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examined a thesis entitled

"Direct Search For The Optimum Of A Simulated
Process Containing Noise"

presented by M. G. Ram Narayan

a candidate for the degree of
Master of Science in Chemical Engineering
and hereby certify that in their opinion it is worthy of acceptance.

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DIRECT SEARCH FOR THE OPTIMUM OF A
SIMULATED PROCESS CONTAINING NOISE

A Thesis
Presented to
the Faculty of the Graduate School
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In Partial Fulfillment
of the Requirements for the Degree
Master of Science in Chemical Engineering

by
M.G. Ram Narayan

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ABSTRACT

The objective of this work was to study the optimization of a function whose measurement contains error or noise. A search method developed for noise free systems was applied to a noisy function using minimum variance estimators to improve the accuracy of the functional values. The results of the new search method are compared to those of a modified stochastic approximation method which has good convergence on noisy systems.

At moderate noise levels ($\sigma \leq 0.5$), the new method appears to converge faster than the best method reported for the modified stochastic approximation although at higher noise levels ($\sigma > 0.5$), this advantage seems to be lost.

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Chapter I

Introduction

The growing use of the digital computer in the process industry gives the general optimization problem increased significance to the engineers. It is of importance to develop search methods which can achieve convergence in the fewest possible number of functional evaluations.

For the situations which are noise free in the measurement of the objective function and decision variables, many techniques for finding the optimum value have been developed and applied to a number of significant problems (Wilde, 1964).

Such optimization techniques are divided into two classes: direct and indirect methods.

Indirect methods only solve the equations rather than search for an optimum. Finding the roots of the equation is closely related to finding the location of the optimum. Lagrange undetermined multipliers method are included with the indirect methods.

Direct methods start at an arbitrary point and proceed stepwise toward the extremum by successive improvement. Direct method divides into two classes:

1. Elimination technique: which by bold moves continuously strive to shrink the region in which the peak must lie, as for example, the Fibonacci search; and

2. Hill climbing technique: which more or less cautiously moves in the direction, based on the local measurements, where the objective appeared to be improving. Some examples are pattern searches including

the Rosenbrock search method which is used in this work.

The noise free searches are successful in the case of unconstrained optimization, but are sometimes less so in case of constrained optimization. However, a number of constrained methods have been described which exhibit convergence with a reasonably high degree of dependability and efficiency in noise free processes.

The situations with respect to optimization of noisy functions is less well developed. Most of the published work may be considered under one of the two categories; interpolation or stochastic approximation.

In interpolation schemes, the response surface is approximated by a second order (or higher) multidimensional polynomial. The extremum of approximating surface is computed and is used as the center point for a new multifactor design to predict a new extremum (Box, 1951, Box & Hunter, 1957). One weak link in this sequence is the difficulty in approaching sufficiently close to the extremum so that the approximating equation is a good representation of the response surfaces. The interpolation method also encounters difficulty with sharp ridges and asymmetric surfaces (Heaps & Wells, 1965). Little work has been done with the interpolating method regarding constrained optima.

Regardless of noise levels, search techniques designed to have at least "convergence in probability" are known as stochastic approximation. Gradient and relaxation methods which were variants of these techniques were studied for the optimization of multiparameter noise disturbed system by Kushner (1963). In spite of proven convergence as number of stages approaches infinity, the convergence rate of stochastic approximation methods tend to be discouragingly slow.

Many studies have been initiated to accelerate convergence.

Ahlgren and Stevens (1966) sacrificed proof of convergence to speed up the response rate. Application of their procedure to a multidimensional chemical engineering problem demonstrated that convergence to the optimum can be accomplished in a reasonable number of runs. These results will be discussed in the later chapter.

There are some limitations to the stochastic approximation techniques. One of them is that performance on the limiting case of noise free functions is similar to steepest ascent method. It is known that convergence rate of steepest ascent is slow for response functions having long, narrow valleys. Another limitation is that little work has been done on the constrained stochastic systems for finding optima.

In this work, optimization will be achieved using searches developed for noise free systems. Minimum variance estimators for functional values will be used to reduce the deleterious effects of noise. This approach allows use of methods that can operate successfully on curved ridges and even permits use of constrained algorithms.

This approach and some variations of it were described and evaluated by Luecke (1970) on several simple test functions. The objective of the present work is to test the performance of this method on a simulation of a complex chemical process for several levels of noise. The results are compared to those from a promising study in stochastic approximation.

Chapter II

Mathematical Development

In this chapter, the method used for the noisy search problem is described in detail. Stochastic approximation and its modification that were used for a comparison purpose are also described. Finally, the process model used as a test problem is developed.

A. Noisy Search Methods

a. Discussion of general methods. The search method proposed here is a tool for the optimization of many types of multiparameter noise corrupted systems. Methods used for the noise free systems were applied to the noisy systems except that the effect of noise was reduced by filtering using minimum variance estimators.

The filters used in this work were obtained by replication alone at the current search point. This type of filter was shown in previous work to yield a significant improvement in search response over traditional stochastic approximation methods (Luecke, 1970).

Rosenbrock's pattern search developed for noise free systems was used as the search method. Screening experiments (Luecke, 1967) indicated that this method is less sensitive than most to the effect of noise. A further advantage is that this search uses only values of objective function at various points unlike gradient techniques which depends on derivatives. This feature allowed a simplified formulation for the minimum variance estimators.

When a point in the search was reached for which the standard search procedure indicated that no further progress toward optimization

was being made, an increased number of replications was made at each functional evaluations. This reduced the effective noise levels by the ratio of the square root of the number of replications.

In the previous study, optimal replication factors were derived by calculus of variations using some information about the function that normally would not be available (Luecke, 1970). For this thesis, replication after search failures was increased by factors two, four, or six. There are approximations to the factors determined by the more complex procedure.

The whole procedure, failure and increased replication process, was repeated until an upper bound on replications was reached or until satisfactory approach to the optimum was attained.

Note that the estimator was realized by replication at the current search location alone. Values obtained at earlier stages are ignored and not used in the function estimates.

b. Rosenbrock technique. The Rosenbrock search used here has been otherwise referred to as the method of rotating coordinates. It has outperformed many other methods on difficult two-dimensional curved ridges (Wilde, 1964).

The method of rotating coordinates differs from other searches mainly in the way it carries out local explorations. Instead of perturbing each of the original variables independently as in other pattern searches, Rosenbrock rotates the coordinate system toward the most efficient direction as estimated in previous trials. The other axes are arranged in the direction normal to the first. Instead of taking a fixed step in each direction, this procedure continuously adjusts the

step sizes. The combined rotation of search vector and scale adjustment is extremely effective on object functions with curved ridges.

The effect of this method is that if a change was successful (criterion function is greater than or equal to the value at the previous base point for functions having maxima), then the next time a step size is made in the same direction, and three times as far. But, if the step was unsuccessful, then when the time comes to use that particular step, it will be in the opposite direction and will have only half the length. This method adjusts the steps by itself to the required magnitude.

A stage is completed when there has been at least one success and one failure in every coordinate direction. Coordinate directions for the next stage are then obtained by constructing a set of orthogonal vectors around a base vector that reaches from the initial point to the final point of the just completed stage.

B. Stochastic Approximation Technique

Among the more successful optimization methods for noisy systems is stochastic approximation. Some recent developments and extensions for the technique are described in this section.

a. Kiefer-Wolfowitz procedure. After the work of Robins and Monroe (1951) was published, Kiefer and Wolfowitz (1952) (K - W) adapted stochastic approximation to the problem of finding the maximum of unimodal functions obscured by noise.

The K - W technique is a one-dimensional procedure. It differs from the other methods in that instead of estimating the derivatives $\Delta\phi/\Delta X$. At one point X_n the dependent variable, is measured at two points at a distance of C_n on either side of X_n (Figure 1). C_n is

defined as the distance between the most recent pair of observations.

From these two observations $z(X_n - C_n)$ and $z(X_n + C_n)$, the average slope is calculated as:

$$\left[z(X_n + C_n) - z(X_n - C_n) \right] / 2C_n \quad (2-1)$$

The sign of the slope indicates the direction in which to locate the next pair of experiments.

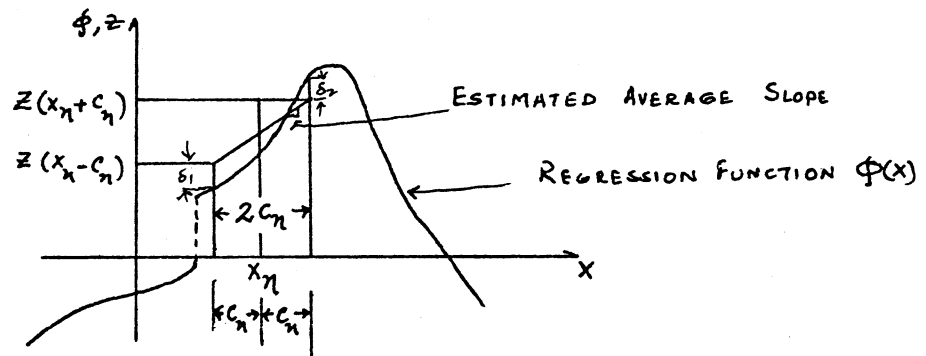


Figure 1.

Kiefer-Wolfowitz Estimation of Average Slope.

The center point, X_{n+1} , of the next pair of the experiments is determined as:

$$X_{n+1} = X_n + A_n \left[\frac{z(X_n + C_n) - z(X_n - C_n)}{2C_n} \right] \quad (2-2)$$

where A_n is one of the sequence of positive numbers determining the step size.

The values of observation z are given by the equation

$$z(X_n) = \phi(X_n) + \delta_n \quad (2-3)$$

where δ_n are the normally distributed random variables with zero mean and standard deviation σ . $\phi(X_n)$ is the criterion function at the point X_n . The K - W technique requires certain restrictions on the stepping sequence and the distance between the observations.

$$\begin{aligned} \text{Lim } A_n &= 0 \\ n &\rightarrow \infty \end{aligned} \quad (2-4)$$

$$\begin{aligned} \text{Lim } C_n &= 0 \\ n &\rightarrow \infty \end{aligned} \quad (2-5)$$

These conditions guarantee that the process will eventually converge. To be certain there is enough corrective action to avoid stopping short of the peak, the stepping sequence must be such that,

$$\sum_{n=1}^{\infty} A_n = \infty \quad (2-6)$$

But to cancel out cumulative noise effects and to guarantee convergence, we must have

$$\sum_{n=1}^{\infty} \left(\frac{A_n}{C_n} \right)^2 < \infty \quad (2-7)$$

The K - W method can be inefficient because it needs an infinite number of runs to ensure convergence. In practice, it is not possible to use infinite numbers of trials to determine the optimum set of operating variables. It is very desirable that convergence be rapid.

It is assumed that noise is unbiased, since any bias would distort the perception of the underlying criterion function. That is its expected value is zero.

$$E[\delta_n] = 0 \quad (2-8)$$

b. Normalized Kiefer-Wolfowitz procedure. Cruz-Diaz (Wilde, 1964)

observed that the K - W technique was very slow in the flat regions far from the optimum.

In Figure 2(a), a more complicated unimodal function is shown. Its average slope, given in Figure 2(b), is certainly not monotonic, having as it does a minimum and a maximum corresponding to the inflection points of ϕ . The K - W procedure would be very slow in the flat regions far from the maximum X^* , and as soon as it reaches the left inflection point it would jump over the peak into the flat region to the right. Thus, it takes a lot of time to come out of the plains.

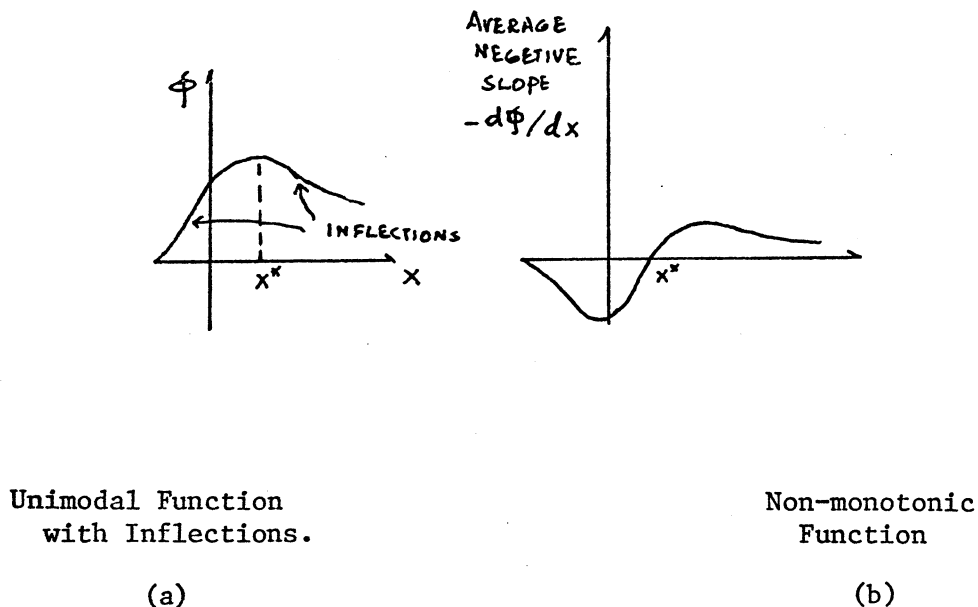


Figure 2.

Function Requiring Normalization

In this way, assymetry in a peak can confound the K - W technique and greatly retard its speed of convergence. Under these circumstances it would be better to use only the sign instead of the magnitude of the

average slope. The normalized version can be written as

$$X_{n+1} = X_n + A_n \operatorname{Sgn} \left[\frac{z(X_n + C_n) - z(X_n - C_n)}{2C_n} \right] \quad (2-9)$$

where $\operatorname{Sgn}[U]$ denotes the sign of the quantity inside the brackets. The new base point, X_{n+1} , is determined from the previous base point, X_n , plus the current value of stepping sequence A_n multiplied by the sign of the average estimated slope at the base point X_n .

Use of the sign of estimated slope rather than its numerical value has been shown empirically to improve performance of the method for certain ill-behaved criterion functions (Wilde, 1964).

The restrictions on the stepping sequence and the distance between recent observations are the same as given in K - W procedure in equations (2-4) through (2-7) in section a. of this chapter.

c. Kesten's accelerated procedure. Kesten modified the K - W procedure to accelerate the convergence process under more restrictive assumptions (Wilde, 1964). This procedure is extended to more general functions and convergence is faster.

Kesten's accelerated procedure merely eliminates shortening of the step size when movement is apparently toward the optimum. Kesten reasoned that far from the peak there will be fewer reversals in the search directions because direction reversing error will be relatively unlikely. The step size, therefore, is shortened only after a reversal of the average slope. This method brings the search close to the optimum more quickly than the unaccelerated schemes. Near the goal one can expect overshooting because of the oscillations from one side to the other, so that short step sizes rapidly result.

The equation for this procedure is the same as given in Equation (2-2), except that the stepping sequence will change only when the sign of the slope changes. The restrictions imposed are the same as given in Equations (2-4), (2-6), and (2-7). Additional restrictions required by Kesten are: Each member of the sequence must be less than all preceding members;

$$A_{n+1} < A_n \quad \text{for all } n \quad (2-10)$$

and

$$C_n = \text{Constant} \quad \text{for all } n = 1, 2, 3, \dots \quad (2-11)$$

These replace the condition given in Equation (2-5) for the unaccelerated procedure.

d. Ahlgren and Steven's modified method. Ahlgren and Stevens (1966) suggested a further modification of the Kesten - Kiefer - Wolfowitz search, in that after a given number of sign changes, the whole procedure was reinitiated with the step size relengthened back to the initial size A_1 . The last basepoint is then considered as a new starting point. This technique, of course, destroys all the rigorous mathematical conditions for convergence. By experimental testing, Ahlgren and Stevens showed that modified procedure was more efficient than the other methods as error was increased.

The results for the Kesten - Kiefer - Wolfowitz method on the test function, taken from Ahlgren and Stevens (1966) are shown here for comparison with the present work. Results for the A & S modified procedure are also shown.

Functional evaluations, used as the criteria for merit in this work, were computed by multiplying the number of search stages as reported by

A & S by eight since, in the four-dimensional system, there are eight explorations at each base point.

C. Test Problem

a. System structure. The present optimization problem is taken from the model proposed by Williams (1961). A diagram of the plant is shown in Figure 3.

This model was used so that the results of the new method could be directly compared with those reported by Ahlgren and Stevens (1966) for the modified stochastic approximation approach. We note here parenthetically, that several difficulties that involved much lost time were incurred because of a typographical error in an equation from the A & S paper (sign in the denominator) and because of a change of a coefficient in the A & S program for this function ($-60 V_R$). To be consistent with the other results, this latter change in Equation 2-30 was retained here although this makes the computed object function slightly incorrect.

The plant consists of a continuous stirred tank reactor, a separation device consisting of a settling tank (decanter) and a distillation column. Before sending the reactor effluent to the decanter it is cooled. The decanter overflow is sent for distillation. In the reactor, three irreversible exothermic, temperature sensitive reactions take place to yield a mixture of six components in the reactor effluent. The temperature of the reactor is assumed controllable at any desired temperature. Column bottoms which would contain the product and some other material is recycled to the reactor for further reaction. A discard stream is taken off the distillation column bottoms and sent to the plant fuel.

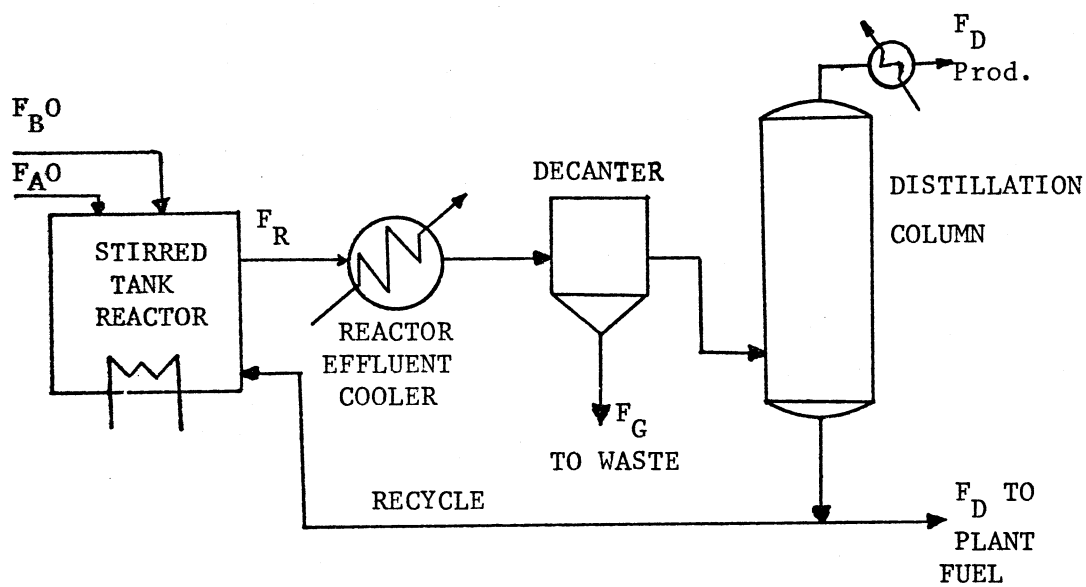


Figure 3.

Block Diagram of Model Plant.

The plant in the present study is to produce 40,000,000 lbs. per year of distillate product, P. Reactants A and B are the only two which produce the product. The reactor effluent contains both raw materials A and B; the desired product, P; an intermediate, C; an inert, E; and a residual substance, G. In the cooler, the residual substance becomes insoluble in the reactor effluent. Residual product (F_G) is separated in the decanter. The desired product is removed by distillation. In the column bottoms an azeotrope is formed. Part of the substance is recycled to the reactor and rest to the plant fuel to control the concentration.

b. Simplifying assumptions. Several simplifying assumptions are made:

1. The reactor can be considered well stirred and reactants and products are at all times completely mixed, i.e., composition in the outlet would be same as the reactants.
2. The decanter is considered well mixed in the layer of material serving as feed to the distillation column and there is no mixing between the light and heavy layer.
3. Loss of heat is considered negligible for all units.
4. Volume is expressed as pounds of contained liquids.
5. All compositions are expressed as weight fractions.
6. If production must exceed 40,000,000 lb. annually (OR 4763 lb/hr considering 8400 operative hours) then that excess is discarded.
7. Molecular weights (M_i) for each components:

Components	A, B, P	100
Components	C, E	200
Components	G	300

c. Equations. Now the equations used to simulate the operation of the model plant are discussed. These equations merely serve to simulate a measured response for a given set of decision variables. Error is generated artificially and introduced in the object function.

1. Chemical reactions: Product P is produced by or takes part in the following chemical reactions:



Initial reactant materials, A and B, are available in pure form from outside sources. Components C, E, and G are intermediate by-products of the reactions. They have no sale value as chemical products, but can be disposed of as fuels.

Rate of Reactions:

$$r_1 = k_1 C_{AR} C_{BR} \quad \text{reaction coefficient} \quad (2-15)$$

$$r_2 = k_2 C_{BR} C_{CR} \quad \text{reaction coefficient} \quad (2-16)$$

$$r_3 = k_3 C_{CR} C_{PR} \quad \text{reaction coefficient} \quad (2-17)$$

Reaction coefficients: The reaction coefficients k_1, k_2, k_3 have been evaluated. Their value can be expressed by the Arrhenius equation:

$$k_i = Q_i e^{-N_i/T} \quad (2-18)$$

Coefficients Q and N are pre-exponential factor and activation energy where

$$Q_1 = 5.9755 \times 10^9/\text{hr.} \quad \text{weight fraction}$$

$$N_1 = 12,000 \text{ }^\circ\text{R} \quad \text{BASIS: 1 lb. of A or B}$$

$$Q_2 = 2.5962 \times 10^{12}/\text{hr.} \quad \text{weight fraction}$$

$$N_2 = 15,000 \text{ } ^\circ\text{R} \quad \text{BASIS: 1 lb. of B}$$

$$Q_3 = 9.6283 \times 10^{15}/\text{hr.} \quad \text{weight fraction}$$

$$N_3 = 20,000 \text{ } ^\circ\text{R} \quad \text{BASIS: 1 lb. of C}$$

2. Process constraints: Material balances were written for various components and the following set of equations were derived. All material balances assume steady state operations. These steady state equations are to be solved for various values of decision variables.

- (a) Material balance on component A (in terms of reactor concentration of A).

$$F_{AO} + (K - 1) F_R C_{AR} - k_1 V_R C_{AR} C_{BR} = 0 \quad (2-19)$$

where K is recycle ratio (weight fraction).

- (b) Material balance on component B (in terms of reactor concentration of B).

$$F_{BO} + (K - 1) F_R C_{BR} - k_1 V_R C_{AR} C_{BR} - k_2 V_R C_{BR} C_{CR} = 0 \quad (2-20)$$

- (c) Material balance on component C (in terms of reactor concentration of C).

$$(K - 1) F_R C_{CR} + \frac{M_C}{M_A} k_1 V_R C_{AR} C_{BR} - \frac{M_C}{M_B} k_2 V_R C_{BR} C_{CR} - k_3 V_R C_{CR} C_{PR} = 0 \quad (2-21)$$

- (d) Material balance on component E (in terms of reactor concentration of E).

$$(K - 1) F_R C_{ER} + \frac{M_E}{M_B} k_2 V_R C_{BR} C_{CR} = 0 \quad (2-22)$$

(e) Material balance on component G.

$$-F_R C_{GR} + \frac{M_G}{M_C} k_3 V_R C_{CR} C_{PR} = 0 \quad (2-23)$$

(f) Material balance on component P.

$$\begin{aligned} (K - 1) F_R C_{PR} - K F_P + \frac{M_P}{M_C} k_2 V_R C_{BR} C_{CR} \\ - \frac{M_P}{M_C} k_3 V_R C_{CR} C_{PR} = 0 \end{aligned} \quad (2-24)$$

(g) Constraint on the concentrations in the reactor.

$$C_{AR} + C_{BR} + C_{CR} + C_{ER} + C_{PR} + C_{GR} = 1.0 \quad (2-25)$$

(h) Constraint on the distillation separation efficiency is:

$$F_R C_{PR} - 0.1 F_R C_{ER} - F_P = 0 \quad (2-26)$$

(this results from the Williams', $F_P = (C_{PS} - 0.1 C_{ES}) F_S$).

(i) Overall material balance.

$$F_{AO} + F_{BO} = F_P + F_R C_{GR} + F_D \quad (2-27)$$

These are fourteen variables and nine nonlinear constraint equations.

Hence, there are five independent variables and nine dependent variables.

The independent variables are F_P , F_{BO} , V_R , T , and K . Since we assumed that the product P is fixed at 40,000,000 lb./yr., there are only four

independent variables which are to be varied in the search for the

optimum. Dependent variables are C_{AR} , C_{BR} , C_{CR} , C_{ER} , C_{PR} , C_{GR} , F_R , F_D , and F_{AO} . To calculate the criterion function it is necessary to ini-

tialize these variables.

3. Objective function: Simultaneous solution of the nine non-linear equations for a given set of decision variables permits evaluation of the criterion function.

(% Return)

$$\phi = 100 \frac{8400X - 2.22F_R - (0.124)(8400)(0.3F_P + 0.0068F_D) - 60V_R - 1.3F_R}{300 V_R + 13.0 F_R} \quad (2-28)$$

The above equation (2-28) is modified version of Williams' percent return on investment contains the following assumptions postulated by Williams.

- (a) 8400 operational hours are assumed.
- (b) $F_P = 4763$ lb/hr.
- (c) $X = 0.30 F_P + 0.0068 F_D - 0.02 F_{AO} - 0.03 F_{BO} - 0.001 F_G$.

(Contains sale price and raw material cost of various streams).

- (d) Utility charges are 2.22 multiplied by the reactor effluent flow rate.
- (e) SARE cost (sales, administration, research and engineering cost factor), compounded as gross return is 0.124.
- (f) $300 V_R + 13.0 F_R$ is factor for estimating gross capital and $30 V_R + 1.3 F_R$ is the corresponding factor for depreciation.

Chapter III

Results and Analysis

Noise in the form of a normally distributed random variable having zero mean was added to the criterion function described in the last section of the previous chapter. A search for the optimum was conducted using the method described earlier.

The results of these searches, as well as the best results of searches made by Ahlgren and Stevens (1966) using stochastic approximation are all graphed in the same general format. The ordinate represents the number of functional evaluations (eight times the number of center points for the stochastic approximation methods). All graphs are plotted to the same scale to facilitate comparison.

At each error level four different random number sequences were generated by digital computer (subroutine GAUSS-IBM Scientific subroutine package) to test reproductibility of results. Five levels of error were introduced in the function in order to test the method: $\sigma = 0.0, 0.5, 1.0, 2.0,$ and 5.0 . At the initial state, the value of the object function was 25.8, compared to the optimal or maximal value of the object function of 46.02.

In the present study, the same initial step size was used for all runs. The four free variables were initialized along with step sizes.

With these initial values and constraint equations, the nine dependent variables were calculated. With the dependent variables and decision variables, the value of the object function could be calculated. Noise was added to this functional value. The Rosenbrock search was used to determine the new values of the decision variables.

The results obtained with the different noise levels and random number sequences are given in Table 1 through Table 14. Plots of the results are also given although all the data points are not shown. Only the points at the end of each search stage in the Rosenbrock routine are plotted.

In Table 1 and Table 2, the results are given for the noise free systems. The results in Table 1 are for the Rosenbrock search method and in Table 2 are for Kesten's accelerated search technique (Ahlgren and Stevens, 1966). At the end of the first stage, that is when search progress failed, the object function has increased from 25.8 to 45.83. A total of 86 functional evaluations were required to reach this value. Kesten's accelerated technique required 212 evaluations to reach the same value (Table 2). These results are plotted in Figure 4. It is evident that for the noise free system, the performance of the Rosenbrock method is superior to that of stochastic approximation. Both methods show slower response in the vicinity of optimum as compared to when it is far away.

Additions of substantial quantities of noise produced a slower time response. Tables 3 through 7 show the progress of the optimizer when the noise is a normally distributed random variable with zero mean and a standard deviation of 0.5. Four random noise sequences were tested. When a level was reached for which further significant improvement stopped or at least was very slow, the number of replications of the object function was increased by multiples of two after each failure of search progress. For comparison purposes, tests were also performed wherein the number of replications was increased by multiples of four and six after each failure.

TABLE 1

Rosenbrock Search Results for Noise Free Case

Value of the Object Function	Number of Functional Evaluations
25.8	Initial
44.84	17
45.81	41
45.83*	86

* Indicates failure in search progress.

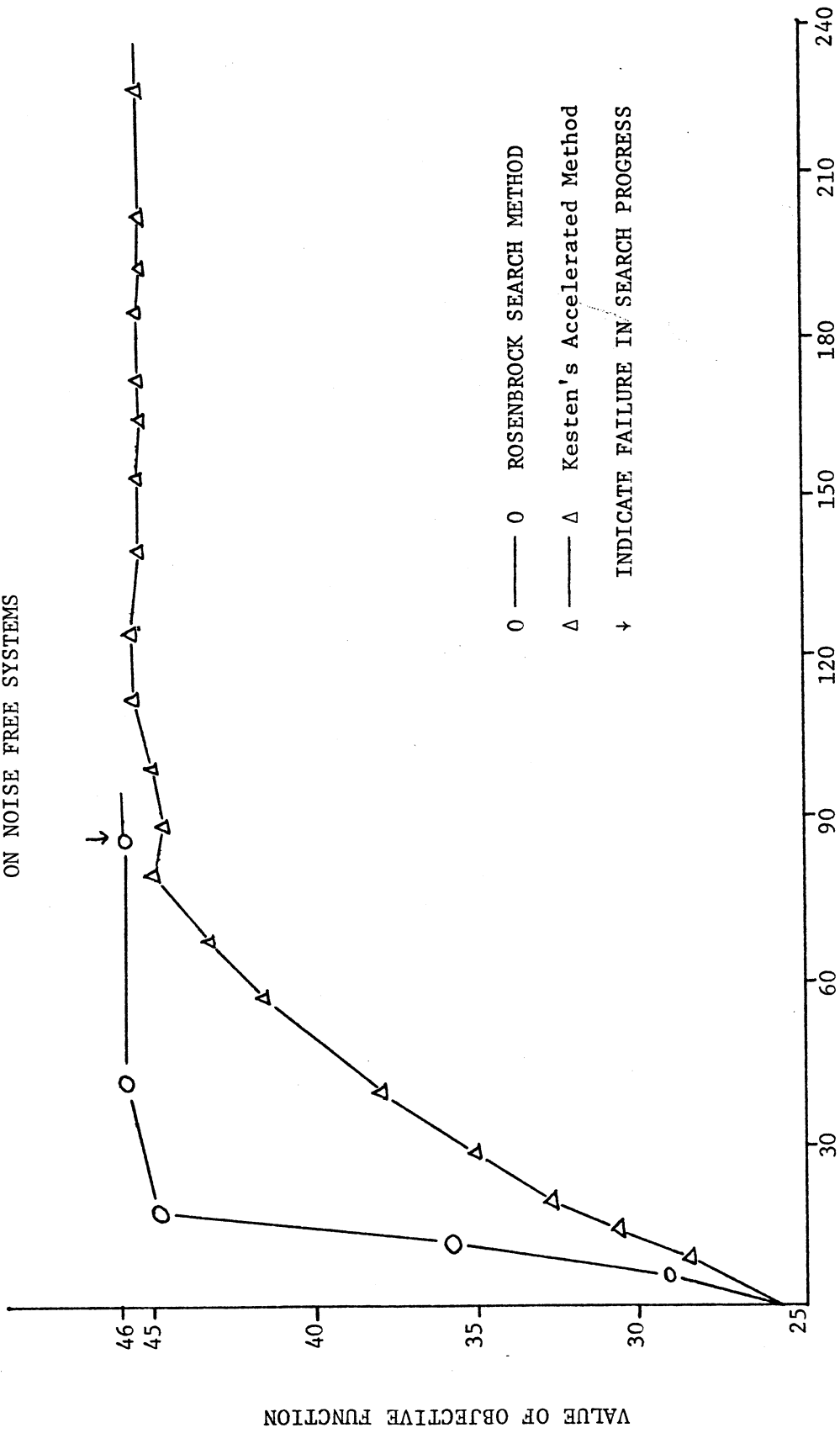
TABLE 2

Kesten's Accelerated Method for Noise Free Case

Value of the Object Function	Number of Functional Evaluations
25.8	Initial
31.4	16
38.0	40
44.8	88
45.8	212

BEHAVIOR OF ROSENBROCK AND KESTEN'S ACCELERATED METHOD

ON NOISE FREE SYSTEMS



N - NUMBER OF FUNCTIONAL EVALUATION

Figure 4.

The results were plotted in Figures 5 and 6 along with results from Ahlgren and Stevens. The arrows in the figure denote the failure in search progress. The failure in search occurs when there is no significant improvement in the object function or response rate is very slow.

Tests with two of the random number sequences (plotted in Figure 5) showed better convergence than that of the best of modified method of Ahlgren and Stevens. And other two random number sequences had convergence rates very similar to that of the best of modified A & S method. On the average, one can say that replication technique is better than the modified method at this error level.

The results for a replication increased by a factor of four and six are shown in Tables 6 and 7. These results are plotted in Figures 7 and 8. In Figure 7, the convergence rate of Rosenbrock search is not better than modified search, but at least it is not worse. In Figure 8, the Rosenbrock shows poor performance compared to the other method.

The noise was doubled to the level of 1.0 and again tests with four random number sequences were made. The results in Tables 8 and 10 are plotted in Figure 9. The best convergence rates of the A & S modified stochastic approximation method was about the same as for the filtered Rosenbrock search for two of the random number sequences, while for two other sequences, replication technique showed a poorer response rate.

In Table 11, the results of convergence rate of the noise level of 2.0 are given and plotted in Figure 11. The best results of the A & S modified method are somewhat better than the filtered Rosenbrock search method, but the responses of both methods are comparable.

TABLE 3

Replication Technique With a Noise Level of 0.5
(For Random Number Sequences 1 & 2)

Random Number Sequence 1		Random Number Sequence 2	
Value of the Criterion Function	Number of Functional Evaluations	Value of the Criterion Function	Number of Functional Evaluations
25.8	Initial	25.8	Initial
33.359	17	43.143	17
40.06	29	45.843*	62
45.508	53	46.034*	154
45.934*	98	45.931	222
46.001*	190	45.931*	402
46.009	226	45.897	506
46.005*	406	46.004*	866
46.011*	774		

* Indicates failure in search progress.

TABLE 4

Replication Technique With a Noise Level of 0.5
(For Random Number Sequences 3 & 4)

Random Number Sequence 3		Random Number Sequence 4	
Value of the Criterion Function	Number of Functional Evaluations	Value of the Criterion Function	Number of Functional Evaluations
25.8	Initial	25.8	Initial
32.88*	46	31.95*	46
37.098	72	38.34	80
41.27*	162	43.52	120
43.687	214	43.88*	210
44.991*	390	45.283*	346
44.942*	758	45.373	714

* Indicates failure in search progress.

TABLE 5

Modified Method of A & S With a Noise Level of 0.5

Value of the Criterion Function	Number of Functional Evaluations
25.8	Initial
34.4	32
39.4	128
43.0	208
45.3	304
45.6	384
45.7	480

SEARCH PROGRESS OF REPLICATION TECHNIQUE AND MODIFIED METHOD

OF A & S WITH A NOISE LEVEL OF 0.5.

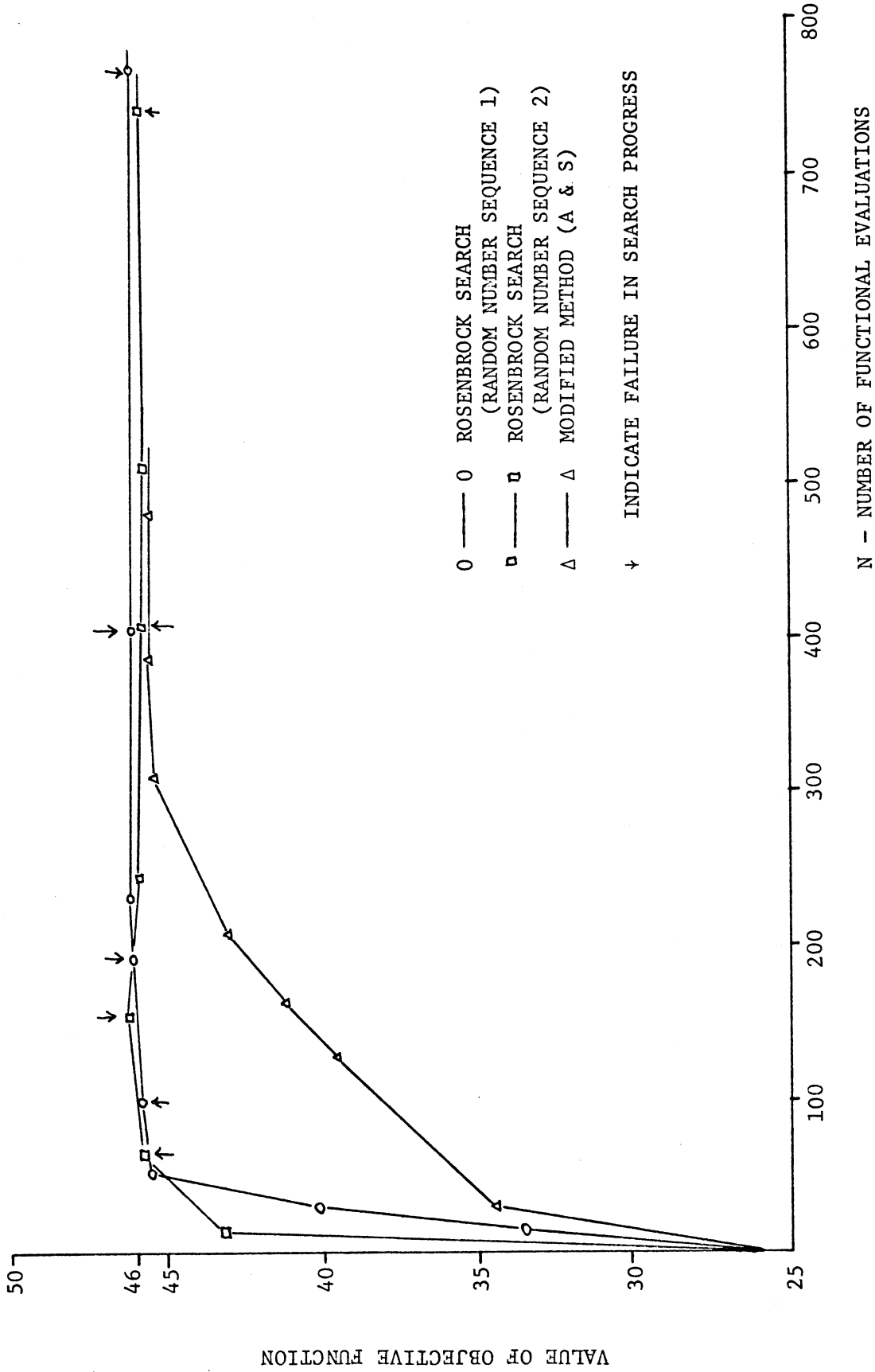


Figure 5.

SEARCH PROGRESS OF REPLICATION TECHNIQUE AND MODIFIED

METHOD (A & S) FOR NOISE LEVEL OF 0.5.

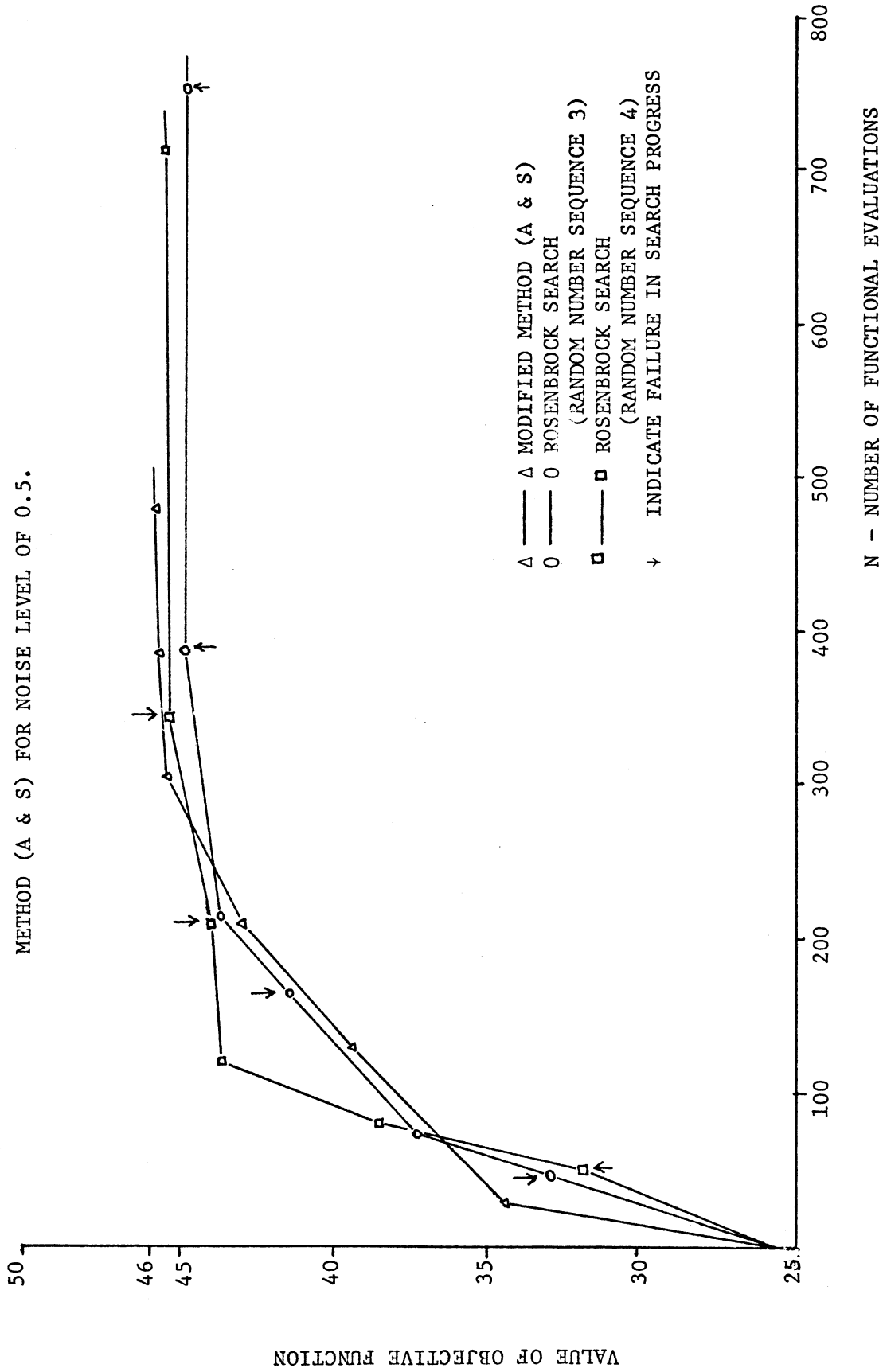


Figure 6.

TABLE 6

Replication Technique With a Noise Level of 0.5
Replication per Stage is Four-Fold

Random Number Sequence 3		Random Number Sequence 4	
Value of Objective Function	Number of Functional Evaluations	Value of Objective Function	Number of Functional Evaluations
25.8	Initial	25.8	Initial
32.88*	46	31.946*	46
45.657*	230	38.28	114
45.73*	966	38.892*	294
		42.813	502
		44.929	694
		45.012*	1414

* Indicates failure in search progress.

COMPARISON OF RATE OF CONVERGENCE OF REPLICATION METHOD
AND MODIFIED METHOD (A & S) FOR NOISE LEVEL OF 0.5.

(REPLICATION PER STAGE IS FOUR-FOLD)

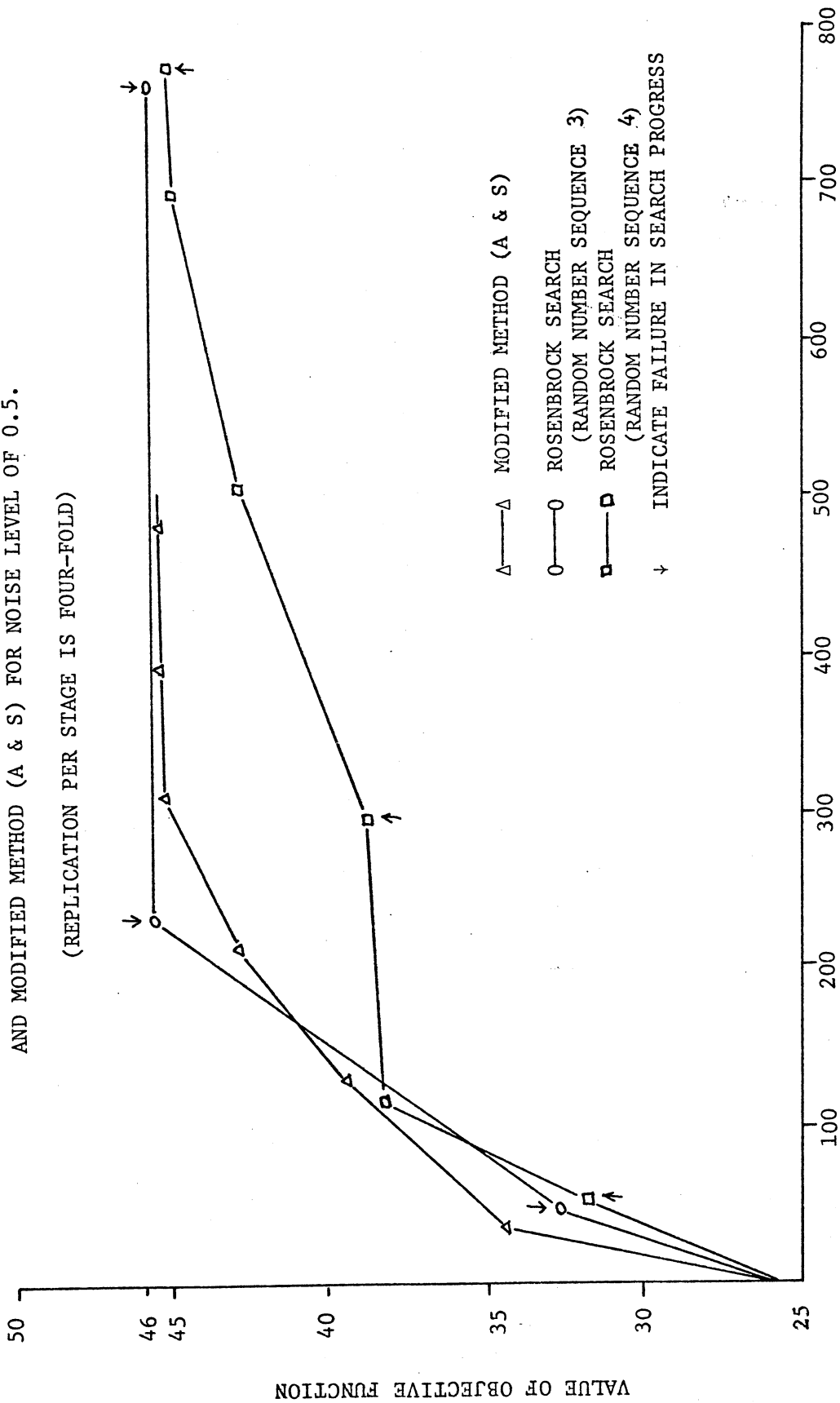


Figure 7.

TABLE 7

Replication Technique With a Noise Level of 0.5.

Replication per Stage is Six-Fold

Random Number Sequence 3

Value of Functional Evaluation	Number of Functional Evaluation
25.8	Initial
32.884*	46
36.935	124
41.702	196
44.665	388
45.088*	688

* Indicates failure in search progress.

SEARCH PROGRESS OF REPLICATION TECHNIQUE AND MODIFIED METHOD

(A & S) FOR NOISE LEVEL OF 0.5.

(REPLICATION PER STAGE IS SIX-FOLD)

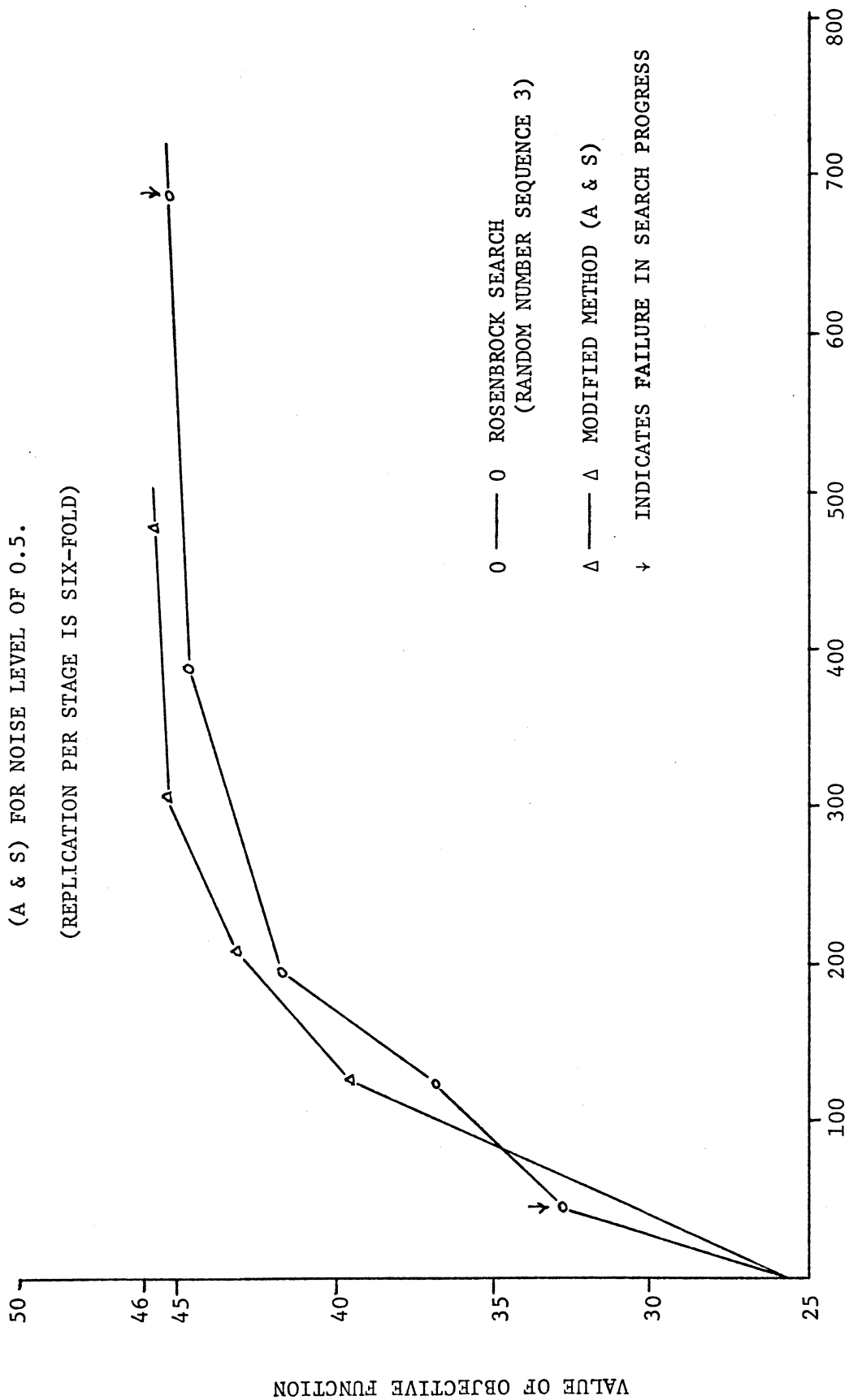


Figure 8.

TABLE 8

Replication Technique With a Noise Level of 1.0

Random Number Sequence 1		Random Number Sequence 2	
Value of Objective Function	Number of Functional Evaluations	Value of Objective Function	Number of Functional Evaluations
25.8	Initial	25.8	Initial
35.577	37	27.841*	46
35.624*	82	34.153*	138
36.514*	174	39.503	190
39.712	226	44.520*	370
41.358	258	44.279	442
44.185	370	45.966*	794
45.591*	550		

* Indicates failure in search progress.

TABLE 9

Replication Technique With a Noise Level of 1.0

Random Number Sequence 3		Random Number Sequence 4	
Value of Objective Function	Number of Functional Evaluations	Value of Objective Function	Number of Functional Evaluations
25.8	Initial	25.8	Initial
33.35*	46	32.653*	58
34.795*	138	35.015*	150
37.364	206	42.617*	330
38.527*	386	44.593*	698
43.497	554	44.767*	1418
43.822*	914	45.107	1706
44.601	1250	45.699	2090
45.1*	1970	46.009*	3530

* Indicates failure in search progress.

TABLE 10

Modified Method of A & S With a Noise Level of 1.0

Value of the Object Function	Number of Functional Evaluation
25.8	Initial
28.6	40
33.0	80
36.0	120
40.2	160
41.0	200
42.4	304
44.4	392
45.04	488
45.0	536
44.4	616
45.1	696

SEARCH PROGRESS OF REPLICATION TECHNIQUE AND
 MODIFIED METHOD (A & S) FOR NOISE LEVEL OF 1.0.

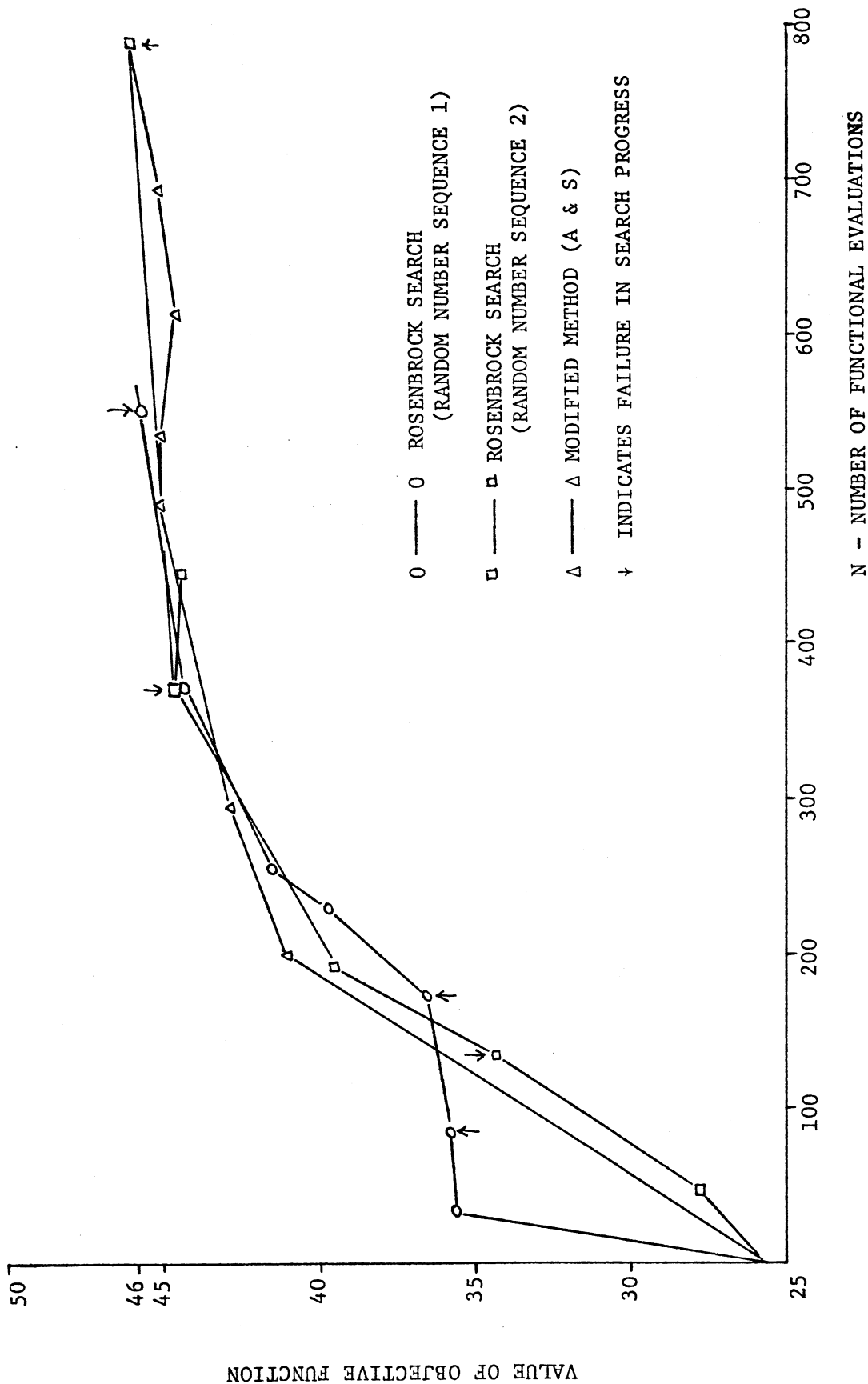


Figure 9.

N - NUMBER OF FUNCTIONAL EVALUATIONS

BEHAVIOR OF REPLICATION TECHNIQUE AND
 MODIFIED METHOD WITH A NOISE LEVEL OF 1.0.

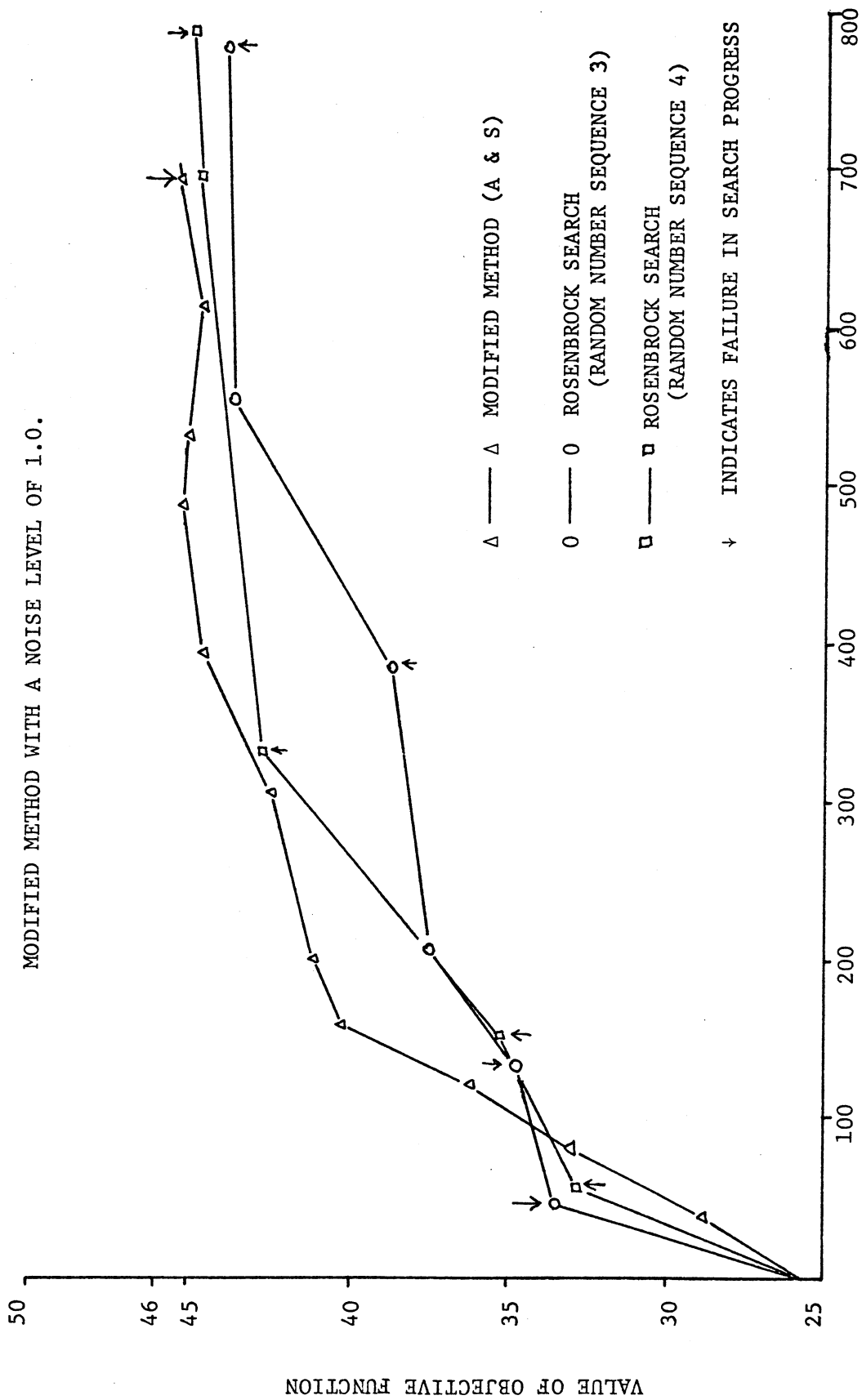


Figure 10.

TABLE 11

Replication Technique With a Noise Level of 2.0

Random Number Sequence 3		Random Number Sequence 4	
Value of Objective Function	Number of Functional Evaluations	Value of Objective Function	Number of Functional Evaluations
25.8	Initial	25.8	Initial
29.16*	46	32.562*	46
33.614	128	33.936	72
34.334*	218	39.986	144
37.164*	402	40.474*	234
40.309	490	39.653	334
45.03	602	40.17*	514
45.784*	962	40.109*	882
46.002*	1698	40.763*	1618

* Indicates failure in search progress.

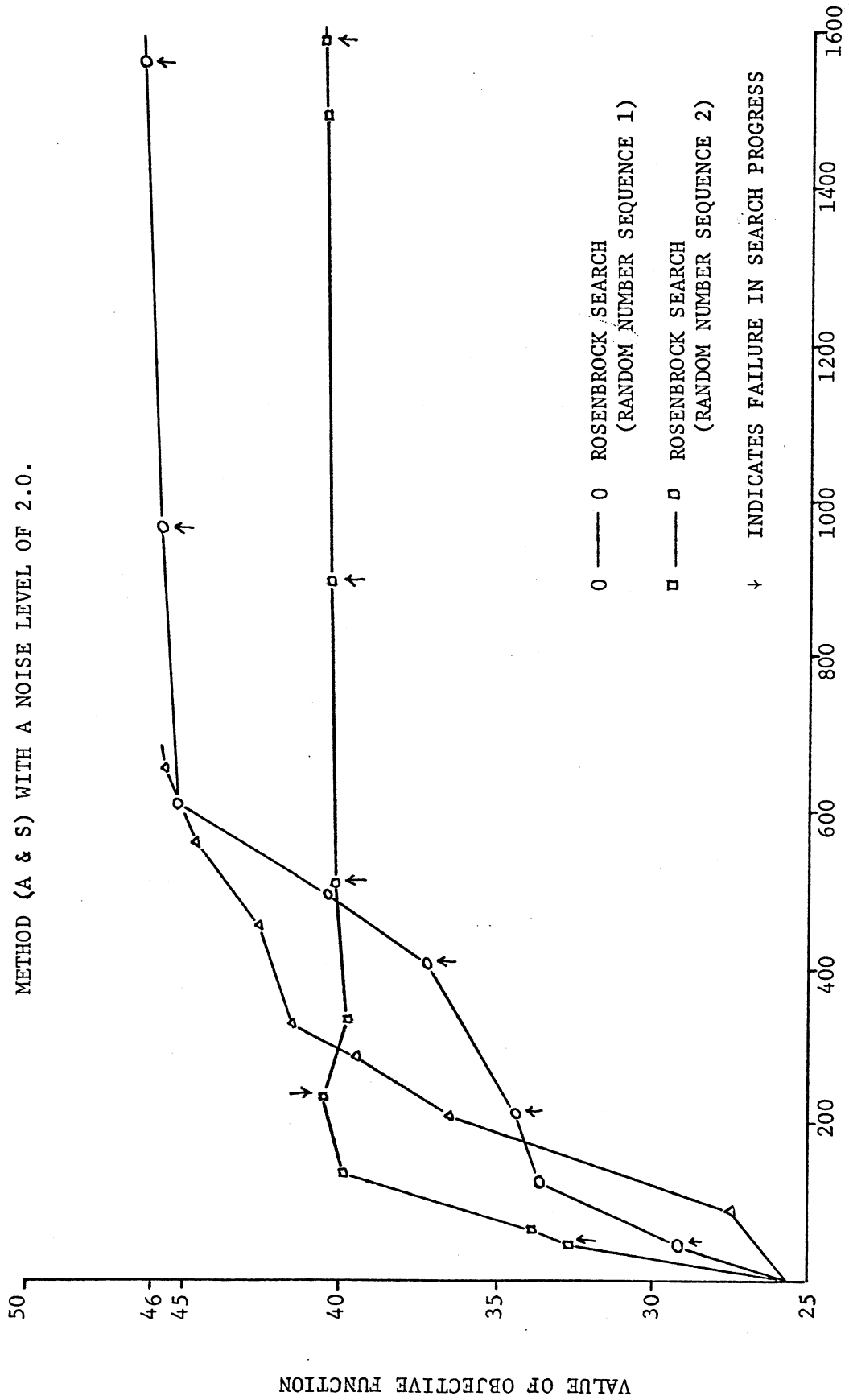
TABLE 12

A & S Modified Method With a Noise Level of 2.0

Value of the Object Function	Number of Functional Evaluation
25.8	Initial
27.4	88
36.4	208
39.2	288
41.4	328
42.6	456
44.6	560
45.4	664

SEARCH PROGRESS OF REPLICATION TECHNIQUE AND MODIFIED

METHOD (A & S) WITH A NOISE LEVEL OF 2.0.



N - NUMBER OF FUNCTIONAL EVALUATIONS

Figure 11.

In the last of them, Table 13 and Figure 12, results of noise level of 5.0 are given. The data in the Table 14, which are plotted in Figure 12, are of Kesten's accelerated method. The results of the A & S modified method are not available. The replication technique showed a faster convergence than Kesten's accelerated technique.

TABLE 13

Replication Technique With a Noise Level of 5.0

Random Number Sequence 3		Random Number Sequence 4	
Value of Objective Function	Number of Functional Evaluations	Value of Objective Function	Number of Functional Evaluations
25.8	Initial	25.8	Initial
33.756*	46	39.549*	46
31.177*	138	34.328	72
29.364*	322	38.613*	162
33.00*	690	35.630*	346
35.872	898	37.049	450
44.709*	1618	38.833*	810
		37.157*	1546

* Indicates failure in search progress.

TABLE 14
Kesten's Accelerated Method With a Noise Level of 5.0

Value of the Object Function	Number of Functional Evaluation
25.8	Initial
31.0	48
30.0	56
31.0	136
31.6	160
33.0	320

CONVERGENCE RATES OF REPLICATION TECHNIQUE AND
 KESTEN'S ACCELERATED METHOD FOR NOISE LEVEL OF 5.0.

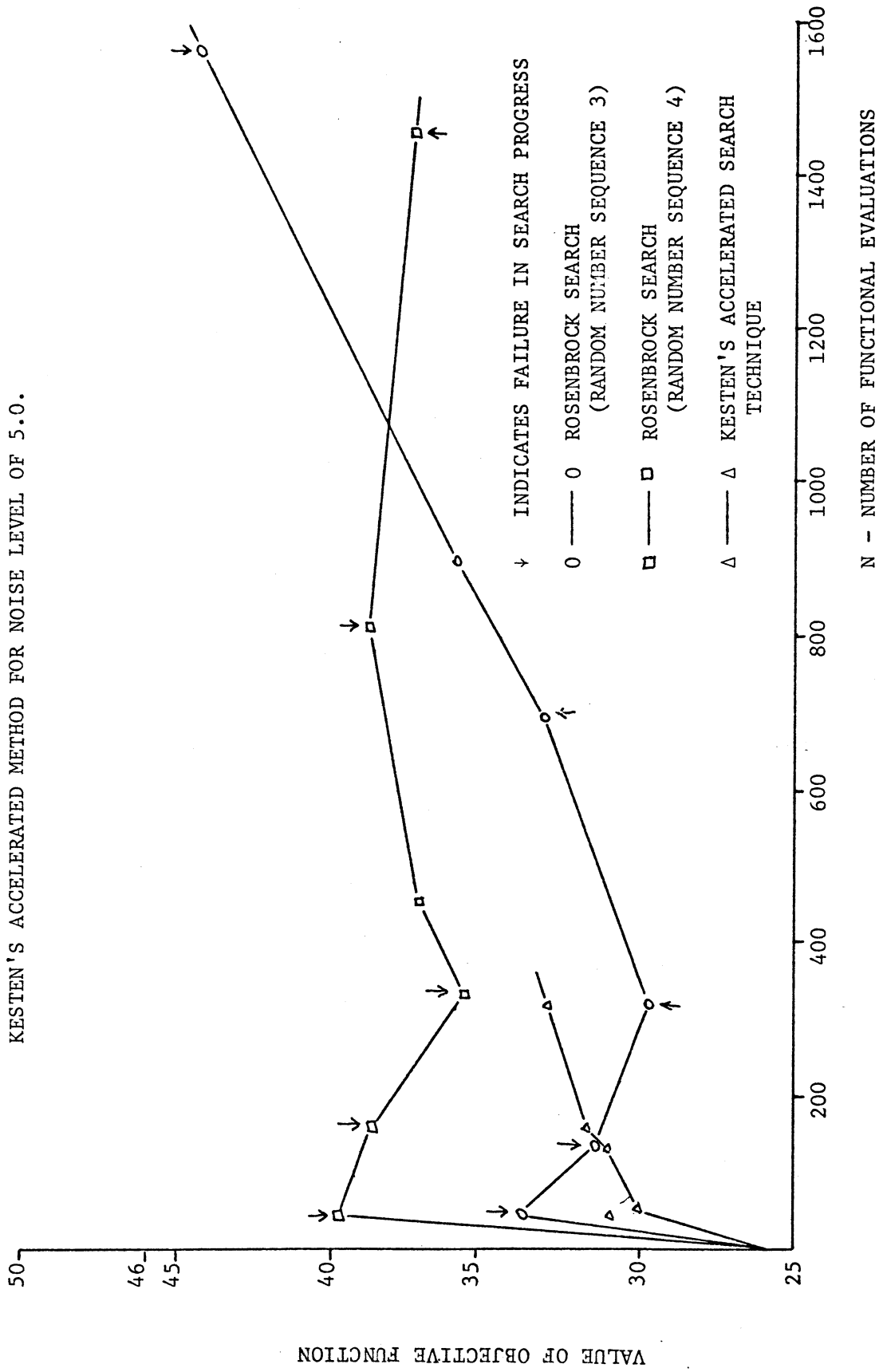


Figure 12.

Chapter IV

Conclusions and Recommendations

The new search method is effective in finding the optimum of this function in the presence of noise. At moderate noise levels ($\sigma \leq 0.5$), the average response rate is faster than that from the best tests reported for the A & S modified stochastic approximation method. At higher noise levels, the average response rate is at a level comparable to that of the best A & S results.

A number of simple changes could enhance the convergence rate of the new method. One is to extend the filter for the functional values to include information from previous search points. Another change might be to modify the way that is used in the Rosenbrock algorithm to decide that search progress had ceased. Too often excessive functional evaluations were made at a maximal value for a given noise and filter level.

Nomenclature

- A = raw material
- a = finite number
- A = sequence of positive numbers used to determine step size
- B = raw material
- C = intermediate product
- C = concentration, lb. material per lb. flowing stream
- c = exploration step size
- E = inert product
- F = flow rate, lb. per hour
- G = residual product
- K = recycle ratio = lb. recycled to reactor/lb. from
distillation column bottoms
- k = reaction rate constant
- M = molecular weight
- N = activation energy x gas constant
- P = desired product
- Q = pre-exponential factor
- r = rate of reaction
- T = temperature, °R
- V = volume, lb.
- X = term containing value of process streams
- x = true value of a decision variable
- z = value of criterion function with error

Greek Letters

δ = error in evaluation of criterion function

ϕ = true value of the criterion function

σ = standard deviation of error

ξ = random number

Subscripts and Superscripts

A = feed material A

B = feed material B

C = feed material C

D = material to plant fuel

E = inert product E

G = residual product

i = dummy index

n = number of base points

O = initial

P = desired product

R = from (of) reactor

S = from decanter

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APPENDIX A

Appendix A
Description (Computer Program)
of Replication Technique

In the Rosenbrock search, the main steps which are applied in finding the optimum conditions are the following.

1. Initial estimates of the decision variables \underline{a}_1 (where $\underline{a}_1 = (x_1^0, x_2^0, \dots, x_4^0)$) are read. In our case, we have four decision variables (volume of the reactor, V_R ; initial flow rate of component B, F_{B0} ; temperature in the reactor, T ; recycle ratio, K). The product, P , is fixed at 40,000,000 lbs. per year. (or 4763 lbs/hr.).

2. Initial estimates of the dependent variables \underline{b}_1 (where $\underline{b}_1 = (x_6^0, x_7^0, \dots, x_{14}^0)$) are fed into the computer. In this case, there are nine dependent variables (compositions of components A, B, C, E, G, P; i.e. $C_{AR}, C_{BR}, C_{CR}, C_{ER}, C_{GR}, C_{PR}$ and cooler effluent, F_R ; by-product stream, F_D ; feed stream, F_{AO}).

3. Initial estimates of step size \overline{DEL}_1 (where $\overline{DEL}_1 = (Del_1, Del_2, Del_3, Del_4)$) are read.

4. Objective function ϕ is evaluated at the initial values of $(x_1^0 \dots x_{14}^0)$. (For this we have to make use of the simultaneous equation solver, SMLIQ).

5. Now we change the one decision variable x_1^0 by the amount of the step size Del_1 .

6. The constraint equation is solved with the help of subroutine EQSLN and objective function is computed again at the new points.

In the subroutine Rosenbrock, $LA = 2$, means still search is continued; $LA = 4$, is stage is complete and no need of functional value;

LA = 5, no change in value and cannot continue; LA = 8 is when answer is found. At the initial entry, LA = 1.

When first time LA = 5 is gotten, then the functional evaluations are averaged to give better value; i.e. if first the NREP = 1, then after we get LA = 5, then NREP = NREP + 2. So that functional value $\phi_{ave} = \sum_{i=1}^4 \phi_i / 2$. That is next time we get LA = 5, then NREP would be equal to 4 and $\phi_{ave} = \sum_{i=1}^{16} \phi_i / 4$ etc.

If $\phi(x_1^0 + \text{Del}_1, x_2^0, \dots, x_k^0) > \phi(x_1^0, x_2^0, \dots, x_k^0)$, then $(x_1^0 + \text{Del}_1, x_2^0, \dots, x_k^0)$ would be new temporary head. A_{11} , let $x_1^0 + \text{Del}_1 = x_{11}$, then go to Step 9 directly, otherwise go to next step.

7. If the new functional value is lower than the previous functional value, then initial value is reduced by the same step size and ϕ is evaluated and again compared to the functional values. If this ϕ is larger than the previous one, then the new values of variables are called new temporary head.

That is, if $\phi(x_1^0 + \text{Del}_1, x_2^0, \dots, x_k^0) > \phi(x_1^0, x_2^0, \dots, x_k^0)$, then previous variable is reduced by the same step size and ϕ is evaluated.

If $\phi(x_1^0 - \text{Del}_1, x_2^0, \dots, x_k^0) > \phi(x_1^0, x_2^0, \dots, x_k^0)$, then the new temporary head would be $a_{11} = (x_1^0 - \text{Del}_1, x_2^0, \dots, x_k^0)$ and let $x_{11} = x_1^0 - \text{Del}_1$, and go to Step 9.

8. Similarly, if $\phi(x_1^0 - \text{Del}_1, x_2^0, \dots) > \phi(x_1^0, x_2^0, \dots)$, then retain original values and next variable is now disturbed by the amount of step size Del_2 and the above procedure is repeated till all the decision variable is computed and then go to Step 10.

Next variable $x_{21} = x_2^0 + \text{Del } 2$ and $x_{11} = x_1^0$.

9. At this point $a_{11} = (x_1^1, x_2^0, \dots)$ and ϕ is evaluated and continuously disturbing the other variables.

10. After one set of decision variables (x_1 through x_4) are varied, then we come back to the first variable and, depending on the success or failure in the previous calculation of objective function, it is varied.

11. Suppose that in the previous calculation of ϕ_1 was a success; i.e. $\phi_1 > \phi$ for $x_{11} = x_1^0 + \text{Del}_1$, so when we came back to this variable after all the decision variables are over, then we evaluate the ϕ at $x_{21} = x_{11} + 3 * \text{Del}_1$.

12. But, suppose that previous calculation of ϕ_1 was a failure; i.e., $\phi_1 < \phi$ for $x_{11} = x_1^0 + \text{Del}_1$, so when we came back to this variable after all the decision variables are over, then we evaluated the ϕ at $x_{21} = x_{11} - \frac{1}{2} * \text{Del}_1$.

The value 3 and $-\frac{1}{2}$ were determined by numerical experiments to give good efficiency in a moderately difficult problem (Rosenbrock and Storey, 1966).

In the computer program the values of 1X are the following:

1X = 387654321 (Random Number Sequence 1)

1X = 487654321 (Random Number Sequence 2)

1X = 123456789 (Random Number Sequence 3)

1X = 7654321 (Random Number Sequence 4)

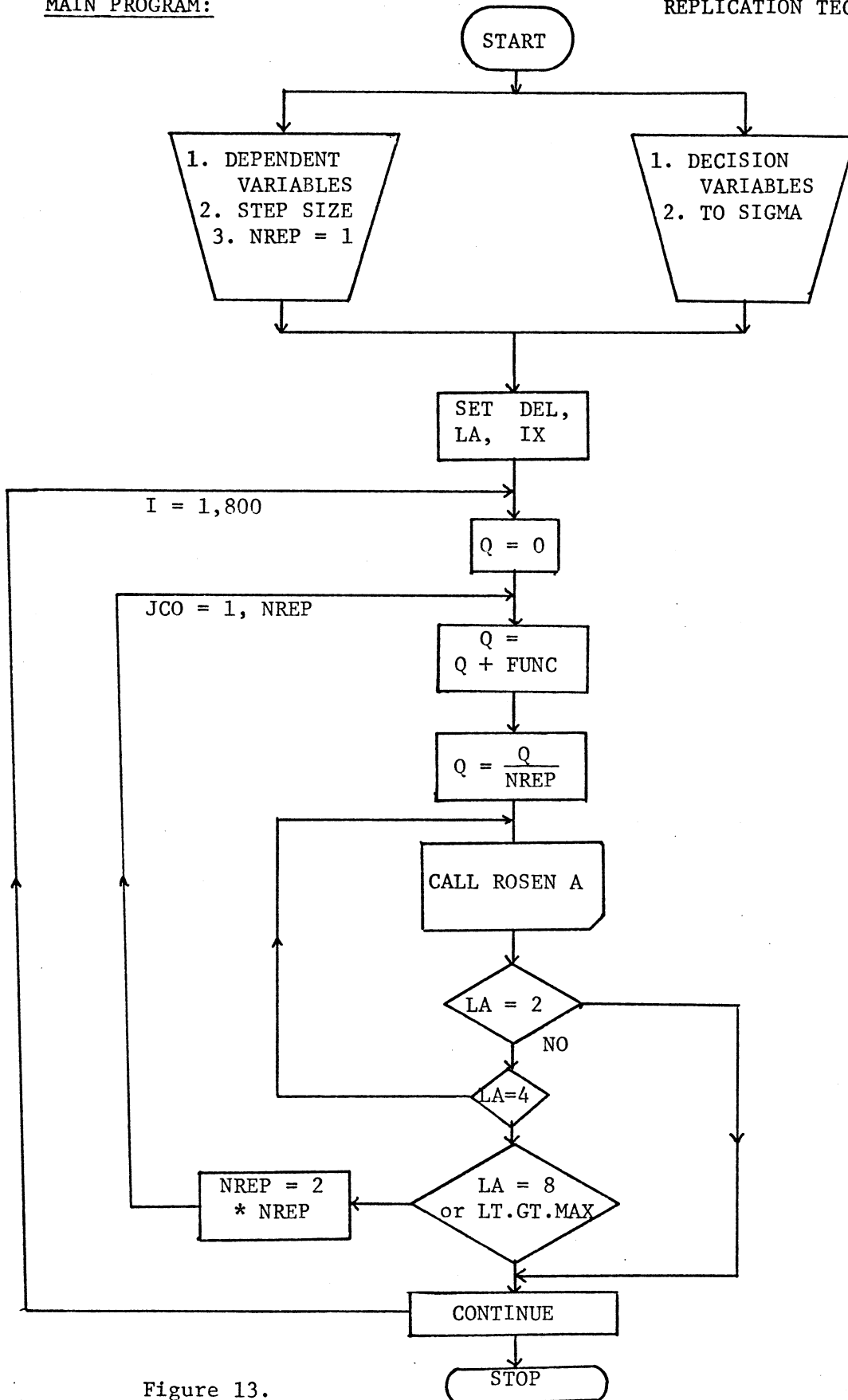


Figure 13.

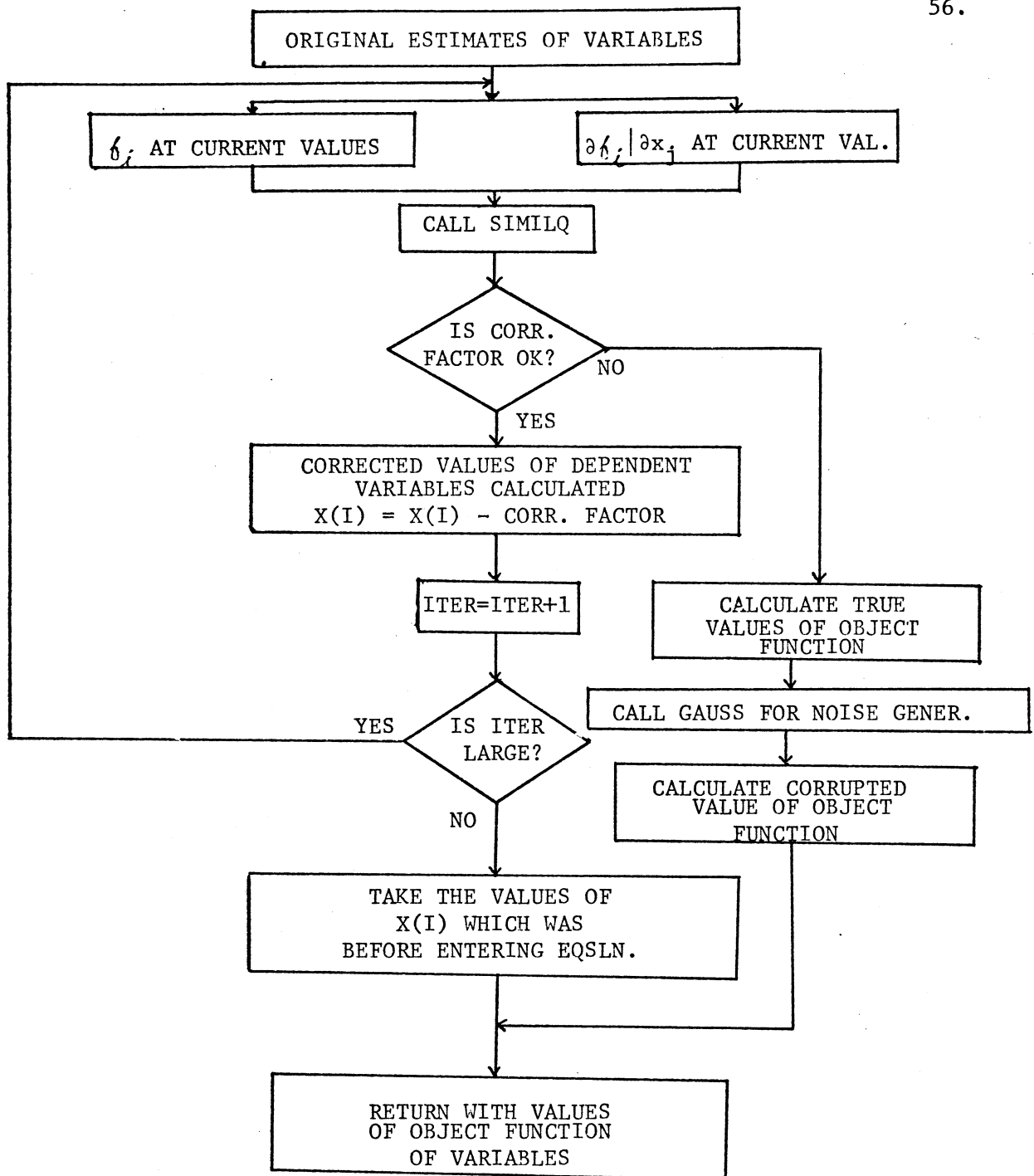


Figure 14.

Subroutine EQSLN

```

C      MAIN PROGRAM
C      ROSEN BROCK SEARCH
C      INITIALIZE X(1) THROUGH X(5) AND X(6) THROUGH X(14).
C      FINDING THE MAXIMUM OF THE OBJECT(CRITERION) FUNCTION
C      FINDING THE MINIMUM OF THE SUM OF THE SQUARES
      DIMENSION X(14),DEL1(5),C(9),DEL(5)
      COMMON /GAUS/ IX,SIGMA
      DATA LL/0/,LT/0/
      TOL=1.E-6
      IX=123456789
      DO 231 I231=1,2
      SIGMA=1.
      KMAX=1000
      LL=0
      LT=0
      NREP=4
      DEL1(5)=0.
      X(1)=4450.0
      X(2)=33500.0
      X(3)=638.0
      X(4)=0.55
      X(5)=4763.0
      X(6)=.131
      X(7)=0.386
      X(8)=0.027
      X(9)=0.337
      X(10)=0.036
      X(11)=0.083
      X(12)=97540.
      X(13)=40180.0
      X(14)=14920.
      K=4
      DEL1(1)=50.
      DEL1(2)=500.
      DEL1(3)=1.
      DEL1(4)=.015
      PRINT 99,SIGMA,IX
14 DO 15 I=1,5
15 DEL(I)=DEL1(I)
      LA=1
      DO 23 I=1,800
      Q1=0.
      DO 20 J=1,NREP
      LT=LT+1
20 Q1=Q1+FUNC1(X,LA)
      Q1=Q1/NREP
      LL=LL+1
21 CALL ROSENA (K,Q1,X,LA,DEL,TOL)
24 PRINT 111,LA,Q1,(X(J),J=1,K),LL,LT
      IF(LA.EQ.2) GO TO 23
      IF(LA.EQ.4) GO TO 21
25 IF( (LA.EQ.8) .OR. (LT.GT.KMAX )) GO TO 229
      NREP=NREP*2
      GO TO 14

```



```

23 CONTINUE
229 IX=7654321
231 CONTINUE
99 FORMAT(1H1,3X,17HROSEN BROCK SEARCH,10X,'SIGMA= ',
$F5.2,10X,'IX= ',I9/1H0)
111 FORMAT(1X,3HLA=,I5,4X          ,E12.5,5X,4E13.5,
$'LL',I5,'LT',I5)
STOP
END
FUNCTION FUNC1(Y,LA)
DIMENSION A(9,10),X( 9),Y(14)
COMMON TEMP,REK,VR,FAO,FBO,CAR,CBR,CCR,CER,CGR,
$CPR,FR,X,A,NC,NV,FG,FP,FD,OPT2,ITER,LLA
LLA=LA
VR=Y(1)
FBO=Y(2)
TEMP=Y(3)
REK=Y(4)
FP=Y(5)
CAR=Y(6)
CBR=Y(7)
CCR=Y(8)
CER=Y(9)
CGR=Y(10)
CPR=Y(11)
FR=Y(12)
FD=Y(13)
FAO=Y(14)
CALL EQSLN
Y(1)=VR
Y(2)=FBO
Y(3)=TEMP
Y(4)=REK
Y(5)=FP
Y(6)=CAR
Y(7)=CBR
Y(8)=CCR
Y(9)=CER
Y(10)=CGR
Y(11)=CPR
Y(12)=FR
Y(13)=FD
Y(14)=FAO
FUNC1=OPT2
RETURN
END
SUBROUTINE EQSLN
DIMENSION A(9,10),X(9),Z(9)
COMMON TEMP,REK,VR,FAO,FBO,CAR,CBR,CCR,CER,CGR,
$CPR,FR,X,A,NC,NV,FG,FP,FD,OPT2,ITER,LLA
COMMON /GAUS/ IX,SIGMA
DATA LCA/1/
Z(1)=CAR
Z(2)=CBR

```

```

Z(3)=CCR
Z(4)=CER
Z(5)=CGR
Z(6)=CPR
Z(7)=FR
Z(8)=FD
Z(9)=FAO
ITER=0
AK1=(5.9755E9)*EXP(-12.0E3/TEMP)
AK2=(2.5962E12)*EXP(-15.0E3/TEMP)
AK3=(9.6283E15)*EXP(-20.0E3/TEMP)
VRK1=VR*AK1
VRK2=VR*AK2
VRK3=VR*AK3
15 A(1,10)=FAO+(REK-1.0)*FR*CAR-VRK1*CAR*CBR
A(2,10)=FBO+(REK-1.0)*FR*CBR-VRK1*CAR*CBR-VRK2*CBR*CCR
A(3,10)=(REK-1.0)*FR*CCR+2.0*VRK1*CAR*CBR-2.0*
VRK2*CCR*CBR-VRK3*CCR*CPR
A(4,10)=(REK-1.0)*FR*CER+2.0*VRK2*CBR*CCR
A(5,10)=CAR+CBR+CCR+CER+CGR+CPR-1.0
A(6,10)=-FR*CGR+1.5*VRK3*CCR*CPR
A(7,10)=(REK-1.0)*FR*CPR-REK*FP+VRK2*CBR*CCR-0.5*VRK3*
$CCR*CPR
A(8,10)=FR*CPR-0.1*FR*CER-FP
A(9,10)=FAO+FBO-FP-FD-FR*CGR
A(1,1)=(REK-1.0)*FR-VRK1*CBR
A(1,2)=-VRK1*CAR
A(1,3)=0.0
A(1,4)=0.0
A(1,5)=0.0
A(1,6)=0.0
A(1,7)=(REK-1.0)*CAR
A(1,8)=1.0
A(1,9)=0.0
A(2,1)=-VRK1*CBR
A(2,2)=(REK-1.0)*FR-VRK1*CAR-VRK2*CCR
A(2,3)=-VRK2*CBR
A(2,4)=0.0
A(2,5)=0.0
A(2,6)=0.0
A(2,7)=(REK-1.0)*CBR
A(2,8)=0.0
A(2,9)=0.0
A(3,1)=2.0*VRK1*CBR
A(3,2)=2.0*VRK1*CAR-2.0*VRK2*CCR
A(3,3)=(REK-1.0)*FR-2.0*VRK2*CBR-VRK3*CPR
A(3,4)=0.0
A(3,5)=0.0
A(3,6)=-VRK3*CCR
A(3,7)=(REK-1.0)*CCR
A(3,8)=0.0
A(3,9)=0.0
A(4,1)=0.0
A(4,2)=2.0*VRK2*CCR

```

```
A(4,3)=2.0*VRK2*CBR
A(4,4)=(REK-1.0)*FR
A(4,5)=0.0
A(4,6)=0.0
A(4,7)=(REK-1.0) *CER
A(4,8)=0.0
A(4,9)=0.0
A(5,1)=1.0
A(5,2)=1.0
A(5,3)=1.0
A(5,4)=1.0
A(5,5)=1.0
A(5,6)=1.0
A(5,7)=0.0
A(5,8)=0.0
A(5,9)=0.0
A(6,1)=0.0
A(6,2)=0.0
A(6,3)=1.5*VRK3*CPR
A(6,4)=0.0
A(6,5)= -FR
A(6,6)=1.5*VRK3*CCR
A(6,7)= -CGR
A(6,8)=0.0
A(6,9)=0.0
A(7,1)=0.0
A(7,2)=VRK2*CCR
A(7,3)=VRK2*CBR-0.5*VRK3*CPR
A(7,4)=0.0
A(7,5)=0.0
A(7,6)=(REK-1.0)*FR-0.5*VRK3*CCR
A(7,7)=(REK-1.0)*CPR
A(7,8)=0.0
A(7,9)=0.0
A(8,1)=0.0
A(8,2)=0.0
A(8,3)=0.0
A(8,4)=-0.1*FR
A(8,5)=0.0
A(8,6)=FR
A(8,7)=CPR-0.1*CER
A(8,8)=0.0
A(8,9)=0.0
A(9,1)=0.0
A(9,2)=0.0
A(9,3)=0.0
A(9,4)=0.0
A(9,5)=-FR
A(9,6)=0.0
A(9,7)=-CGR
A(9,8)=1.0
A(9,9)=-1.0
NC=9
CALL SIMILQ(NC,A,X,NOGO)
```

```

DO 5 I=1,9
  IF(ABS(X(I)).GT.0.05) GO TO 10
5 CONTINUE
  GO TO 100
10 CAR=CAR-X(1)
  CBR=CBR-X(2)
  CCR=CCR-X(3)
  CER=CER-X(4)
  CGR=CGR-X(5)
  CPR=CPR-X(6)
  FR=FR-X(7)
  FAO=FAO-X(8)
  FD=FD-X(9)
  ITER=ITER+1
  IF(ITER.LE.10)GO TO 15
16 OPT2=0.
  CAR=Z(1)
  CBR=Z(2)
  CGR=Z(5)
  CCR=Z(3)
  CER=Z(4)
  CPR=Z(6)
  FR=Z(7)
  FD=Z(8)
  FAO=Z(9)
  GO TO 31
100 FG=FK*CGR
C   CALCULATING THE CRITERION (OBJECT) FUNCTION
  P=0.3*FP+.0068*FD-.02*FAO-.03*FBO-.01*FG
  OPT2=100.*(8400.*P-2.22*FR-.124*8400.*(0.30*FP+.0068
1*FD)-60.*VR-1.30*FR)/(300.*VR+13.0*FR)
  CALL GAUSS(IX,SIGMA,0.0,YRAND)
  OPT2=OPT2+YRAND
31 CONTINUE
  IF(LLA.EQ.2 .GR. LCA.EQ.0) GO TO 8
  WRITE(6,7)(X(I),I=1,NC)
  WRITE(6,3)
  WRITE(6,4) TEMP,REK,VR,FAO,FBO
  WRITE(6,60)
  WRITE(6,4) FP,FD
  WRITE(6,6)
  WRITE(6,4) CAR,CBR,CCR,CER,CGR,CPR,FR
  WRITE(6,807) ITER
  WRITE(6,841) OPT2
8 CONTINUE
  LCA=1
  IF (LLA.EQ.1) LCA=0
7 FORMAT( 3X,9E12.5)
3 FORMAT(4X,4HTEMP,11X,3HREK,12X,2HVR,13X,3HFAO,
$12X,3HFBO)
4 FORMAT(7(3X,E12.5))
6 FORMAT(4X,3HCAR,12X,3HCBR,12X,3HCCR,12X,3HCER,
112X,3HCGR,12X,3HCPR,12X,3HFR )
60 FORMAT(4X,2HFP,13X,2HFD )

```

```

807  FORMAT(4X,5HITER=,I3)
841  FORMAT(4X,'RATE OF RETURN',6X ,E14.6)
843  FORMAT(4X,'RATE OF RETURN')
      RETURN
      END
      SUBROUTINE GAUSS(IX,S,AM,V)
      A=0.0
      DO 50 I=1,12
      CALL RANDU(IX,IY,Y)
      IX=IY
50    A=A+Y
      V=(A-6.0)*S+AM
      RETURN
      END
      SUBROUTINE RANDU(IX,IY,YFL)
      IY=IX*65539
      IF(IY)5,6,6
5    IY=IY+2147483647+1
6    YFL=IY
      YFL=YFL*.4656613E-9
      RETURN
      END
      SUBROUTINE ROSENA ( NM, SS, PN, LAA, DEL, TOL )

```

```

C
C*****
C
C      NM = NUMBER OF INDEPENDENT VARIABLES
C              SET NM + TO FIND MAX, - TO FIND MIN
C
C
C      SS IS OBJECT FUNCTION AND MUST BE EVALUATED ON INITIAL
C      ENTRY
C      PN IS THE VECTOR OF COORDINATE POINTS IN THE SEARCH
C      --ON ANY ENTRY
C      INTO PROGRAM, S = SS(PN), ON EXIT PN IS MOVED TO A
C      NEW POINT
C
C      LAA = 1 ON INITIAL ENTRY
C           = 2 WHEN SEARCHING
C           = 4 AFTER COMPLETE STAGE (DO NOT NEED FUNCTION
C           VALUE)
C           = 5 CORRECTION STEP DID NOT CHANGE VALUES - CAN
C           NOT CONTINUE
C           = 8 WHEN CONVERGED
C
C      DEL VECTOR IS ABSOLUTE INITIAL STEP SIZE
C      INITIAL DEL ALSO USED AS SCALE FACTOR
C
C      C IS THE CONVERGENCE TOLERANCE ON SUCCESSIVE VALUES
C      OF SS
C*****
C
C

```

```

DIMENSION SA(2,30),PW(20,20),A(20,20),AI(20,20)
DIMENSION DEL(1),PN(1),P2(30),DELSV(30,2),P1(30)
DATA SA/60*0./,PW/400*0./,A/400*0./,AI/400*0./,DELSV/
160*0./, P1/30*0./,P2/30*0./

```

C

```

1 LA = LAA
2 SN = SS
3 N = IABS (NM)
4 NN = N
9 IF( LA - 4 ) 10,2000,10
10 IF( LA - 1 ) 11,11,13
11 SBD = SN
   RNM = NM
12 SNM = SIGN (1.0,RNM)
13 IF( SNM ) 14,14,16
14 SBD = AMAX1(SBD,SN+1.0)
15 GO TO 20
16 SBD = AMIN1(SBD,SN-1.0)
20 CONTINUE
21 IF( LA - 2 ) 22,110,90
22 LA = 2
30 SBASE = SN
31 SBA = SBASE
32 IF( TOL ) 33,33,40
33 TOL = 1.0E-7
40 DO 48 J=1,N
42 P2(J) = 0.0
43 DELSV(J,1) = DEL(J)
44 DELSV(J,2) = PN(J)
45 DEL(J) = 1.0
46 DO 47 I=1,N
47 A(I,J) = 0.0
48 A(J,J) = 1.0
49 DO 60 J=1,N
50 DO 60 I=1,2
60 SA(I,J) = 0.0
70 NCT = 1
80 P2(NCT) = P2(NCT) + DEL(NCT)

```

C

C

C

OBTAIN ORIGINAL VARIABLES AND RETURN

```

   NSWT = 0
81 DO 87 J=1,N
   PNT = PN(J)
82 PNSUM = 0.0
83 DO 84 I=1,N
84 PNSUM = PNSUM + A(I,J)*P2(I)
85 PN(J) = DELSV(J,1)*PNSUM + DELSV(J,2)
87 IF( PNT .NE. PN(J) ) NSWT = 1
88 IF( NSWT .LE. 0 ) LA = 5
90 SS = SN
91 LAA = LA
   RETURN
110 IF( SNM*(SBASE- SN) ) 111,111,210

```

```

111 SA(1,NCT) = SA(1,NCT) + 1.0
120 DEL(NCT) = 3.0*DEL(NCT)
130 SBASE = SN
140 NCT = NCT + 1
141 IF( NCT .LE. N ) GO TO 80
142 IF((SA(1,1) + SA(2,1)).LE. 10.0 ) GO TO 160
143 NSWT = -100
144 GO TO 195
160 DO 190 J=1,N
170 DO 190 I=1,2
    IF( SA(I,J) .EQ. 0. ) GO TO 70
190 CONTINUE
191 LA = 4
192 IF( ABS(SBASE-SBA) .LE. TOL ) LA = 8
193 NSWT = 1
195 SBA = SBASE
196 SN = SBASE
197 GO TO 81
210 P2(NCT) = P2(NCT) - DEL(NCT)
220 DEL(NCT) = -0.5*DEL(NCT)
230 SA(2,NCT) = SA(2,NCT)+ 1.0
240 GO TO 140
2000 LA = 2
2005 DO 2060 I=1,N
2010 DO 2060 J=1,N
2020 IF( I-J ) 2050,2050,2030
2030 PW(I,J) = 0.0
2040 GO TO 2060
2050 PW(I,J) = P2(J) - P1(J)
2060 CONTINUE
2070 DO 2210 I=1,N
2080 J = I - 1
2090 IF( J ) 2160,2160,2100
2100 DO 2150 K=1,J
2110 SUM = 0.
2120 DO 2130 L=1,N
2130 SUM = SUM + PW(I,L)*PW(K,L)
2140 DO 2150 L=1,N
2150 PW(I,L) = PW(I,L) - SUM*PW(K,L)
2160 SUM = 0.
2170 DO 2180 K=1,N
2180 SUM = SUM + PW(I,K)**2
2190 SUM = SQRT (SUM)
2200 DO 2210 K=1,N
2210 PW(I,K) = PW(I,K)/SUM
3000 DO 3040 I=1,N
3010 DO 3040 J=1,N
3020 AI(I,J) = 0.0
3030 DO 3040 K=1,N
3040 AI(I,J) = AI(I,J) + PW(I,K)*A(K,J)
3050 DO 3120 I=1,N
3060 DO 3120 J=1,N
3120 A(I,J) = AI(I,J)
4000 DO 4030 I=1,N

```

```

4010 P1(I) = 0.0
4020 DO 4030 J=1,N
4030 P1(I) = P1(I) + PW(I,J)*P2(J)
4040 DO 4050 J=1,N
4050 P2(J) = P1(J)
4060 GO TO 49
      END
      SUBROUTINE SIMILQ(N,A,X,NOGO)
      DIMENSION A(9,10),X(1)
      NOGO=0
      N1=N+1
      N2=N-1
      DO 3 L=1,N2
      L1=L+1
      K=L
      DO 5 J=L1,N
      IF( ABS(A(K,L))- ABS(A(J,L)))4,5,5
4 K=J
5 CONTINUE
  IF(A(K,L))6,18,6
6 IF(K-L)12,12,13
13 DO 10 J=L,N1
  S=A(K,J)
  A(K,J)=A(L,J)
10 A(L,J)=S
12 D=1./A(L,L)
  DO 14 J=L1,N1
14 A(L,J)=A(L,J)*D
  DO 3 I=L1,N
  IF(A(I,L))15,3,15
15 DT=1./A(I,L)
  DO 16 J=L1,N1
16 A(I,J)=A(I,J)*DT-A(L,J)
3 CONTINUE
  IF(A(N,N))17,18,17
18 NOGO=1
  RETURN
17 X(N)=A(N,N1)/A(N,N)
  DO 19 J=1,N2
  M=N-J
  DO 20 I=1,M
20 A(I,N1)=A(I,N1)-X(M+1)*A(I,M+1)
19 X(M)=A(M,N1)
  RETURN
      END

```


APPENDIX B

Appendix B

Solution of the Constraint Equation

In solving steady state equations describing the system, the Newton-Raphson method for solving simultaneous equations is used (Scarborough, 1955). This method is extended to a system of m equations and n unknowns.

Given the simultaneous equations:

$$\begin{aligned}
 F_1(x_1, x_2, \dots, x_n) &= 0 \\
 F_2(x_1, x_2, \dots, x_n) &= 0 \\
 &\dots \dots \dots \dots \dots \dots \\
 &\dots \dots \dots \dots \dots \dots \\
 F_m(x_1, x_2, \dots, x_n) &= 0
 \end{aligned}
 \tag{1}$$

and if $(x_1^0, x_2^0, \dots, x_n^0)$ are approximate values of a set of solutions and (L_1, L_2, \dots, L_n) are corrections such that;

$$\begin{aligned}
 x_1 &= x_1^0 + L_1 \\
 x_2 &= x_2^0 + L_2 \\
 &\dots \dots \dots \dots \dots \dots \\
 &\dots \dots \dots \dots \dots \dots \\
 x_n &= x_n^0 + L_n
 \end{aligned}
 \tag{2}$$

Then substituting in Equations 1;

$$\begin{aligned}
 F_1(x_1^0 + L_1, x_2^0 + L_2, \dots, x_n^0 + L_n) &= 0 \\
 F_2(x_1^0 + L_1, x_2^0 + L_2, \dots, x_n^0 + L_n) &= 0 \\
 &\dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \\
 &\dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \\
 F_m(x_1^0 + L_1, x_2^0 + L_2, \dots, x_n^0 + L_n) &= 0
 \end{aligned}
 \tag{3}$$

Expanding these by Taylor's Theorem around the point $(x_1^0, x_2^0, \dots, x_n^0)$ we get the simple simultaneous equation:

$$F_i(x_1^0 + L_1, x_2^0 + L_2, \dots, x_n^0 + L_n) =$$

$$F_i(x_1^0, x_2^0, \dots, x_n^0) + \left. \frac{\partial F_i}{\partial x_1} \right|_0 L_1 + \left. \frac{\partial F_i}{\partial x_2} \right|_0 L_2 + \dots$$

$$\dots + \left. \frac{\partial F_i}{\partial x_n} \right|_0 L_n + \text{terms} = 0$$

in higher planes of (L_1, L_2, \dots, L_n) .

Neglecting terms of order greater than 1;

$$F_1(x_1^0, x_2^0, \dots, x_n^0) + \left. \frac{\partial F_1}{\partial x_1} \right|_0 L_1 + \left. \frac{\partial F_1}{\partial x_2} \right|_0 L_2 \dots$$

$$\dots + \left. \frac{\partial F_1}{\partial x_n} \right|_0 L_n = 0$$

$$F_2(x_1^0, x_2^0, \dots, x_n^0) + \left. \frac{\partial F_2}{\partial x_1} \right|_0 L_1 + \left. \frac{\partial F_2}{\partial x_2} \right|_0 L_2 \dots$$

$$\dots + \left. \frac{\partial F_2}{\partial x_n} \right|_0 L_n = 0 \tag{4}$$

$$F_m(x_1^0, x_2^0, \dots, x_n^0) + \left. \frac{\partial F_m}{\partial x_1} \right|_0 L_1 + \left. \frac{\partial F_m}{\partial x_2} \right|_0 L_2 \dots$$

$$\dots + \left. \frac{\partial F_m}{\partial x_n} \right|_0 L_n = 0$$

The above equations represent a set of homogeneous linear equations with unknowns (L_1, L_2, \dots, L_n) .

Subroutine SIMILQ is called to solve the set of equations for the unknown L_1, L_2, \dots, L_n .

After achieving solutions for (L_1, L_2, \dots, L_n) , the value of $(x_1^0, x_2^0, x_3^0, \dots, x_n^0)$ are changed by the value of the correction terms.

$$\begin{aligned} x_1 &= x_1^0 + L_1 \\ x_2 &= x_2^0 + L_2 \\ \text{---} & \text{---} \text{---} \\ \text{---} & \text{---} \text{---} \\ x_n &= x_n^0 + L_n \end{aligned} \tag{5}$$

The new values of (x_1, x_2, \dots, x_n) are used to calculate the value of coefficients in Equation (4) and new values of (L_1, L_2, \dots, L_n) are obtained by the Gaussian elimination procedure. The process is repeated until the values of corrections (L_1, L_2, \dots, L_n) are as close to zero as required to obtain the desired accuracy. As (L_1, L_2, \dots, L_n) approach zero,

$$F_i(x_1, x_2, x_3, \dots, x_n) \rightarrow F_i(x_1^0, x_2^0, \dots, x_n^0)$$

where $i = 1, 2, \dots, m$ by equation.

The initial approximation $(x_1^0, x_2^0, \dots, x_n^0)$ should be reasonably close to the true value. Poor approximation might lead to no convergence.

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