Adaptive random search

"ADAPTIVE RANDOM SEARCH"

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Abstract

Random search methods for multivariable function minimization are considered. Beginning with a theoretical method having an optimum step size [2], directional information is added, and the resulting improvement in performance is calculated for the function $Q(\underline{x}) = \sum_{i=1}^{n} x_i^2$. Practical algorithms, with and without adaptation of step size and search direction, are tested for several functions. For each algorithm the number of function evaluations required for minimization increases linearly with the number of variables. Theoretical and numerical results indicate that directional adaptation improves performance significantly.

Contents

1. Introduction

A topic of much current interest is the development of efficient computational methods for solving the following problem: Find the values of a set of parameters, $\underline{x} = (x_1, x_2, \ldots, x_n)^T$, which minimize a (real valued) objective function $Q(\underline{x})$.

"Random search" methods for function minimization have been studied and used by several researchers [1]. Like other direct search methods, random search algorithms have the advantage of requiring neither measurements of the gradient of $Q(\underline{x})$ nor one-dimensional minimizations of $Q(\underline{x})$- operations which can be numerically troublesome and/or costly in computational effort. Schumer and Steiglitz [2] have analyzed a random search method with optimum step size and have found that, under certain conditions, the number of evaluations of $Q(\underline{x})$ required for minimization is a linear function of the number of parameters.

In the present paper we postulate and analyze the performance of two theoretical random methods which have both optimum step size and also information concerning the direction in which $Q(\underline{x})$ decreases. Our method of analysis is similar to that of Schumer and Steiglitz. A practical algorithm, which attempts to realize the theoretical ones by adapting both step size and the search direction to the function being minimized, is developed from a method proposed by Matyas [3]. Numerical results are given for this algorithm as applied to several test functions.

2. Theoretical random search methods.

For the development of the theoretical random search methods, we assume a quality function of the form

$$Q(\underline{x}) = \sum_{i=1}^{n} x_i^2 = \underline{x}^T\underline{x} = \rho^2$$

where $\rho = |\underline{x}|$. Figure 1 shows a 2-dimensional view of the parameter space, where the search is currently located at point A. $\underline{\Delta x}$, a typical random step of length s forms an angle θ with the negative-gradient direction AO. The random search method examines $Q(\underline{x}+\underline{\Delta x})$, and if $Q(\underline{x}+\underline{\Delta x}) < Q(\underline{x})$, the search moves to the point $\underline{x} + \underline{\Delta x}$. Otherwise the search remains at $\underline{x}$. The $(k+1)^{\underline{st}}$ step is described by

$$\underline{x}(k+1) = \underline{x}(k) + \delta(k)\ \underline{\Delta x}(k) \tag{1}$$

where

$$\delta(k) = \begin{cases} 1 & \text{if} \quad Q(\underline{x}+\underline{\Delta x}) < Q(\underline{x}) \\ 0 & \text{if} \quad Q(\underline{x}+\underline{\Delta x}) \geq Q(\underline{x}) \end{cases}$$

We consider two methods for choosing $\underline{\Delta x}$, each method assuming a certain amount of information concerning the direction in which $Q(\underline{x})$ decreases.

2.1. Optimum directional random search (ODRS).

It is first assumed that the search method has a large amount of directional information: it can control the distribution of the random steps such that each one is successful. Furthermore, it chooses the step length $s = |\underline{\Delta x}|$ so as to maximize the average progress toward the optimum. (The "optimum step size random search" (OSSRS) of Schumer & Steiglitz assumes no directional information, but does optimize the step size.) Thus, for "optimum direction random search" (ODRS) we consider the tip of the random vector $\underline{\Delta x}$ to be uniformly distributed over the spherical surface of an n-dimensional hypercone with vertex at $\underline{x}$, an axis of length s lying along the negative-gradient direction OA, and an aperture angle $\theta_o = \arccos(s/2\rho)$. The probability density function of the angle θ is then (see Appendix A)

$$f_\theta(\theta) = \frac{\sin^{n-2}\theta}{\int_0^{\theta_o} \sin^{n-2}\theta d\theta} \qquad 0 \leq \theta < \theta_o \tag{2}$$

$$\theta_o = \arccos(s/2\rho) \tag{3}$$

The normalized expected improvement in $Q(\underline{x})$ per step is defined as

$$I_\theta \equiv \frac{E\{-\Delta Q\}}{Q(\underline{x})} \tag{4}$$

where $E\{.\}$ denotes the expectation operation and, with reference to (1), $\Delta Q \equiv Q(\underline{x}(k+1))-Q(\underline{x}(k))$. ΔQ is negative for successful steps and zero for a failure. From Fig. 1, note that

$$-\Delta Q = \rho^2 - \rho'^2 \qquad \text{if} \quad \theta < \theta_o$$

$$= \begin{cases} 2\, s\rho \cos\theta - s^2 & \text{if } \theta < \theta_o \\ 0 & \text{if } \theta \geq \theta_o \end{cases} \tag{5}$$

With ODRS all steps are successful, and

$$E\{-\Delta Q\} = \int_0^{\theta_o} (2\, s\rho\cos\theta - s^2) f_\theta(\theta)\, d\theta \tag{6}$$

Substituting (2) and (6) in (4), we have

$$I_\theta(n,\eta) = \frac{2\eta \int_0^{\theta_o} \cos\theta \sin^{n-2}\theta\, d\theta}{\int_0^{\theta_o} \sin^{n-2}\theta\, d\theta} - \eta^2 \tag{7}$$

where $\eta = s/\rho$, the relative step length. In order to obtain the step length for a maximum normalized expected improvement per step, $I_\theta(\eta,\eta)$ is differentiated with respect to η, and the result is set equal to zero. This yields an equation in η_o, the optimum relative step length:

$$(n-1)\eta_o B^2(\eta_o) - \left(1-\frac{\eta_o^2}{4}\right)^{\frac{n-3}{2}} \left(1-n\frac{\eta_o^2}{4}\right) B(\eta_o) - \frac{\eta_o}{2}\left(1-\frac{\eta_o^2}{4}\right)^{n-2} = 0 \tag{8}$$

where $B(\eta_o) = \int_0^{\theta_o} \sin^{n-2}\theta\, d\theta$. Under the assumptions that n is large and that η_o is small for large n, $B(\eta_o)$ may be approximated by (see Appendix II of [2])

$$B(\eta_o) \approx \sqrt{\frac{\pi}{2n}} - \int_0^{\eta_o/2} \cos^{n-2}\theta \, d\theta$$

$$\approx \sqrt{\frac{\pi}{2n}} - \frac{\eta_o}{2} + \frac{n-2}{48}\eta_o^3 - \frac{(n-2)(n-3)}{1280}\eta_o^5 + \cdots \qquad (9)$$

Substituting (9) in (8) and writing the binomial series for the terms in (8), we obtain an equation of the following form for η_o.

$$\frac{a_o}{\sqrt{n}} + a_1\eta_o + a_2\sqrt{n}\,\eta_o^2 + \cdots + a_m\eta_o^m (n)^{\frac{m-1}{2}} + \cdots \approx 0 \qquad (10)$$

were the a_m's are constants. This equation provides the result that $\eta_o = \alpha/\sqrt{n}$, with α a constant to be determined. Direct solution of (10) was abandoned in favor of numerically maximizing $I_\theta(\eta_o,n) = I_\theta(\alpha/\sqrt{n},n)$ with respect to α (see Appendix B). The results are:

$$\eta_o \approx \frac{2.290}{\sqrt{n}} \qquad (11)$$

$$I_\theta = (\eta_o,n) = \frac{k_\theta}{n} \approx \frac{2.159}{n} \qquad (12)$$

Analogous results for OSSRS (where for notational purposes we denote by ϕ the angle between $\underline{x}$ and the negative gradient) are [2]

$$\eta_o \approx \frac{1.225}{\sqrt{n}} \qquad \text{(OSSRS)} \qquad (13)$$

$$I_\phi\ (\eta_o,n) = \frac{k_\theta}{n} \approx \frac{.406}{n} \qquad \text{(OSSRS)} \qquad (14)$$

It is noteworthy that, while the average improvement is greater for ODRS than for OSSRS, the assumption of directional information in ODRS has not changed the nature of the relationship between the average improvement and the number of parameters; it remains inversely proportionalto n.

2.2. Optimum half-space random search (OHSRS)

In ODRS a great amount of directional information is assumed to be known. In an effort to have a theoretical method which is slightly closer to a realizeable algorithm, we postulate a method in which all random steps lie in the half-space defined by the hyperplane tangent to $Q(\underline{x})$ at $\underline{x}$.

The tip of $\Delta\underline{x}$ is assumed to be uniformly distributed over the spherical surface of an n-dimensional half-hypersphere, which has radius s, center at $\underline{x}$, and a flat side defined by the aforementioned tangent plane.

For "optimum half-space random search" (OHSRS) the angle between $\Delta\underline{x}$ and the negative gradient is denoted by ψ, $0 \leq \psi \leq \pi/2$. The probability density function of ψ is (see Appendix A)

$$f_\psi(\psi) = \frac{\sin^{n-2}\psi}{\int_0^{\pi/2} \sin^{n-2}\psi d\psi} \qquad 0 \leq \psi \leq \pi/2 \tag{15}$$

For OHSRS the normalized expected improvement in $Q(\underline{x})$, denoted by $I_\psi(\eta,n)$, is defined as in (4) and (5). We have

$$E\{-\Delta Q\} = \int_0^{\pi/2} (-\Delta Q) f_\psi(\psi) d\psi$$

$$= \int_0^{\theta_o} (2s\rho\cos\psi - s^2) f_\psi(\psi) d\psi \tag{16}$$

Substitution of (15) and (16) in (4) yields

$$I_\psi(\eta,n) = \frac{\int_0^{\theta_o} (2\eta\cos\psi - \eta^2)\sin\psi d\psi}{\int_0^{\pi/2} \sin^{n-2}\psi d\psi} \tag{17}$$

$$= 2\, I_\theta(\eta,n)$$

where $I_\theta(\eta,n)$ is the average improvement obtained for OSSRS (see Eq. (7) of [2]). Thus, η_o is the same for OHSRS and OSSRS, and for OHSRS

$$I_\psi(\eta_o,n) = 2\, I_\theta(\eta_o,n)\, \frac{k_\psi}{n} \approx \frac{.812}{n} \tag{18}$$

Again, the expected improvement per step is inversely proportional to the number of parameters.

2.3. Comparison of OSSRS, ODRS and OHSRS

We now compare the number of evaluations of the quality function required by the three theoretical methods for minimization of $Q(\underline{x}) = \rho^2$. Let Q_o be the value of $Q(x)$ at the beginning of the search, and let the search be ended when an $\underline{x}$ is found such that $Q(\underline{x}) \leqslant Q_f$. Then under the assumptions that n is large and that the improvements at each step are independent, the number of steps M (and therefore the number of function evaluations) required to minimize $Q(\underline{x})$ is [2]

$$M \approx -\frac{1}{k} \ln \left(\frac{Q_f}{Q_o}\right) \cdot n \tag{19}$$

where

$$\frac{1}{k} = \begin{cases} \dfrac{1}{k_\phi} = 2.463 & \text{for OSSRS} \\ \dfrac{1}{k_\psi} = 1.213 & \text{for OHSRS} \\ \dfrac{1}{k_\theta} = 0.463 & \text{for ODRS} \end{cases} \tag{20}$$

From (20) we see that OHRS requires half as many function evaluations as OSSRS, and ODRS requires roughly one-fifth as many as OSSRS.

3. Adaptive directional random search (ADRS)

Matyas [3] has proposed a practical random search algorithm with adaptive direction and step size, which is used here in an attempt to realize (to a limited degree) the properties of ODRS or OHSRS. The algorithm, adaptive directional random search (ADRS), is described by (1), where $\underline{\Delta x}(k)$, $k = 1,2,\ldots,$ is determined by the following expressions ((21)-(27)):

$$\underline{\Delta x}(k) = \underline{d}(k) + b(k)\underline{z}(k) \tag{21}$$

$$\underline{d}(k) = c_o\underline{d}(k-1) + c_1\,\underline{\Delta x}(k-1) \tag{22}$$

with $\underline{\Delta x}(0) = 0$ and $\underline{d}(0) = \underline{0}$, and where for $\delta(k-1) = 1$ (last step a success)

$$c_o = c_{os};\ c_1 = c_{1s} \tag{23}$$

$$0 < c_{os} < 1;\quad c_{1s} > 0;\quad c_{os}+c_{1s} > 1 \tag{24}$$

and for $\delta(k-1) = 0$ (last step a failure)

$$c_o = c_{of};\quad c_1 = c_{1f} \tag{25}$$

$$0 < c_{of} < 1;\quad c_{1f} < 0;\ |c_{of} + c_{1f}| < 1 \tag{26}$$

Finally, $|\underline{d}(k)|$ is limited by

$$|\underline{d}(k)| < D\,b(k) \tag{27}$$

Should (22) result in a violation of (27), $\underline{d}(k)$ is normalized so that $|d(k)| = D\,b(k)$. $\underline{z}(k)$ is a random vector generated by selecting each component from a distribution uniform on $[-1, 1]$ and normalizing the resulting vector such that $|\underline{z}(k)| = 1$.

$b(k)$ and D are scalars. $\underline{d}(k)$, the mean value of $\underline{\Delta x}(k)$, is weighted positively by $\underline{d}(k-1)$ and is weighted in the direction of the last step following a success, or in the opposite direction following a failure. When successes occur in the same general direction, inequalities (24) tend to bias $\underline{\Delta x}$ in this direction and to increase $|\underline{\Delta x}|$. Following failures, inequalities (25) tend to remove directional bias and to decrease $|\underline{\Delta x}|$. The inequality (27) prevents $\underline{\Delta x}$ from being "overdetermined" by $\underline{d}$.

As values for c_{os}, c_{1s}, c_{of}, c_{1f}, $b(k)$ and D are not provided in [3], they were chosen on the basis of numerical experiments with $Q(\underline{x}) = \underline{x}^T\underline{x}$. The values selected are

$$\begin{aligned} c_{os} &= 0.75,\ c_{1s} = 1.25 \\ c_{of} &= 0.75,\ c_{1f} = -0.75 \\ D &= 3 \end{aligned} \tag{28}$$

b(k) is given an initial value and is multiplied by a factor of 1/10 following 20 consecutive unsuccessful steps. The complete algorithm is shown in Fig. 2. For the purpose of comparing results, we have chosen the basic structure of the flow diagram to be the same as that for the "adaptive step size random search" (ASSRS) of [2]

One more algorith, which we call "ordinary random search" (ORS), is constructed according to (1) and (21) with the restriction that $\underline{d}(k) \equiv \underline{0}$ for all k. It is also described by the flow diagram of Fig. 2. ORS does not adapt the search direction, and adapts the step size only in the sense that b(k) is reduced following 20 consecutive failures. It is used as a basis for judging the effectiveness of the adaptive algorithms ASSRS of [2] and ADRS.

4. Numerical results.

The algorithms ADRS and ORS were tested for several functions. Comparisons are made with results reported for ASSRS [2].

For $Q(\underline{x}) = \underline{x}^T\underline{x}$, 10 independent optimizations were performed for n = 5, 10, 15 and 20. The initial step size is b(0) = 0.1, the starting point is $\underline{x}(0) = (1,1,\dots,1)$, and the search is stopped when $Q(\underline{x}) < Q_{min} = 10^{-8}$. The results for ADRS, ORS and ASSRS are shown in Fig. 3. The numbers of function evaluations required by ORS and ADRS are approximately linear in n. This result for ORS is especially noteworthy, because this linear relationship has been predicted theoretically only for an algorithm with optimum step size. The directional adaptation of ADRS results in an improvement over ORS, and ORS is slightly more efficient than ASSRS. Apparently the adaptation of step size in ASSRS is costly in terms of function evaluations. From the experimental results it is possible to calculate approximate values of 1/k in (19):

	ADRS	ORS	ASSRS
1/k	2.63	3.60	3.67

These values, which are proportional to the number of function evaluations required to minimize $Q(\underline{x}) = \underline{x}^T\underline{x}$, may be compared with the values for the theoretical algorithms (20). The practical methods fall well short of the theoretical limits.

For the function

$$Q(\underline{x}) = \sum_{i=1}^{n} a_i x_i^2 \tag{29}$$

where the a_i's are random numbers chosen from a distribution uniform on [.1, 1], 10 independent trials were performed for n = 5, 10, 15 and 20. b(0) = 0.1, $\underline{x}(0) = (1,1,\dots,1)$ and $Q_{min} = Q(1,1,\dots,1)/1000$. The results, shown in Fig. 5, are qualitatively the same as for $Q(\underline{x}) = \underline{x}^T\underline{x}$, although the relative improvement of ADRS over ORS and ASSRS is greater here than for $Q(\underline{x}) = \underline{x}^T\underline{x}$. This might be expected, because the directional adaptation of ADRS should be helpful in moving along the valleys of (29).

Similar results were obtained for $Q(\underline{x}) = \sum_{i=1}^{n} x_i^4$ with 10 independent trials, b(0) = 0.1, $\underline{x}(0) = (1,1,\dots,1)$, and $Q_{min} = 0.5 \times 10^{-8}$. numbers of function evaluations are approximately described by 53 n for ASSRS [2], 51.n for ORS, and 32.n for ADRS.

ADRS was tested for Rosenbrock's function,

$$Q(\underline{x}) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2 \tag{30}$$

with $b(0) = 0.1$, $\underline{x}(0) = (-1.2,1)$, and $Q_{min} = 10^{-3}$.
Convergence was very slow. Multiplying the step size by a factor of 1/10 following 20 consecutive failures (Fig. 2) soon resulted in a very small step size. For a reducing factor of only 1/2 and with $D = 6$, 399 evaluations (average of four trials) were required for minimization. This is inferior to results for other "direct search" methods, such as pattern search, the simplex method, and Rosenbrock's method [5].

5. Conclusions

Two theoretical random search methods, optimum directional random search (ODRS) and optimum half-space random search (OHSRS), have been analyzed in an attempt to evaluate the improvement in performance resulting from the inclusion of directional information in a random search algorithms. Although the improvement is significant in comparison with a similar method without directional information (OSSRS [2]), the number of function evaluations required by ODRS and OHSRS to minimize $Q(\underline{x}) = \sum_{i=1}^{n} x_i^2$ remains a linear function of n.

The performances of three practical algorithms have been compared: adaptive directional random search (ADRS) based on [3], which attempts to adapt both step size and search direction to the function being minimized; adaptive step size random search (ASSRS [2]) which adapts only step size; and ordinary random search (ORS) which only reduces its step size following some number of consecutive failures. For the functions $Q(\underline{x}) = \sum_{i=1}^{n} x_i^2$, $Q(\underline{x}) = \sum_{i=1}^{n} a_i x_i^2$, and $Q(\underline{x}) = \sum_{i=1}^{n} x_i^4$, the number of function evaluations required for minimization is approximately linear in n for all three algorithms. ADRS requires about .74 times as many evaluations at ORS for $Q(\underline{x}) = \underline{x}^T\underline{x}$, and about 0.6 times as many as ORS for the other two functions. ORS performs slightly better than ASSRS for each function. These results suggest that spending an extra function evaluation at each step in order to adapt the step size (as in ASSRS) is not profitable. The strategy of ADRS, which attempts to step size and search direction only with information collected from past steps, is more successful. This follows the basic strategy of direct search algorithms: use every function evaluation to try to step immediately toward the minimum and collect information only from such steps.

The performance of ADRS on Rosenbrock's function indicates that the algorithm is still inferior to other direct search methods for functions with narrow, curving valleys. Random search algorithms appear to be most useful for rather "smooth" functions of many variables.

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APPENDIX A.

1. Probability density of θ.

The distribution of $\underline{\Delta x}$ is given in section 2.1.
Then the distribution function $F_\theta(\theta)$ of θ is

$$F_\theta(\theta) = \frac{S(\theta)}{S(\theta_o)} \tag{31}$$

where $S(\theta)$ is the area of the spherical surface of an n-dimensional cone with axis of length s and aperture angle θ. The probability density of θ is

$$f_\theta(\theta) = \frac{d}{d\theta} F_\theta(\theta)$$

$$= \frac{dS(\theta)}{d\theta} \quad \frac{1}{S(\theta_o)} \tag{32}$$

From [4] we have

$$\frac{dS(\theta)}{d\theta} = a_{n-1} \; (n-1)s^{n-1} \; \sin^{n-2}\theta \tag{33}$$

where

$$a_n = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2}+1)} \tag{34}$$

Integrating (33) to obtain $S(\theta_o)$ and substituting in (32), we obtain

$$f_\theta(\theta) = \frac{\sin^{n-2}\theta}{\int_0^{\theta_o} \sin^{n-2}\theta d\theta} \qquad 0 \leq \theta \leq \theta_o \tag{35}$$

2. Probability density of ψ.

The distribution of $\underline{\Delta x}$ is given in section 2.2.
Then the distribution function $F_\psi(\psi)$ of ψ is

$$F_\psi(\psi) = \frac{S(\psi)}{\frac{1}{2}S(\pi)} \tag{36}$$

where $S(\psi)$ is defined analogously to $S(\theta)$ above, and $S(\pi)$ is the surface area of an n-dimensional hypersphere.
Again using (32), we obtain

$$f_\psi(\psi) = \frac{\sin^{n-2}\psi}{\int_0^{\pi/2} \sin^{n-2}\psi d\psi} \qquad 0 \leq \psi \leq \pi/2 \tag{37}$$

APPENDIX B. Maximization of $I_\theta(\alpha/\sqrt{n},n)$ with respect to α.

In the numerator of the first term of (7) we have

$$\int_0^{\theta_o} \cos\theta \sin^{n-2}\theta d\theta = \frac{1}{n-1}\left(1 - \frac{\eta_o^2}{4}\right)^{\frac{n-1}{2}} \tag{38}$$

$$= \frac{1}{n-1}\left\{1 - \frac{\alpha^2}{8} + \frac{\alpha^4}{128} - \frac{\alpha^6}{2560} + \ldots\right\}$$

where we have expanded the binomial series with $\eta_o = \alpha/\sqrt{n}$. The denominator is approximated by (9) with $\eta_o = \alpha/\sqrt{n}$. Substitution of (9) and (38) in (7) yields for large n

$$n\ I_\theta(\alpha/\sqrt{n},n) = 2\alpha \frac{1 - \frac{\alpha^2}{8} + \frac{\alpha^4}{128} - \frac{\alpha^6}{1536} + \ldots}{\sqrt{\frac{\pi}{2}} - \frac{\alpha}{2} + \frac{\alpha^3}{48} - \frac{\alpha^5}{1280} + \ldots} - \alpha^2 \tag{39}$$

The sums in the numerator and denominator of (39) can be shown to be absolutely convergent for any α.

The maximum value of the right side of (39) was found numerically to be attained for $\alpha \approx 2.290$. This yields

$$\eta_o \approx \frac{2.290}{\sqrt{n}} \tag{40}$$

$$I_\theta(\eta_o,n) \approx \frac{2.159}{n} \tag{41}$$

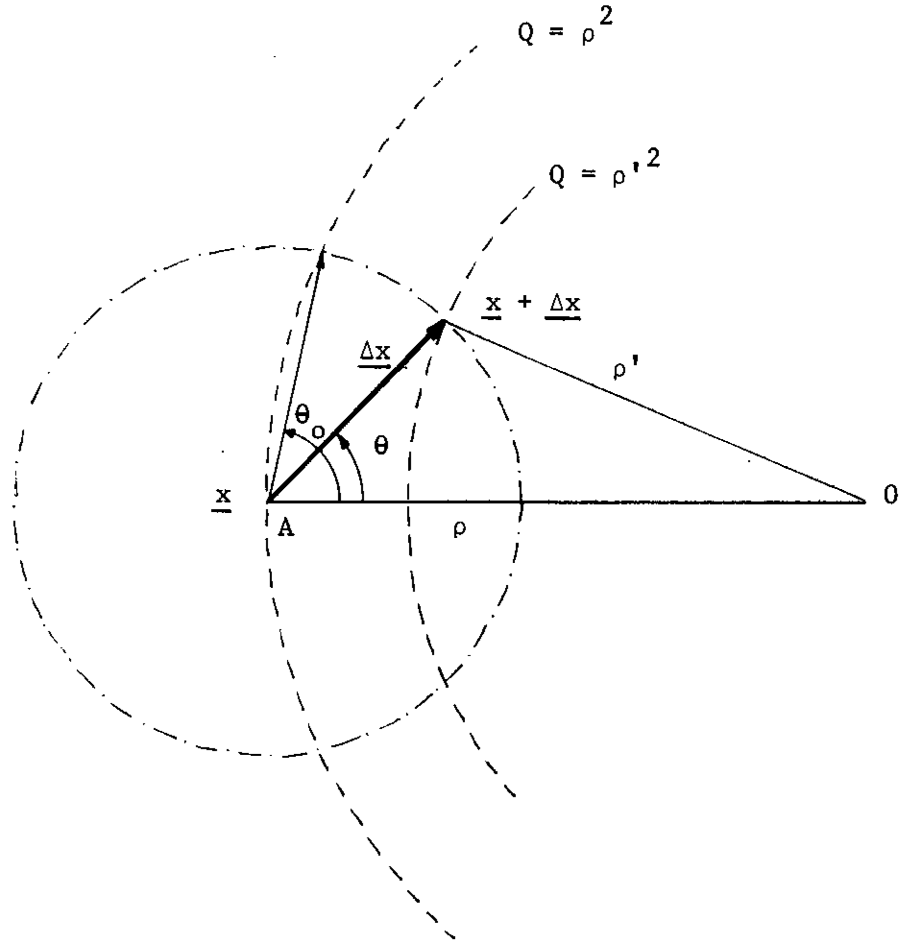

Fig. 1. A 2-dimensional view of the parameter space.

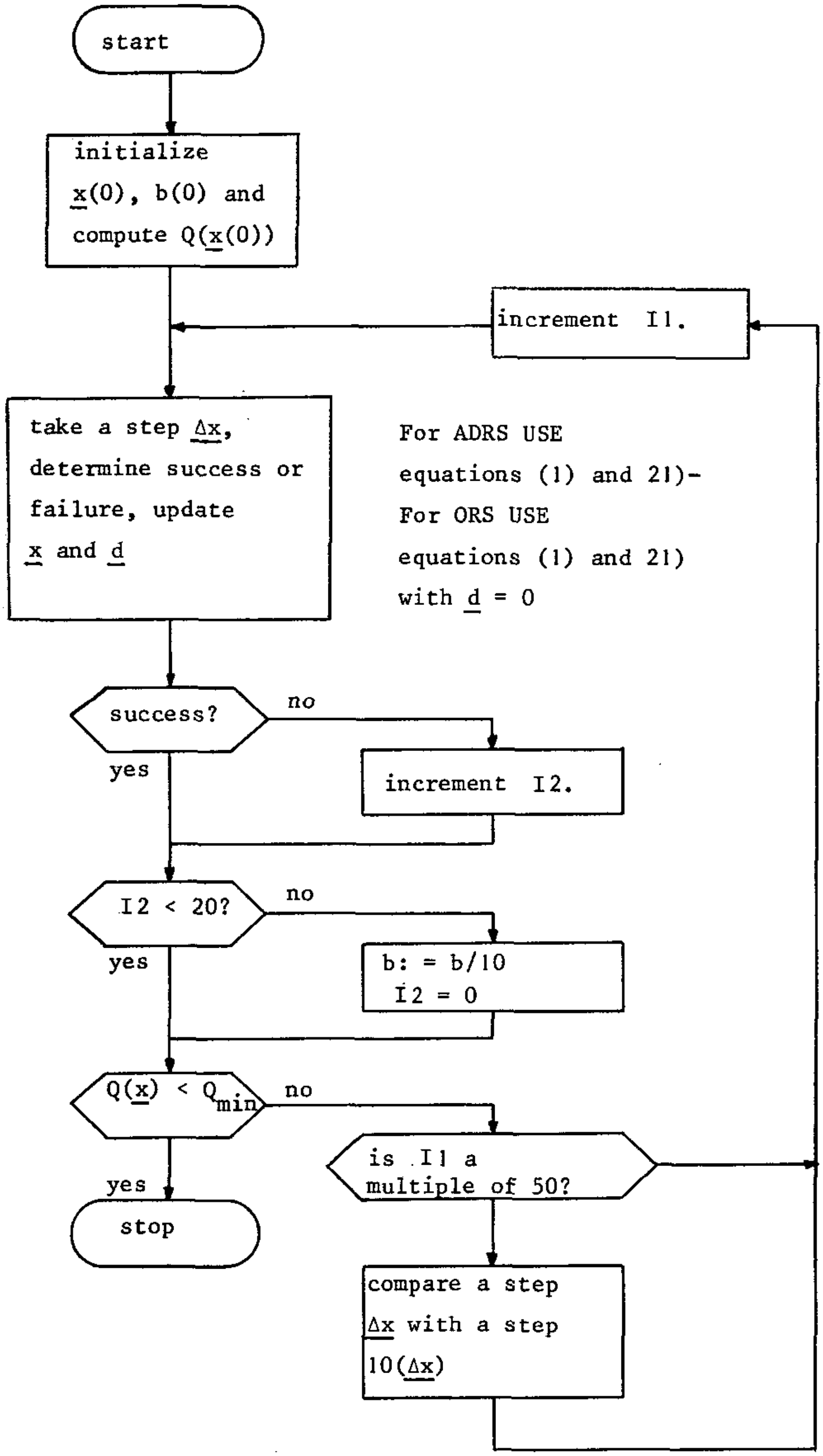

Fig. 2. Flow diagram for ADRS and ORS

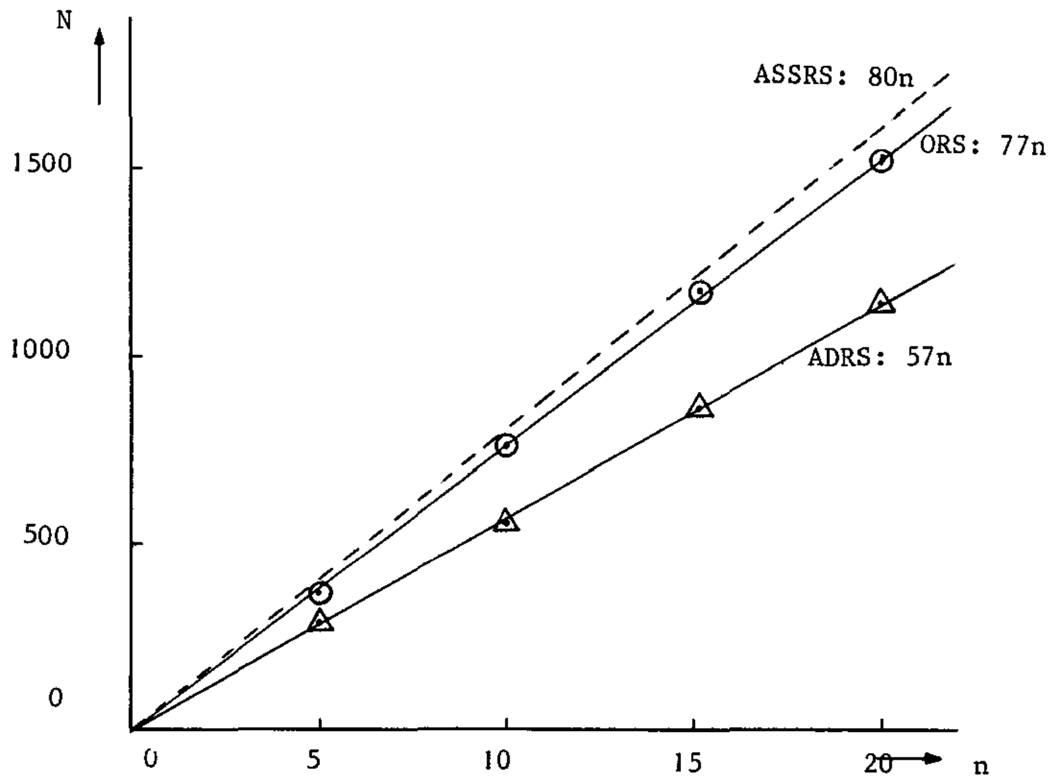

Fig. 3. Average number of function evaluations N vs. dimension n required by ASSRS, ORS and ADRS for $Q(\underline{x}) = \underline{x}^T\underline{x}$.

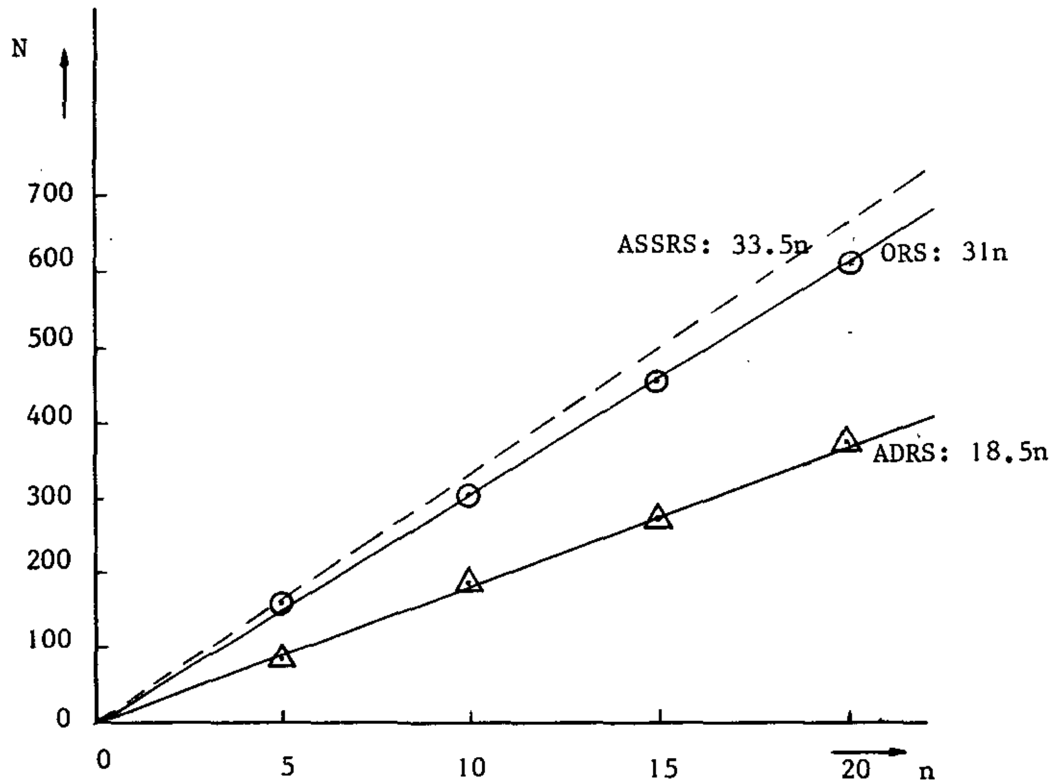

Fig. 4. Average number of function evaluations N vs. dimension n required by ASSRS, ORS and ADRS for $Q(\underline{x})=\sum_{i=1}^{n} a_i x_i^2$

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