A Simulation–Optimization Method: Its Convergence and Utility

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An optimization method is given for solving problems where a portion of the explicit mathematical form is unknown but can be evaluated. The solution scheme is an iterative process utilizing optimization and subsystem evaluation (such as via simulation). Conditions for the convergence of the iterative process are given. Several published application articles are noted as using this basic methodology. The method is superior to most other numerical optimization procedures. However, the class of problems for which the method is applicable is restricted to problems with enough known structure to generate a convergent iterative procedure. Three numerical examples are given and comparisons made with several other methods of optimizing unknown systems.

1. INTRODUCTION

Realistic problems are often encountered which require the optimization of a system for which the explicit mathematical formulation is either unknown or at least extremely complex. In certain instances, it is possible to develop mathematical and/or computer models of these systems. The development of these models often takes the form of a computer simulation model. The optimization of these modeled systems can require, however, an intolerable number of simulations or system evaluations. Some of these simulators are so complex that even a few evaluations can become cost prohibitive. This cost limitation for simulators is particularly apparent for policy optimization schemes which utilize numerical derivatives. As was pointed out by Smith [28], one normally must be satisfied, for such systems, with an improved but not necessarily optimal policy.

General, nonstructure-oriented, optimization procedures for unknown or simulated systems are available in the literature [1–3,15,16]. However, these improvement methods become costly even for a small number of variables and a coarse variable grid [27]. Holloway [14] assumed a convexity structure for his unknown system (the objective function and a set of constraints being known explicitly) and devised convergent optimization methods based on inner and outer linearization (numerical derivative approximations) of the unknown constraints. In a conceptually similar method, Heller and Staats [13] used linearized approximations to optimize systems not precisely known but which can be approximated by fitted response surfaces. Daughety and Turnquist [6] used spline functions for the response surface approximations. These methods, excluding Holloway's, do not take advantage of any known structure to

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reduce the number of system simulations required. Nolan and Sovereign [20], on the other hand, proposed a recursive linear programming–simulation scheme for the analysis of large-scale transportation system problems. The concepts of an iterative optimization–simulation scheme is not unique to their approach, having been proposed independently in at least three other articles [4,25,26]. These iterative algorithms utilize the known structure of the system, with certain relationships still being treated as unknown or simulated, to generate highly efficient (in terms of the number of simulations) policy improvement schemes. Farrell [7] gives a survey of simulation–optimization work up to 1977. Several of the references of his paper were omitted from his survey. Garcia-Diaz, Hogg, and Tari [8] compare several algorithms for machine inference problems.

There are two basic drawbacks to the general utility of the iterative optimization-simulation scheme. The method does not necessarily converge to the optimal solution, as was demonstrated for Simmons' application by Hartfiel and Curry [10]. The second complication, which is actually the most important consideration for complex systems, is that this scheme is not necessarily a convergent process. That is, the solution need not stabilize with an increasing number of iterations. There is, however, a restrictive class of problems which have the necessary convergent structure. Within this structure class, convergence generally occurs exceedingly quick, in ten simulations or less, and for highly complex problems the method seems to obtain a considerable degree of system cost improvement. Curry and Hartfiel [5] report the total iterative result, for an eight-variable inventory problem, costing \$0.20, while the optimal solution, starting from the iterative policy, required an additional \$100 of computer time. The optimal solution was only \$12, 3% of the total cost, better than the iterative solution.

The thrust of this article is to develop a convergence theory for a class of iterative optimization–simulation (subsystem evaluation) algorithms. Conditions that the mathematical structure of the unknown subsystem must satisfy for convergence are specified. The basic concept for the algorithm class is that the unknown subsystem can be evaluated (simulated) but derivatives for the subsystem are not obtainable. Numerical derivatives for the subsystem are not considered because of their excessive expense which can be due to a large number of variables and/or an inaccuracy in the evaluation necessitating a considerable number of repetitions for an acceptable gradient. Thus, the algorithm class is restricted to problems with enough known structure to generate a convergent iterative procedure requiring only one (or possibly a few) subsystem evaluations per iteration. In fact, the structure studied allows the decomposition of multiple-decision-variable problems into a series of much smaller problems. The interrelated effect of the subproblem variables enters the problem through the simulation measurements. Other studies of structural forms which lead to convergent iterative optimization–functional evaluation processes are those of Hartfiel and Curry [11,12]. In their 1977 paper [11], the structural form was different from that posed here; the 1981 paper [12] was concerned with an approximation method for forcing the iterative procedure to the global optimum. The numerical evaluation of the approximating Jacobian matrix of the unknown function (simulator) puts this method computationally in the class of the nonstructural optimization methods.

2. MATHEMATICAL STRUCTURE

Simulation models and mathematical submodels can both be thought of as mathematical mappings with complex relationships. Even if the exact functions are not

known explicitly, knowledge of the properties that these functions must satisfy is useful in the development of solution procedures for the associated problems.

The proposed solution method is basically a relaxation technique. The general procedure is based on constraint relaxation, parametric programming for multicriterion functions, and contraction mappings. However, it is not necessary to solve the general nonlinear parametric programming problem since the technique utilizes only selected values of the general solution functions. These values can be obtained by merely solving an associated numerical nonlinear problem.

Consider problem (P1) below. The problem as stated is not separable in the objective function but is separable in the constraints. It is the purpose of this article to develop an approximation solution for the problem and to demonstrate that the approximation problem's solution can be obtained by a decomposition procedure. Three ideas are basic to this method: relaxation, general parametric solutions, and contraction maps.

(P1)
$$\begin{aligned} &\text{minimize} && \sum_{i=1}^{N} \{g_i(\mathbf{x}) f_i^1(\mathbf{x}_i) + [1 - g_i(\mathbf{x})] f_i^2(\mathbf{x}_i)\}, \\ &\text{subject to} && \mathbf{h}_i(\mathbf{x}_i) \leq \mathbf{0} \quad \text{for } i = 1, \ldots, N, \\ & && \mathbf{0} \leq \mathbf{g}(\mathbf{x}) \leq \mathbf{1}, \end{aligned}$$

where $\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$, $\mathbf{h}_i$ is a vector function each component of which is convex, the feasible region $X = \{\mathbf{x} | \mathbf{h}_i(\mathbf{x}_i) < \mathbf{0} \text{ for all } i\}$ is nonempty and bounded, the functions f_i^1 and f_i^2 are strictly convex over X, and the functions g_i are continuous over X.

Problem (P1) can be restated as problem (P2) which is the form that will be addressed.

(P2)
$$\begin{aligned} &\text{minimize} && \sum_{i=1}^{N} \{y_i f_i^1(\mathbf{x}_i) + (1 - y_i) f_i^2(\mathbf{x}_i)\}, \\ &\text{subject to} && \mathbf{h}_i(\mathbf{x}_i) \leq \mathbf{0} \text{ for all } i, \\ & && \mathbf{0} \leq \mathbf{y} = \mathbf{g}(\mathbf{x}) \leq \mathbf{1}. \end{aligned}$$

Before proceeding, two basic lemmas from mathematical analysis are needed.

LEMMA 1: If f is a continuous mapping from X to Y and if g is a continuous mapping from Y to Z, then the mapping $f \circ g$ from X to Z is also continuous [30].

LEMMA 2: Let f be a continuous mapping of a compact convex subset X of R^n into itself. Then there is a point $\mathbf{x} \in X$ such that $f(\mathbf{x}) = \mathbf{x}$ [24].

To obtain a separable form of (P2), relaxation [17] is utilized for the equality constraints $\mathbf{y} = \mathbf{g}(\mathbf{x})$. Then each subproblem (P3) is a convex program since $0 \leq y_i \leq 1$ for all i.

(P3)
$$\begin{aligned} &\text{minimize} && y_i f_i^1(\mathbf{x}_i) + (1 - y_i) f_i^2(\mathbf{x}_i), \\ &\text{subject to} && \mathbf{h}_i(\mathbf{x}_i) \leq \mathbf{0}, \\ & && y_i \in [0,1]. \end{aligned}$$

Theorem 3 below establishes under certain assumptions the existence of a solution $(\mathbf{x}^*, \mathbf{y}^*)$ to (P2). However, the solution is not necessarily optimal. The parametric solution to subproblem (P3) is denoted by $\mathbf{x}_i^*(y_i)$, while the solutions of the total collection of these problems is denoted by $\mathbf{x}^*(\mathbf{y})$. Several additional restrictions need to be made on the functions of the problem:

(a) If $y_i \in [0,1]$ and $\mathbf{x}_i^*(y_i)$ is an optimal parametric solution to subproblem (P3), then the matrix whose rows are gradients $\nabla_{\mathbf{x}} h_i^j(\mathbf{x}_i)$, for j such that $h_i^j(\mathbf{x}_i) = 0$ is of maximal rank.

(b) $\mathbf{h}_i$, f_i^1, f_i^2 are analytical on some open region containing X.

(c) $\nabla \mathbf{h}_i$, ∇f_i^1, ∇f_i^2 are bounded on X.

THEOREM 3: (P3) has optimal solutions which can be expressed as continuous functions of y_i, $\mathbf{x}_i^*(y_i)$. Also there exists a feasible solution $[\mathbf{x}^*(\mathbf{y}^*), \mathbf{y}^*]$ to (P2).

PROOF: From Geoffrion [9] there exist unique optimal solutions $\mathbf{x}_i^*(y_i)$ to (P3) and the $\mathbf{x}_i^*(y_i)$ are continuous solutions. Thus, $[\mathbf{x}^*(\mathbf{y}), \mathbf{y}]$, where $\mathbf{y} = \mathbf{g} \circ \mathbf{x}^*(\mathbf{y})$, is feasible in (P2) if a solution to $\mathbf{y} = g(\mathbf{x}^*)$ exists. Since $\mathbf{x}^*$ is continuous and $\mathbf{g}$ is continuous then by Lemma 1 $\mathbf{g} \circ \mathbf{x}^*$ is a continuous function such that $\mathbf{g} \circ \mathbf{x}^* : S \to S$ where S, the domain of $\mathbf{y}$, is a compact convex set. Thus, by Lemma 2, a solution to $\mathbf{y} = \mathbf{g} \circ \mathbf{x}^*(\mathbf{y})$ exists. Q.E.D.

The characterization of the general form of the optimal parametric solutions to (P3) was given by Geoffrion [9]. Under the restrictions imposed on the functions, these characteristics are:

(a) $\mathbf{x}_i^*(y_i)$ is unique and continuous for $y_i \in [0,1]$,

(b) the solution $\mathbf{x}_i^*(y_i)$ consists of connected segments $\mathbf{x}_i^s(y_i)$ which are analytic over their range of validity, and

(c) the number of segments $\mathbf{x}_i^s(y_i)$, and hence the number of points of connection, is finite.

The optimal solutions $\mathbf{x}^*(\mathbf{y})$ of (P3) can be shown to satisfy a Lipschitz condition under the additional restrictions that gradients of the functions are bounded.

LEMMA 4: The optimal solution $\mathbf{x}_i^*(y_i)$ to subproblem (P3) satisfies a Lipschitz condition for $y_i \in [0,1]$; and $\nabla_{\mathbf{x}_i} f_i^2(\mathbf{x}_i)$, and $\nabla_{\mathbf{x}_i} \mathbf{h}_i(\mathbf{x}_i)$ are bounded.

PROOF: Let $\mathbf{x}_i^s(y_i)$ be the segment of $\mathbf{x}_i^*(y_i)$ which is optimal when the constraints indexed by s are strict equalities and all other constraints are inequalities. By Geoffrion [9], $\mathbf{x}_i^s(y_i)$ is analytic. Thus, by definition $\mathbf{x}_i^s(y_i)$ has a continuous derivative with respect to y_i.

Since $\mathbf{x}_i^*(y_i) = \mathbf{x}_i^s(y_i)$ for the range of y_i where the index s remains valid, $\mathbf{x}_i^*(y_i)$ is analytic except possibly at the points of y_i where s changes. However, by Geoffrion [9], there are only a finite number of points of change on $[0,1]$. Hence, $\mathbf{x}_i^*$ is analytic a.e. (almost everywhere).

Since $\mathbf{x}_i^s$ is analytic on each region of $[0,1]$ where s remains constant, then $d[\mathbf{x}_i^s(y_i)]/dy_i$ is bounded there. Thus, $d[\mathbf{x}_i^*(y_i)]/dy_i$ is bounded except possibly at the points of change. Therefore,

$$\left| \frac{d[\mathbf{x}_i^*(y_i)]}{dy_i} \right| \leq \alpha_i < \infty \quad \text{a.e.}$$

By the Lebesque theorem [22], $d[\mathbf{x}_i^*(y_i)]/dy_i$ is Riemann integrable, since it is a bounded function on [0,1] and the set of discontinuities has measure zero. Furthermore, $d[\mathbf{x}_i^*(y_i)]/dy_i$ is measurable and Lebesque integrable by Proposition 4 [22], which states that a bounded function over a closed and bounded region which is Riemann integrable is measurable and Lebesque integrable.

Since

$$\mathbf{x}_i^*(y_i) = \int_0^{y_i} \frac{d[\mathbf{x}_i^*(z)]}{dz} \, dz + \mathbf{x}_i^*(0),$$

and hence by theorem 13 [22] $\mathbf{x}_i^*$ is absolutely continuous.

From [29] a function which is absolutely continuous and has a derivative a.e., such that the derivative is bounded, satisfies a Lipschitz condition. Therefore,

$$\|\mathbf{x}_i^*(y_i^1) - \mathbf{x}_i^*(y_i^2)\| \leq \alpha_i \|y_i^1 - y_i^2\| \text{ for all } i.$$

Hence,

$$\|\mathbf{x}^*(\mathbf{y}^1) - \mathbf{x}^*(\mathbf{y}^2)\| \leq \alpha \|\mathbf{y}^1 - \mathbf{y}^2\|. \qquad \text{Q.E.D.}$$

LEMMA 5: If the relaxed constraints $\mathbf{g}(\mathbf{x})$ satisfy a Lipschitz condition with a constant of β, then the composition function $\mathbf{g} \circ \mathbf{x}^*$ satisfies a Lipschitz condition with a constant $\alpha\beta$.

PROOF: By Lemma 4 and the assumption on $\mathbf{g}(\mathbf{x})$,

$$\|\mathbf{x}^*(\mathbf{y}^1) - \mathbf{x}^*(\mathbf{y}^2)\| \leq \alpha_i \|\mathbf{y}^1 - \mathbf{y}^2\|,$$
$$\|\mathbf{g}(\mathbf{x}^1) - \mathbf{g}(\mathbf{x}^2)\| \leq \beta \|\mathbf{x}^1 - \mathbf{x}^2\|.$$

$$\begin{aligned} \|\mathbf{g} \circ \mathbf{x}^*(\mathbf{y}^1) - \mathbf{g} \circ \mathbf{x}^*(\mathbf{y}^2)\| &= \|\mathbf{g}[\mathbf{x}^*(\mathbf{y}^1)] - \mathbf{g}[\mathbf{x}^*(\mathbf{y}^2)]\| \\ &\leq \beta \|\mathbf{x}^*(\mathbf{y}^1) - \mathbf{x}^*(\mathbf{y}^2)\| \leq \alpha\beta \|\mathbf{y}^1 - \mathbf{y}^2\|. \end{aligned}$$

Therefore $\mathbf{g} \circ \mathbf{x}^*$ satisfies a Lipschitz condition with constant $\alpha\beta$. Q.E.D.

The framework has now been established for the development of a solution procedure for (P2). The method consists of three steps and the proof of convergence of the method is given in Theorem 6 below. Again it should be emphasized that the procedure converges to the solution $\mathbf{x}^*(\mathbf{y})$ of problem (P4):

(P4)

$$\begin{aligned} \text{minimize} \quad & \sum_{i=1}^{N} \{y_i f_i^1(\mathbf{x}_i) + (1 - y_i) f_i^2(\mathbf{x}_i)\}, \\ \text{subject to} \quad & \mathbf{h}_i(\mathbf{x}_i) \leq \mathbf{0} \quad \text{for all } i, \\ & \mathbf{g}[\mathbf{x}^*(\mathbf{y})] = \mathbf{y}. \end{aligned}$$

The solution $[\mathbf{x}^*(\mathbf{y}^*), \mathbf{y}^*]$ to this problem is of course feasible for (P2) but it need not be the optimal solution.

Iterative Procedure

STEP 0. Set $k = 1$ and select an initial $\mathbf{y}^k$ such that $y_i^k \in (0,1)$ for all i and establish an ϵ convergence tolerance.

STEP 1. Solve subproblem (P3) for the optimal solutions $\mathbf{x}_k^*$ where $\mathbf{y}^k$ is a specified numerical vector and k designates the iteration number.

STEP 2. Obtain $\mathbf{y}^{k+1} = \mathbf{g}(\mathbf{x}_k^*)$; if $\|\mathbf{y}^{k+1} - \mathbf{y}^k\| \leq \epsilon$ convergence has occurred, otherwise set $k = k + 1$ and repeat Steps 1 and 2.

THEOREM 6: The iterative procedure converges to the unique solution of (P4), if the product $\mathbf{g} \circ \mathbf{x}^*$ is contractive.

PROOF: By Theorem 3 a solution to (P4) exists since (P4) is merely the explicit statement of a solution pair $[\mathbf{x}^*(\mathbf{y}^*), \mathbf{y}^*]$ that is feasible for (P2). Since $\mathbf{g} \circ \mathbf{x}^*$ is contractive, $\alpha\beta < 1$, then by the Banach fixed-point theorem [23, p. 54] there exists a unique solution $\mathbf{y}^*$ to $\mathbf{g} \circ \mathbf{x}^*(\mathbf{y}) = \mathbf{y}$ and the sequence $\{\mathbf{y}^k\} \to \mathbf{y}^*$, where $\mathbf{y}^{k+1} = \mathbf{g}(\mathbf{x}_k^*)$. Since $\mathbf{x}^*(\mathbf{y}^*)$ are optimal solutions to subproblem (P3) which satisfy the relaxed constraints $\mathbf{y} = \mathbf{g}(\mathbf{x})$, then $[\mathbf{x}^*(\mathbf{y}^*), \mathbf{y}^*]$ solves (P4). Q.E.D.

3. EXAMPLES

Three examples of the procedure and comparisons with other optimization methods follow. In the first example, a known system of equations is utilized as the "simulation" model so that the mathematical structure underlying the convergence property can be emphasized. The remaining examples are multiple-product joint-order inventory systems with different numbers of products. For these problems, a production system [4], using actual daily product demand sequences, was used as the simulation component.

EXAMPLE 1

Consider solving the following problem:

$$\begin{aligned}
\text{minimize} \quad & y_1(x_1 - 1)^2 + (1 - y_1)(x_1 - 2)^2 \\
& + y_2(x_2 - 0)^2 + (1 - y_2)(x_2 - 4)^2 \\
& + y_3(x_3 - 3)^2 + (1 - y_3)(x_3 - 6)^2, \\
\text{subject to} \quad & 1 \leq x_1 \leq 2, \\
& 0 \leq x_2 \leq 4, \\
& 3 \leq x_3 \leq 6, \\
& \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{10} & \frac{1}{20} & \frac{1}{12} \\ \frac{1}{8} & \frac{1}{12} & \frac{1}{18} \\ \frac{1}{10} & \frac{1}{20} & \frac{1}{10} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.
\end{aligned}$$

Relaxing the equality constraints of the form $\mathbf{y} = \mathbf{Ax}$ and solving the remaining system for the parametric solution, denoting the upper and lower bounds on x_i by b_i and a_i, respectively, then

$$\mathbf{x}_i^*(y_i) = b_i + (a_i - b_i)y_i \qquad \forall i.$$

Obtaining the composition functions

$$\mathbf{y} = \mathbf{g} \circ \mathbf{x}^*(\mathbf{y}) = \mathbf{A} \cdot [\mathbf{b} + (\mathbf{a} - \mathbf{b})\mathbf{y}],$$
$$\mathbf{y} = \mathbf{By} + \mathbf{d},$$

with

$$\mathbf{B} = \begin{bmatrix} -\frac{1}{10} & -\frac{1}{5} & -\frac{1}{4} \\ -\frac{1}{8} & -\frac{1}{3} & -\frac{1}{6} \\ -\frac{1}{10} & -\frac{1}{5} & -\frac{3}{10} \end{bmatrix} \text{ and } \mathbf{d} = \begin{bmatrix} 0.9 \\ 0.917 \\ 1.0 \end{bmatrix}.$$

This system of equations has a solution and can be solved by the iterative procedure [18]. Starting with $\mathbf{y}^1 = (1,1,1)$, after 20 iterations the answer is

$$\mathbf{x}^* = \begin{bmatrix} 1.427 \\ 1.784 \\ 4.080 \end{bmatrix}, \qquad \mathbf{y}^* = \begin{bmatrix} 0.572 \\ 0.554 \\ 0.640 \end{bmatrix},$$

with the objective function value of 6.272. The convergence criterion used was a change of 0.0001 units in the objective function value. The true optimal solution to this problem is $\mathbf{x}^* = (1.602, 1.795, 4.148)$ with an objective function value of 6.216. The iterative solution value is within 0.9% of the optimal value.

For comparison purposes, two nonadaptive search techniques [27] and an adaptive search method [19] are employed to optimize this system. The results of these investigations are:

(i) the factorial design method yielded results (two different setups) which are 0.02 and 0.10% better than the iterative method at a cost of 1331 function evaluations (a 63.4-fold increase),

(ii) the random search method yielded a 0.66% improvement over the iterative method at a cost of 1000 function evaluations (a 50-fold increase), and

(iii) an adaptive search method, the flexible polyhedron search [19] improved the required function evaluations to 86 and 77 for two separate runs but yielded results 1.60 and 6.1% higher than the iterative method.

EXAMPLE 2

An iterative algorithm was presented by Simmons [26] for a multiproduct continuously reviewed inventory system with joint replenishment of all products to be ordered in a scheduling period. The replenishment cost consists of a constant plus a variable cost for each product ordered. A simulation model of this process for the two-product case with backlogging of orders was developed, and several optimization

procedures compared with the contractive mapping method. The results are displayed in Figure 1.

The methods compared are (i) factoral design, (ii) random search over selected points on a factorial design grid, (iii) cyclic iterations through one-dimensional coordinate axes searches, (iv) nonderivative conjugate direction search method [21], (v) flexible polyhedron search [19], and (vi) iterative solution procedure. As is evident from Figure 1, the iterative procedure converges to its best solution in a very small number of iterations (five or less), while none of the other methods approach this cost region in less than 50 simulation evaluations.

EXAMPLE 3

A multiproduct inventory system operating under a joint replenishment policy was solved by the iterative procedure by Curry, Skeith, and Harper [4]. The reordering policy, called a can-order policy, operates as follows: A product reaches its reorder point; all other products which are below their respective can-order inventory levels are also ordered. The ordering cost is a fixed cost plus an individual cost per product replenished. A simulation model of this process for a four-product system was developed. The random factorial design, cyclic coordinate, Powell's method [21], Nelder–Mead [19], and iterative search procedures were all used to find the decision parameter values. Figure 2 illustrates that the iterative contractive mapping procedure converges much faster than the other methods. For this problem, Powell's method required 130 simulation evaluations, and the Nelder–Mead method 450 simulations to reach essen-

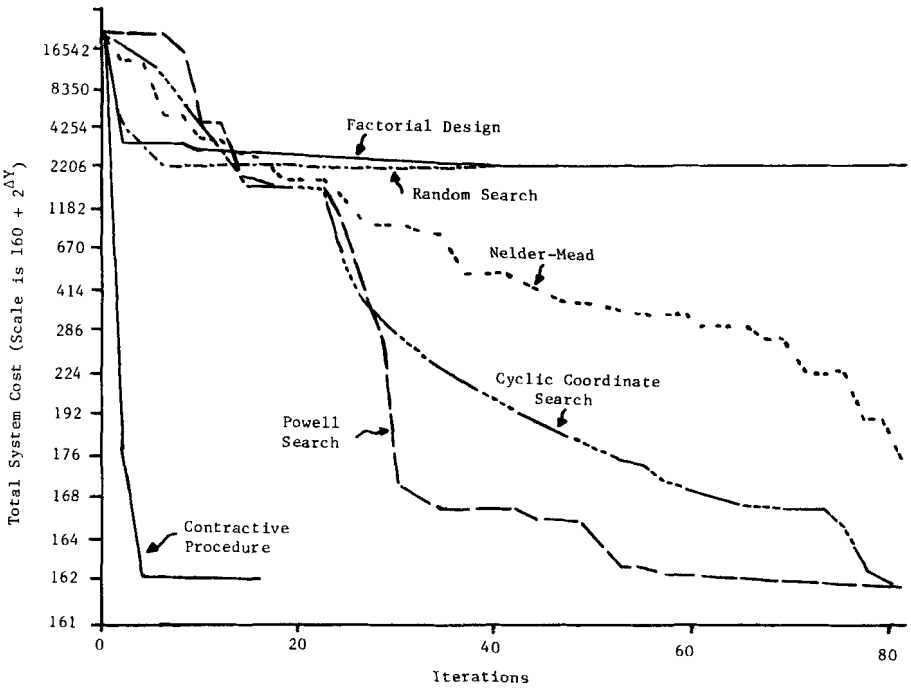

Figure 1. Solution algorithm comparisons for a two-product inventory problem with a random joint replenishment policy.

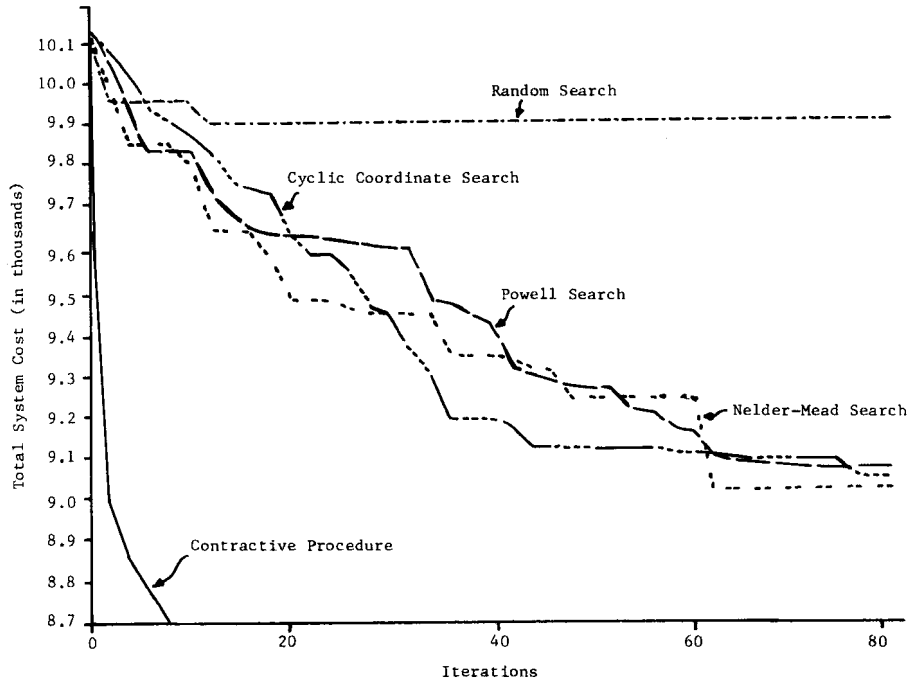

Figure 2. Solution algorithm comparisons for a four-product inventory problem with a can-order replenishment policy.

tially the same system cost as the iterative procedure obtained in six simulation evaluations.

4. SUMMARY

The optimization of complex problems that require simulation or a subsystem evaluation can be an expensive process. The number of functional evaluations required sometimes can be reduced significantly by the development of an iterative optimization–simulation procedure. This method in general will not yield the optimal solution. However, the savings in computational effort sometimes greatly overshadows the loss in optimization refinement. The method's main limitation is the restrictive class of problems for which the iterative optimization–simulation scheme is contractive. This method has been applied with good utility to a class of practical inventory problems of the joint setup cost type.

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