtained by applying any of the efficient unconstrained descent algorithms (such as the Davidon-Fletcher-Powell method) to minimize the function $f(x)$ while being careful not to penetrate the boundary of S. We shall now consider several strategies which try to ensure that the local solution we finally accept is, in fact, a global minimum.

III. Strategies For Avoiding Local Solutions

Six different strategies for organizing a global optimization are compared in this paper. These are briefly described below with references to more complete descriptions when they exist.

Strategy S1 (From the folklore)

a. Set $k = 1$.

b. Let x^k be a vector chosen at random in the search region S. Starting at x^k perform an unconstrained minimization search on the function $f(x)$ terminating at the local minimum x^{k*}.

c. Replace k with $k + 1$ and go to step b. At each stage retain the best local solution obtained to date.

S1 is the strategy suggested in section I. Intuitively the problem with this strategy is that it may repeatedly search to the same local minimum if the starting points x^k happen to be chosen within the "range of attraction" of that local minimum. The next three strategies attempt to solve this problem.

Strategy S2

a. Set $k = 1$, $f^* = +\infty$

b. Randomly select points $x \in S$ until one is found with $f(x) < f^*$. Call this point x^k.

c. Starting at x^k perform an unconstrained minimization search terminating at a new local minimum x^{k*}.

d. Set $f^* = f(x^{k*})$, replace k with $k + 1$, and go to step b.

In S2 a minimization (step c.) is initiated at x^k only if $f(x^k)$ is smaller than the best solution found to date. Hence, each successive minimization gives a new local minimum which is better than any

found so far. The same local minimum cannot be located twice. It is, however, much more difficult to determine the starting points x^k for strategy S2 than for S1.

Strategy S3 (Bocharov [1])

a. Choose x^1 randomly in S. Set $k = 1$.

b. Starting from x^k perform an unconstrained minimization terminating at the local minimum x^{k*}.

c. Choose a direction $d^k \in E^n$ at random and consider $f(x^{k*} + \alpha d^k)$ as the positive scalar α increases. Moving away from x^{k*} in direction d^k, the function f must initially increase (since x^{k*} is a local minimum). Continue to increase α until f begins to decrease when $\alpha = \alpha^k$.

d. Let $x^{k+1} = x^{k*} + \alpha^k d^k$, replace k with $k + 1$, and go to step b.

Strategy S4 (Bocharov [1])

S4 is the same as S3 except that in step c, instead of choosing the direction at random, d^k is chosen to be the direction of overall progress from the most recent minimization

$$d^k = x^{k*} - x^k \tag{2}$$

Both S3 and S4 attempt to prevent repeated minimization to the same local optimum by moving out of the region of attraction of the

most recent local solution before starting the next minimization. By continuing in the direction (2), strategy S4 hopes to also avoid local minima detected before the most recent minimum.

Strategies S5 and S6 are considerably different from the first four methods. While S1 - S4 attempt to choose good starting points for repeated local minimizations, S5 and S6 attempt to gain information about the entire search region S, gradually concentrating their attention on portions of S which are in some sense "likely" to contain the global minimum. S5 and S6 are most easily described for problems where S is determined by lower and upper bounds on each variable:

$$S = \{x \in E^n \mid \ell_i \leq x_i \leq L_i \ , \ i = 1,\ldots,n\}$$

For ease of presentation we will restrict our attention to such problems.

Strategy S5 (Piecewise Coordinate Projection - Zakharov [5])

a. Set up an initially empty list of points, and let $\hat{S} = \{x \in E^n \mid \hat{\ell}_i \leq x_i \leq \hat{L}_i \ , \ i = 1,\ldots,n\}$ be the "remaining feasible region." Let $\hat{S} = S$ initially.

b. Randomly choose N points $x^k \in \hat{S}$, compute $f(x^k)$ for each, and adjoin them to the list.

c. For each coordinate x_i of x $(i = 1,\ldots,n)$ separate the remaining feasible interval $[\hat{\ell}_i, \hat{L}_i]$ into m equal subintervals.

Let $X_{ij} = \{x^k$ in the list whose i^{th} component is in the j^{th} subinterval of $[\hat{\ell}_i, \hat{L}_i]\}$

$= \{x^k \mid (j-1)(\hat{L}_i - \hat{\ell}_i)/m \leq x_i^k - \hat{\ell}_i < j(\hat{L}_i - \hat{\ell}_i)/m\}$

for $i = 1,\ldots,n$ and $j = 1,\ldots,m$. Then $X_{i1}, X_{i2}, \ldots, X_{im}$ describe the projection of the list of points x^k into the m subintervals of the i^{th} coordinate axis.

d. By considering $\{f(x^k) \mid x^k \in X_{ij}\}$ $(i = 1,\ldots,n$; $j = 1,\ldots,m)$ select the subinterval set X_{st} which is considered most likely to contain the global minimum (for details see Zakharov [5]).

e. By redefining $\hat{\ell}_s$ and $\hat{L}_s$ delete the subinterval sets X_{sj} $(j = 1,\ldots,m$; $j \neq t)$ from the remaining feasible region. Delete all points in the list which are in a deleted subinterval. Go to step b.

As the remaining feasible region $\hat{S}$ gradually shrinks, the global minimum will be more and more closely bracketed. The problem with this method is that the most promising subinterval must be determined on the basis of the sample of points x^k chosen so far. There is always a chance that a subinterval chosen for deletion will, in fact, contain the global minimum solution, and once it is deleted it can never be recovered.

Strategy S6 attempts to solve this problem by retaining the entire region S throughout and using a probabilistic allocation device to concentrate attention on areas in S which are most

promising. This algorithm is new and is still under development. Initial results show some promise, but considerable improvement is still necessary.

Strategy S6 (Coordinatewise Allocation)

a. Define a marginal probability distribution function Φ_i on the feasible interval $[\ell_i, L_i]$ of each coordinate axis $i = 1,\ldots,n$. In the absence of other information, a uniform distribution seems reasonable for the initial distribution.

b. Randomly choose N points $x^k \in S$ and compute $f(x^k)$ for each. The probability distribution functions Φ_i govern these choices in that the i^{th} component x_i^k of x^k is chosen as a random sample point from the distribution Φ_i. Thus, the Φ_i determine the allocation of trial points to various regions in S.

c. Based on the results of the trials to date, modify the Φ_i to increase the allocation of future points to regions considered likely to contain the global minimum. Go to step b.

Strategy S6 can have many realizations depending on the method of handling step c. In the version of S6 reported in this paper, step c is performed as following for each coordinate $i = 1,\ldots,n$.

1. The feasible interval $[\ell_i, L_i]$ is split into m subintervals.
2. A "success" is defined as a value of $f(x^k)$ in the bottom 25% of all $f(x^k)$ values, and the ratios r_{ij} of the number of successes in subinterval j of coordinate i to the total number of points in subinterval j are computed for all i and j.
3. The modified probability for subinterval j of coordinate i is given by $p_{ij} = r_{ij} / \sum_{j=1}^{j=m} r_{ij}$ the normalized success ratio.

Several improvements on this allocation scheme are being considered for future testing.

In early tests it became apparent that performance of the various strategies fluctuated considerably, depending on the particular test problem under investigation. For example, relative to the other strategies, S2 performed spectacularly on some problems but miserably on others. On closer examination it was found that S2 did well on problems for which the global f value was significantly lower than the local minima and for which the global region of attraction was quite large; that is, on problems which were rather easy to solve. This suggests the need for a benchmark strategy to be used for assessing problem difficulty. The benchmark strategy should have as little structure as possible. We have chosen to use the pure random search method for this purpose.

Strategy S0 (Pure Random - Brooks [2])

a. Set $k = 1$.

b. Randomly select $x^k \in S$. Evaluate $f(x^k)$.

c. Replace k with $k + 1$. Go to step b. At each stage retain the best f value found to date.

This strategy may be regarded as a benchmark method since it makes no attempt to take advantage of the information gathered at previous stages. In this sense it is probably the most primitive strategy possible. We can use S0 in two ways:

1. If a strategy does not do considerably better than S0, it should be discarded.
2. If a test problem is such that S0 can solve it nearly as well as the other strategies, then the problem is not very difficult and probably is not useful for discriminating among strategies.

IV. Computational Experiments

A number of computational experiments were performed to compare the various strategies presented above. For each of the test functions employed, each strategy was run 30 times with different random number sequences. A run was allowed to continue until the algorithm had required 1000 evaluations of the objective function $f(x)$.

Test problems with predictable local and global solutions were constructed using the objective function

$$f(x) = - \sum_{j=1}^{j=m} c_j \exp[(x-p_j)' A_j (x-p_j)]$$

This function consists of the superposition of m modes, where mode j has depth $c_j \in E^1$, position $p_j \in E^n$, and shape and width determined by the $n \times n$ negative definite matrix A_j. Particular test functions were obtained by choosing the parameters c_j and p_j from a random number table. A_j was chosen to ensure that the m modes were narrow enough that they did not completely merge into one another.

Strategies S1 through S4 require an unconstrained minimizer. Since the purpose of the study is to compare global strategies, a minimizer is desired which uses the same information as is available to the other strategies - function values but not derivatives. Powell's derivative free method was selected [4].

V. Results

The computational results obtained are summarized in Tables 1 and 2. Table 1 gives characteristics of the test problems used. Table 2 lists for each problem and for each strategy the best f value obtained after 200, 500, and 1000 function evaluations. Each value is the average of the 30 trials conducted for that problem and strategy. The percentage of the 30 trials which did not locate the global minimum after 1000 function evaluations is also given in Table 2. It is

Problem	Number of Variables	Number of Minima	Value of Global Minimum
A	2	4	- 9.0
B	2	10	- 9.9
C	2	10	- 9.3
D	2	10	- 9.8
E	2	10	-13.0
F	5	5	- 9.4
G	5	5	-10.1
H	5	10	-10.0
I	5	10	- 8.9
J	5	20	-11.9

Table 1

Characteristics of Test Problems

Function		S0	S1	S2	S3	S4	S5	S6
A	best f after 200	- 8.6	- 8.5	- 9.0	- 8.2	- 8.6	- 8.5	- 8.7
	best f after 500	- 8.8	- 8.9	- 9.0	- 8.9	- 9.0	- 8.7	- 9.0
	best f after 1000	- 8.9	- 9.0	- 9.0	- 9.0	- 9.0	- 8.8	- 9.0
	% failures	-	0.0	0.0	0.0	0.0	20.0	0.0
B	best f after 200	- 9.0	- 8.9	- 9.7	- 9.0	- 9.5	- 9.1	- 9.1
	best f after 500	- 9.6	- 9.3	- 9.8	- 9.9	- 9.9	- 9.7	- 9.8
	best f after 1000	- 9.7	- 9.8	- 9.9	- 9.9	- 9.9	- 9.8	- 9.9
	% failures	-	3.3	0.0	0.0	0.0	10.0	0.0
C	best f after 200	- 7.6	- 8.3	- 8.1	- 8.8	- 7.8	- 7.8	- 7.7
	best f after 500	- 8.0	- 8.6	- 8.2	- 9.1	- 8.5	- 8.1	- 8.0
	best f after 1000	- 8.3	- 8.9	- 8.6	- 9.2	- 8.7	- 8.2	- 8.2
	% failures	-	33.3	53.3	3.3	43.3	83.3	80.0
D	best f after 200	- 8.6	- 8.9	- 9.2	- 7.8	- 7.4	- 8.8	- 8.8
	best f after 500	- 9.1	- 9.5	- 9.5	- 9.4	- 8.5	- 9.2	- 9.4
	best f after 1000	- 9.4	- 9.7	- 9.6	- 9.7	- 9.6	- 9.2	- 9.6
	% failures	-	10.0	30.0	6.7	33.3	73.3	33.3
E	best f after 200	-10.2	-10.1	-11.8	- 8.3	- 9.5	-10.9	-10.2
	best f after 500	-11.6	-12.1	-12.8	-10.5	-11.2	-12.6	-12.3
	best f after 1000	-12.1	-12.7	-12.9	-12.0	-13.0	-12.7	-12.8
	% failures	-	10.0	3.3	30.0	0.0	6.7	3.3
F	best f after 200	- 0.3	- 6.7	- 5.0	- 6.4	- 5.8	- 0.8	- 0.8
	best f after 500	- 1.0	- 7.9	- 5.0	- 8.0	- 8.7	- 2.9	- 3.1
	best f after 1000	- 1.5	- 8.7	- 5.6	- 8.5	- 8.9	- 7.0	- 7.5
	% failures	-	60.0	86.7	43.3	33.3	80.0	76.7
G	best f after 200	- 4.1	- 7.4	- 7.3	- 7.1	- 7.5	- 5.0	- 4.7
	best f after 500	- 5.5	- 9.3	- 8.8	- 9.7	- 9.7	- 8.3	- 8.2
	best f after 1000	- 6.1	-10.0	- 9.1	- 9.9	-10.1	- 9.5	- 9.3
	% failures	-	3.3	56.7	10.0	0.0	16.7	40.0
H	best f after 200	- 3.4	- 7.6	- 7.0	- 6.8	- 7.4	- 3.7	- 3.6
	best f after 500	- 4.6	- 8.3	- 7.3	- 8.7	- 9.2	- 6.3	- 7.2
	best f after 1000	- 5.2	- 8.9	- 7.7	- 9.2	- 9.7	- 8.2	- 8.9
	% failures	-	73.3	93.3	56.7	20.0	60.0	50.0
I	best f after 200	- 3.9	- 7.6	- 6.3	- 6.5	- 6.7	- 4.2	- 4.2
	best f after 500	- 4.7	- 8.0	- 7.4	- 8.0	- 7.8	- 5.8	- 5.3
	best f after 1000	- 5.3	- 8.8	- 7.6	- 8.4	- 8.6	- 6.9	- 6.1
	% failures	-	10.0	66.7	33.3	36.7	80.0	100.0
J	best f after 200	- 3.3	- 7.4	- 6.3	- 6.7	- 6.5	- 3.8	- 3.6
	best f after 500	- 4.1	- 8.8	- 6.6	- 7.4	- 8.1	- 5.3	- 4.6
	best f after 1000	- 4.8	- 9.7	- 7.2	- 8.8	- 8.3	- 7.4	- 6.5
	% failures	-	43.3	83.3	66.7	76.7	73.3	90.0

Table 2.

Test Results

difficult to obtain a single measure of performance for this kind of problem since we must balance speed of convergence against the chance that the global solution will be missed entirely.

From these test results we can draw some general conclusions:

1. Test functions A and B were not very challenging since S0 did nearly as well as most other strategies.
2. S2 seems to make rapid initial progress but frequently stops short of the global solution - it is not recommended.
3. In general, S1, S3, and S4 perform about the same and better than the other strategies.
4. S5 and S6 exhibit slow initial convergence. Both frequently tend to concentrate the search effort around a good local minimum which is not global.
5. On difficult problems even the best of these methods will frequently fail to locate the global minimum.

It is also interesting to examine the entire graph of the number of function evaluations versus the best function value obtained for each strategy. These curves are shown for test function H in Figure 1. The results for function H are representative of those obtained for the other functions and serve to emphasize conclusions 2, 3, and 4 above.

In conclusion, it is appropriate to note that these six methods do not come near to exhausting the possible techniques for avoiding

local solutions. Methods which are hybrids of these and entirely new methods should be tested. In particular, we hope to develop an algorithm which allocates unconstrained minimizations to various regions similar to the way strategy S6 allocates the individual points x^k. Such a method would combine the rapid local optimizing power of the minimization method with a global analysis of the feasible region.

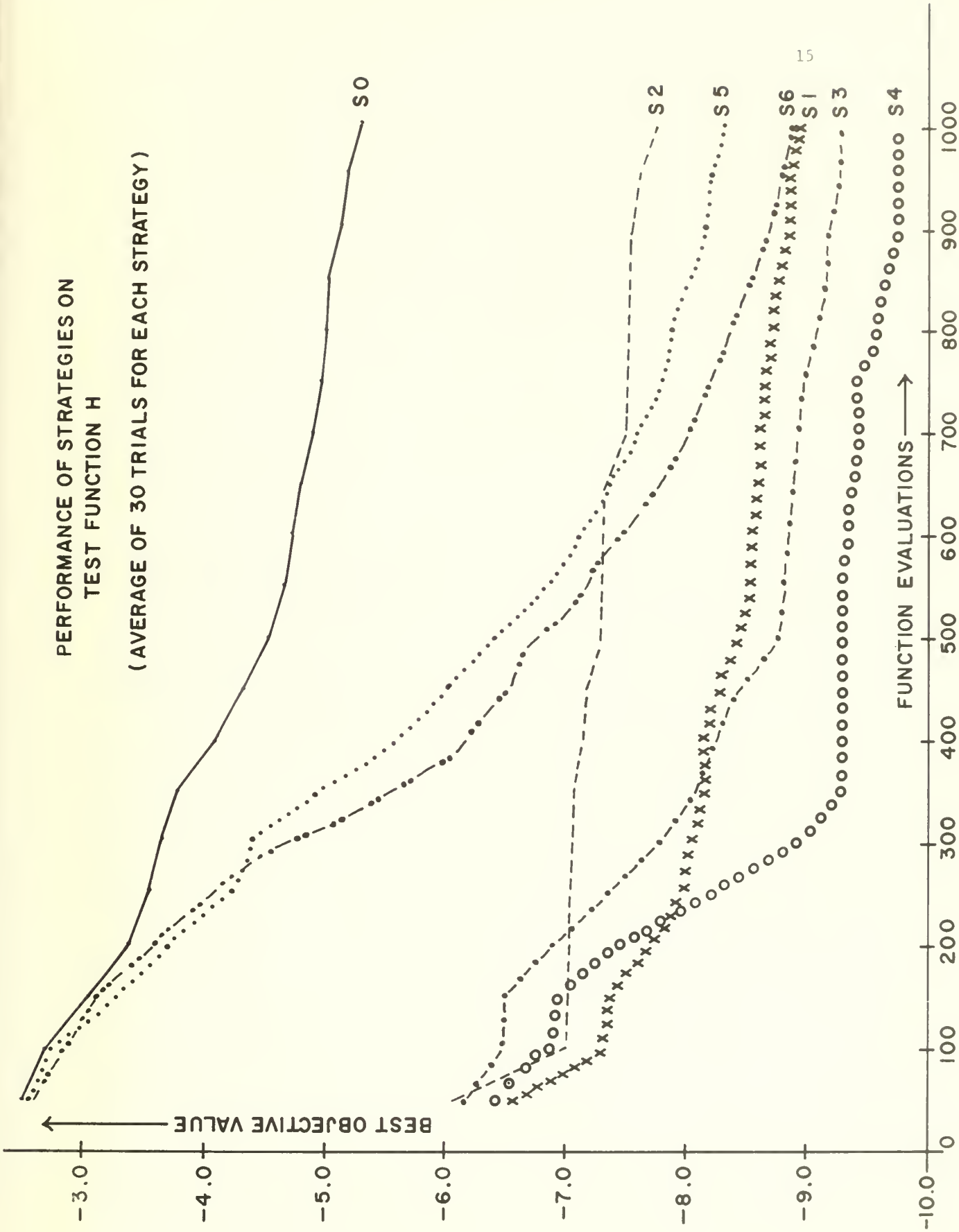
PERFORMANCE OF STRATEGIES ON
TEST FUNCTION H
(AVERAGE OF 30 TRIALS FOR EACH STRATEGY)
BEST OBJECTIVE VALUE
FUNCTION EVALUATIONS
-3.0
-4.0
-5.0
-6.0
-7.0
-8.0
-9.0
-10.0
0
100
200
300
400
500
600
700
800
900
1000
S0
S2
S5
S6
S1
S3
S4

Figure 1.

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13. ABSTRACT

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mathematical programming						
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global optimization						
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