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SHORT COMMUNICATION

Global Optimization Methods for Chemical Process Design: Deterministic and Stochastic Approaches

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Abstract–Process optimization often leads to nonconvex nonlinear programming problems, which may have multiple local optima. There are two major approaches to the identification of the global optimum: deterministic approach and stochastic approach. Algorithms based on the deterministic approach guarantee the global optimality of the obtained solution, but are usually applicable to small problems only. Algorithms based on the stochastic approach, which do not guarantee the global optimality, are applicable to large problems, but inefficient when nonlinear equality constraints are involved. This paper reviews representative deterministic and stochastic global optimization algorithms in order to evaluate their applicability to process design problems, which are generally large, and have many nonlinear equality constraints. Finally, modified stochastic methods are investigated, which use a deterministic local algorithm and a stochastic global algorithm together to be suitable for such problems.

Key words: Global Optimization, Deterministic, Stochastic Approach, Nonconvex, Nonlinear Program

INTRODUCTION

Many chemical process optimization problems can be represented by nonlinear programming (NLP) problems in the following form:

$$\min f(\mathbf{x}) \qquad (P)$$

subject to

$$\mathbf{g}(\mathbf{x}) \le \mathbf{0}$$
$$\mathbf{h}(\mathbf{x}) = \mathbf{0}$$

where $\mathbf{x} \in R^n$, f: $R^n \rightarrow R$, $\mathbf{g}$: $R^n \rightarrow R^l$, $\mathbf{h}$: $R^n \rightarrow R^m$, and n>m. If the objective function and the feasible region are convex, e.g., when f and $\mathbf{g}$ are convex and $\mathbf{h}$ is linear, the problem is called a convex problem, which has only one local minimum that is the global minimum. Most of chemical process optimization problems, however, have a nonconvex feasible region because of nonlinear equality constraints. Therefore, they are nonconvex, and in many cases, have multiple local optima. Furthermore, the size of the problem is generally large. The objective of this study is to find a global optimization algorithm suitable for nonconvex problems which involve a large number of highly nonlinear equations such as obtained from rigorous models of chemical processes.

Most global optimization algorithms belong to one of the two categories: (1) deterministic approach and (2) stochastic approach. Algorithms based on the deterministic approach such as cutting plane [Horst and Tuy, 1993], generalized Benders decomposition [Geoffrion, 1972; Floudas and Visweswaran, 1990; Bagajewicz and Manousiouthakis, 1991], branch and bound [Soland, 1971; Ryoo and Sahinidis, 1995; Adjiman et al., 1996], and interval analysis [Ratschek and Rokne, 1988; Vaidyanathan and El-Halwagi, 1994; Han et al., 1997] guarantee finite ε-convergence (convergence to the global optimum in finite computation steps for a given finite error tolerance) and global optimality of the obtained solution. Algorithms based on the stochastic approach such as simulated annealing [Kirkpatrick et al., 1983] and genetic algorithm [Goldberg, 1989] aim at high probability of finding the global optimum, not guaranteeing the finite ε-convergence or the global optimality of the obtained solution.

METHODOLOGY

The goal of global optimization is achieved if a method is developed which is guaranteed to do one of the following three tasks.

1. Find a Tight Convex Hull

Assume that we have an NLP in which the objective function is linear. Note that any problem can be reformulated to this type of problem by replacing the objective function by a substitution vari-

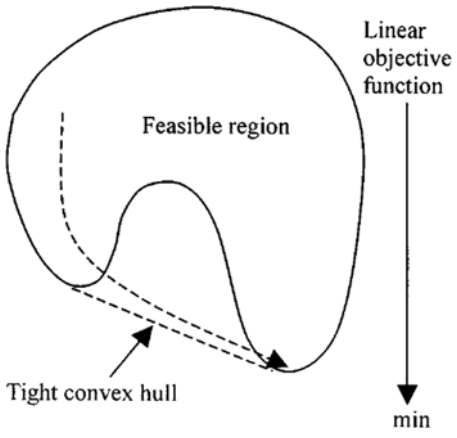

Fig. 1. Convex hull strategy.

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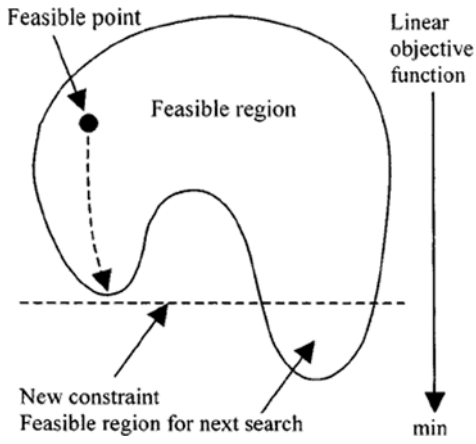

Fig. 2. Feasible point strategy [Choi et al., 1999].

able and declaring its definition equation as a constraint. Now consider a new problem in which the constraints form a tight convex hull for the feasible region of the original problem as shown in Fig. 1. This is a convex problem which can easily be solved by a local optimization technique and whose solution is equivalent to the global solution of the original problem. This is the basic idea of most of the deterministic algorithms.

2. Find a Feasible Point

Assume that we have a method that is guaranteed to find a feasible point if any exists. Given a feasible point, a local optimizer using the generalized reduced gradient method can find a local minimum. We can then add a new constraint that forces the objective function value to be lower than the current local minimum, and search for a new feasible point. This procedure can be repeated until no feasible point exists. Fig. 2 schematically describes this strategy. In order to implement this strategy, we need a global algorithm for finding feasible points and a local algorithm for finding local minima. A stochastic method that uses this strategy is described in this paper.

3. Find All Kuhn-Tucker Points

If a method is available which is guaranteed to find all real roots of systems of nonlinear algebraic equations, the objective function values at all Kuhn-Tucker points can be compared to each other to find the global optimum. This approach is out of the scope of this paper.

DETERMINISTIC APPROACH

The deterministic approach to global optimization of chemical processes has actively been studied since the 1980's, and some history was summarized by Han et al. [1997]. However, since the global optimization of a nonconvex NLP problem is one of the toughest NP-hard problems, the deterministic algorithms that are currently available can usually be applied to small problems only. Detailed discussion of the NP-hardness was presented by Choi et al. [1999].

1. Outer Approximation

A convex hull of a feasible region can be constructed by a set of linear inequality constraints. For example, Horst and Tuy [1993] defined a concavity cut for a region K\G formed by a polyhedral

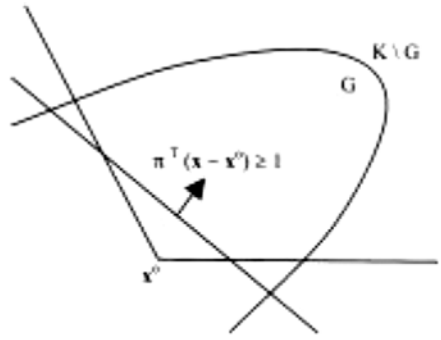

Fig. 3. (G, K)-cut [Horst and Tuy, 1993].

cone K with vertex x^0 and a reverse convex constraint $x \notin \text{int } G$ as shown in Fig. 3. The cut by a new linear inequality constraint excludes some region around the infeasible point x^0 but not any feasible point. However, a big disadvantage of this approach is that the number of constraints increases as the algorithm converges to a tight convex hull, and thus constraint dropping strategies are required as indicated by Horst and Tuy [1993].

Note that any continuous function defined on a finite closed convex domain can be represented by a difference of two convex (d.c.) functions. All we have to do is add and subtract a sufficiently convex function. The cutting plane methods are applicable to d.c. problems where all functions are d.c. on a given convex set [Horst and Tuy, 1993]. However, in general, these methods are suitable only for low rank nonconvex problems, in which only a few of the variables are responsible for the nonconvexity of the problem [Konno et al., 1997].

2. Generalized Benders Decomposition

Consider the following type of problem:

$$\min_{x,y} f(\mathbf{x}, \mathbf{y})$$

subject to

$$\mathbf{g}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0}$$

where f and **g** are convex with respect to **x**, i.e., when **y** is constant, the problem is convex. This problem can be decomposed into two problems as follows.

Primal:

$$\min_{x} f(\mathbf{x}, \mathbf{y})$$

subject to

$$\mathbf{g}(\mathbf{x}, \mathbf{y}) \leq \mathbf{0}$$

where **y** is fixed at a given point. This problem can easily be solved because it is convex. The solution is an upper bound of the global minimum because the feasible region has been narrowed.

Master:

$$\min_{y} y_0$$

subject to

$$L^*(\mathbf{y}; \mathbf{u}) = \min_{x} [f(\mathbf{x}, \mathbf{y}) + \mathbf{u}^T \mathbf{g}(\mathbf{x}, \mathbf{y})] \leq y_0$$
$$\text{for all } \mathbf{u} \geq \mathbf{0}$$

$$L_*(\mathbf{y}; \mathbf{v}) = \min_{\mathbf{x}} \mathbf{v}^T \mathbf{g}(\mathbf{x}, \mathbf{y}) \le 0$$
$$\text{for all } \mathbf{v} \in \{\mathbf{v} | \mathbf{v} \ge \mathbf{0}, \sum_i v_i = 1\}$$

For subsets of **u** and **v**, the solution to this problem is a lower bound for the global minimum.

This technique is useful when **x** and **y** are separable, because the solution **x** and the Lagrange multipliers **u** obtained from the primal can directly be used in the first set of constraints in the master, in which the minimization with respect to **x** is unnecessary.

If the primal is infeasible at a given point **y**, an infeasibility minimization problem can be solved such as the following.

$$\min_{\mathbf{x}} \alpha$$

subject to

$$\mathbf{g}(\mathbf{x}, \mathbf{y}) \le \alpha \mathbf{1}$$

where $\mathbf{1}=[1 \ \dots \ 1]^T$. The solution **x** and the Lagrange multipliers **v** obtained from this problem can be used to construct the second set of constraints in the master, in which the minimization with respect to **x** is again unnecessary.

The algorithm iterates between the primal and the master until the upper and lower bounds converge together. Like outer approximation, this technique also needs constraint dropping strategies, and is suitable for low rank nonconvex problems only.

3. Branch and Bound

This is the most widely used technique for global optimization of various problems. Let us consider the following type of problem.

$$\min f(\mathbf{x})$$

subject to

$$\mathbf{g}(\mathbf{x}) \le \mathbf{0}$$
$$\mathbf{A}\,\mathbf{x} = \mathbf{c}$$

where **A** and **c** are constant matrix and vector respectively.

The algorithm starts from relaxation of the above problem into a convex problem over an initial box $\mathbf{a} \le \mathbf{x} \le \mathbf{b}$. Let us replace the objective function $f(\mathbf{x})$ by a convex envelope such as shown by dashed curves in Fig. 4. A convex hull of the feasible region can be obtained by replacing all nonconvex functions $g_i(\mathbf{x})$ by their convex envelopes. The relaxed problem is now convex, and thus its local solution is guaranteed to be the global minimum. Furthermore, as this is the solution to a relaxed problem, it is a lower bound for the global minimum of the original problem.

The box is subsequently split into parts (branching). The solution to each subproblem is a lower bound in its region. The lowest one of these is the lower bound for the global minimum of the original problem. If a solution satisfies the original constraints as well, the value of the original objective function at that point is an upper bound. The lowest upper bound is stored as a candidate for the global minimum. Meanwhile, every subproblem is discarded if it is infeasible or its solution is higher than the upper bound (bounding). The algorithm stops when the lower bound converges to the upper bound.

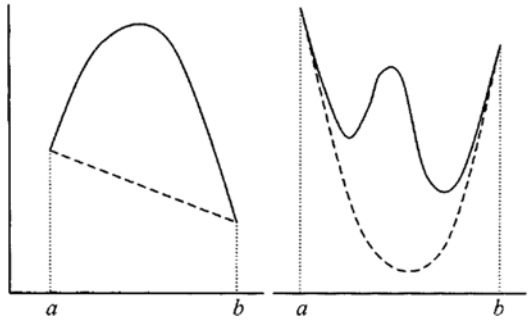

Fig. 4. Convex envelopes.

The efficiency of the branch and bound algorithm mainly depends on the tightness of the convex envelopes. The most commonly used convex envelopes, which are also called underestimators, can be classified as follows.

3-1. Linear Underestimators

A reverse convex term in a separable function $\phi(\mathbf{x})=\sum_j \phi_j(x_j)$ can be replaced by a linear underestimator. For example, if $\phi_j(x_j)=-x_j^2$, $a_j \le x_j \le b_j$, the tightest convex envelope is the following linear function.

$$\psi_j(x_j) = -(a_j+b_j)\,x_j + a_j b_j$$

Note that this approach can be applied to separable problems only. However, any problem can be converted to a separable problem because a nonseparable term $x_1 x_2$ can be replaced by a separable function $w_1^2 - w_2^2$ where w_1 and w_2 are defined by the following linear equality constraints.

$$w_1 = (x_1 + x_2)/2$$
$$w_2 = (x_1 - x_2)/2$$

3-2. Quadratic Underestimators

For general functions, quadratic underestimators can be used as proposed by Adjiman et al. [1996]. For a nonconvex function $\phi(\mathbf{x})$, $\mathbf{a} \le \mathbf{x} \le \mathbf{b}$, a convex envelope can be defined as follows.

$$\psi(\mathbf{x}) = \phi(\mathbf{x}) + \sum_j \alpha_j (x_j - a_j)(x_j - b_j)$$
$$\alpha_j \ge \max\{0, -0.5 \min_k [\mathbf{H}(\phi(\mathbf{x}))]\}$$

where λ_k (k=1, …, n) are the eigenvalues of the Hessian matrix **H**. A problem in this approach is that determination of tight α_j is again a nonconvex optimization problem unless **H** is constant.

4. Interval Analysis

Convex envelopes and hulls can also be obtained by interval analysis based on the following arithmetic.

$$[a, b] + [c, d] = [a+c, b+d]$$
$$[a, b] - [c, d] = [a-d, b-c]$$
$$[a, b] \times [c, d] = [\min(ac, ad, bc, bd), \max(ac, ad, bc, bd)]$$
$$[a, b] / [c, d] = [\min(a/c, a/d, b/c, b/d), \max(a/c, a/d, b/c, b/d)] \text{ if } 0 \notin [c, d]$$

Unlike the case of linear or quadratic underestimators, the branch and bound algorithm can directly be applied to problem (P). Let us start from an interval box X of variables **x**. For any $X^k \subset X$, if lb $\mathbf{g}(X^k) > \mathbf{0}$ or lb $\mathbf{h}(X^k) > \mathbf{0}$ or ub $\mathbf{h}(X^k) < \mathbf{0}$, then the box X^k is infeasible. The box X^k can also be discarded if lb $f(X^k) > f(\mathbf{x}^\circ)$ where $\mathbf{x}^\circ$ is a feasible point. The interval boxes are repeatedly branched and bounded, and the algorithm stops when a feasible point is found near the global lower bound.

The convex envelopes and hulls based on interval analysis are just constants and intervals respectively, and not tight at all. There-

fore, the branch and bound procedure that uses interval analysis in some cases requires extremely many subproblems. However, each subproblem can be solved very efficiently because it only requires simple interval arithmetic.

5. Handling Equalities

Many deterministic algorithms are applicable to specific types of problems only. For example, the generalized Benders decomposition algorithm described in this paper allows inequality constraints only, and the underestimator branch and bound allows inequality constraints and linear equality constraints only. Generally, algorithms can be modified to accept linear equality constraints because they do not cause nonconvexity. However, problems should be modified, except for algorithms such as interval branch and bound, if they have nonlinear equality constraints.

The simplest method is to convert $\mathbf{h}(\mathbf{x})=\mathbf{0}$ into $\mathbf{h}(\mathbf{x})\leq\mathbf{0}$ and $\mathbf{h}(\mathbf{x})\geq\mathbf{0}$. Note that $\mathbf{h}(\mathbf{x})\leq\mathbf{0}$ and $\sum_i h_i(\mathbf{x})\geq 0$ are also equivalent to $\mathbf{h}(\mathbf{x})=\mathbf{0}$. Therefore, m equality constraints can be converted to 2m or m+1 inequality constraints. The generalized Benders decomposition can now be applied to equality constrained problems. The linear underestimator branch and bound can also be applied to any problem because $\mathbf{h}(\mathbf{x})$ can be converted to a separable d.c. function $\mathbf{c}(\mathbf{x})+\mathbf{r}(\mathbf{x})$ where $\mathbf{c}(\mathbf{x})$ is convex and $\mathbf{r}(\mathbf{x})$ is reverse convex. In this case, 2m inequality constraints $\mathbf{c}(\mathbf{x})+\mathbf{r}(\mathbf{x})\leq\mathbf{0}$ and $-\mathbf{c}(\mathbf{x})-\mathbf{r}(\mathbf{x})\leq\mathbf{0}$ are preferred to m+1 inequalities, because summation of reverse convex terms results in a larger gap between the original function and its convex envelope.

The following procedure applies to general d.c. functions $\mathbf{c}(\mathbf{x})+\mathbf{r}(\mathbf{x})$ where $\mathbf{c}(\mathbf{x})$ is convex and $\mathbf{r}(\mathbf{x})$ is reverse convex. Let us define new variables $\mathbf{u}=\mathbf{c}(\mathbf{x})$ and $\mathbf{v}=\mathbf{r}(\mathbf{x})$. Then, $\mathbf{c}(\mathbf{x})+\mathbf{r}(\mathbf{x})=\mathbf{0}$ are equivalent to linear equality constraints $\mathbf{u}+\mathbf{v}=\mathbf{0}$, convex inequality constraints $\mathbf{c}(\mathbf{x})-\mathbf{u}\leq\mathbf{0}$ and $-\mathbf{r}(\mathbf{x})+\mathbf{v}\leq\mathbf{0}$, and reverse convex inequality constraints $-\mathbf{c}(\mathbf{x})+\mathbf{u}\leq\mathbf{0}$ and $\mathbf{r}(\mathbf{x})-\mathbf{v}\leq\mathbf{0}$. Note that the last 2m reverse convex constraints can be summed to form a single reverse convex constraint $\sum_i [-c_i(\mathbf{x})+r_i(\mathbf{x})+u_i-v_i]\leq 0$. Therefore, using 2m extra variables, m nonlinear equality constraints can be converted to m linear equality constraints, 2m convex inequality constraints, and one reverse convex inequality constraint. As a result, all we need, theoretically, is an algorithm that can solve a convex problem with a single reverse convex constraint, and all of the deterministic algorithms reviewed in this paper can do it.

STOCHASTIC APPROACH

Stochastic algorithms, when run sufficiently long, are virtually guaranteed to find the global optimum according to the following convergence theorem [Bäck et al., 1991].

For minimization of objective function $f(\mathbf{x})$,
1) Let $\mathbf{x}^{t+1}=\mathbf{x}^t+N(0,\sigma)\,\mathbf{1}$.
2) If $f(\mathbf{x}^{t+1})<f(\mathbf{x}^t)$, accept $\mathbf{x}^{t+1}$.
Otherwise, $\mathbf{x}^{t+1}=\mathbf{x}^t$.
3) Repeat for next t.
Then, for $\sigma>0$ and $f^{min}>-\infty$, $\lim_{t\to\infty} p\{f(\mathbf{x}^t)=f^{min}\}=1$.

This means that for a random search based on a normal distribution, the probability of global optimality of the obtained solution will eventually approach one. For stochastic algorithms to be efficient, however, balancing is required between exploiting the best solution (local search) and exploring the search space (global search) [Booker, 1987]. The above algorithm is biased towards local search, and two representative methods that can be balanced are summarized as follows.

1. Simulated Annealing

Let us consider a collection of atoms in equilibrium at a given temperature T. Displacement of an atom causes a change ΔE in the energy of the system. If $\Delta E\leq 0$, the displacement is accepted. If $\Delta E>0$, the probability that the displacement is accepted is $\exp(-\Delta E/kT)$ where k is the Boltzmann constant. This process can be simulated in optimization as follows.

For minimization of objective function $f(\mathbf{x})$,
1) Take $\mathbf{x}^{new}$ randomly.
2) If $\Delta f=f(\mathbf{x}^{new})-f(\mathbf{x}^{old})\leq 0$, accept $\mathbf{x}^{new}$.
Otherwise,
a) Take a random number $w\in[0,1]$.
b) If $w\leq\exp(-\Delta f/T)$, then accept $\mathbf{x}^{new}$.
Otherwise, $\mathbf{x}^{new}=\mathbf{x}^{old}$.
3) Control T, and repeat.

This algorithm is mostly applied to combinatorial optimization problems, but suitable for unconstrained function optimization also.

2. Genetic Algorithm

The theory of evolution can also be employed in optimization as follows.

For optimization of fitness function $f(\mathbf{x})$,
1) Select a given size of population $\{\mathbf{x}^t\}$ where $\mathbf{x}^t$ is a chromosome (binary vector).
2) At a given crossover probability, crossover $\mathbf{x}^p$ and $\mathbf{x}^q$ to generate $\mathbf{x}^{p'}$ and $\mathbf{x}^{q'}$.
3) At a given mutation rate, mutate $\mathbf{x}^t$.
4) Repeat.

This algorithm is based on the assumption that the best solutions will be found in regions of the search space containing relatively high proportions of good solutions, and that these regions can be identified by judicious and robust sampling of the space [Booker, 1987]. It is being widely applied case by case to special data structures in which problem specific knowledge is incorporated. Such modified genetic algorithms are referred to as evolution programs [Michalewicz, 1996].

The original genetic algorithm uses binary representation of chromosomes to be suitable for combinatorial optimization. However, this algorithm can also be applied to unconstrained function optimization. In this case, floating point representation is more efficient, in which the following operators can be used.

For randomly selected $j\in\{1,\ldots,n\}$,
1) Simple crossover: $\mathbf{x}^{p'}=[x_1^p,\ldots,x_j^p,x_{j+1}^q,\ldots,x_n^q]$ and $\mathbf{x}^{q'}=[x_1^q,\ldots,x_j^q,x_{j+1}^p,\ldots,x_n^p]$
2) Arithmetical crossover: $\mathbf{x}^{p'}=w\,\mathbf{x}^p+(1-w)\,\mathbf{x}^q$ and $\mathbf{x}^{q'}=(1-w)\,\mathbf{x}^p+w\,\mathbf{x}^q$
3) Uniform mutation: $x_j^t\in[a_j,b_j]$
4) Boundary mutation: $x_j^t=a_j$ or b_j
5) Non-uniform mutation: Fine tune x_j^t.

3. Handling Equalities

Stochastic algorithms do not suffer from the NP-hardness of the

problem, and thus they are considered to be suitable for large problems. However, these algorithms still have difficulties when applied to chemical process design. The stochastic algorithms are based on the random search technique. Since the evaluation of the objective function is meaningful only at feasible points, they are suitable for unconstrained or inherently inequality constrained optimization problems only. However, most chemical process design problems have many equality constraints. Therefore, the problem or the algorithm should be modified.

3-1. Problem Modification

3-1-1. Penalty Function Method

Constrained optimization problems can be converted to unconstrained problems as follows.

$$\min_x F(x, r)=f(x)+1/(2r)\ \mathbf{c}(x)^T \mathbf{c}(x)$$

where r is a penalty parameter (>0), and $\mathbf{c}(x)$ is a vector of all active constraint functions. As $r \rightarrow 0$, $\mathbf{x}$ converges to a local minimum $\mathbf{x}^*$, but the Hessian matrix $\mathbf{H}[F(x, r)]$ becomes ill-conditioned. Furthermore, when there are too many equality constraints as in chemical process design problems, it is difficult to keep the reformulated problem numerically stable.

3-1-2. Feasible Point Strategy

In order to avoid dealing with equality constraints in a stochastic algorithm, a feasible point strategy can be adopted, in which feasible points can be found by solving an infeasibility minimization problem such as the following.

$$\min \mathbf{c}(x)^T \mathbf{c}(x)$$

where $\mathbf{c}(x)$ is a vector of all violated constraint functions. Another form of infeasibility minimization problem is as follows.

$$\min \max\{\mathbf{g}(x), \mathbf{h}(x), -\mathbf{h}(x)\}$$

As shown by Choi et al. [1999], finding a feasible point for a nonconvex problem is an NP-complete problem, and thus can be considered easier than finding the global optimum, which is NP-hard.

An equality constrained simulated annealing algorithm proposed by Choi et al. [1999] solves the following inequality constrained infeasibility minimization problem.

$$\min \alpha \qquad \text{(I)}$$

subject to

$$\mathbf{g}(x) \le \alpha \mathbf{1}$$
$$\mathbf{h}(x) \le \alpha \mathbf{1}$$
$$-\mathbf{h}(x) \le \alpha \mathbf{1}$$
$$f(x) \le f^* - \varepsilon + \alpha$$

where $\mathbf{1}=[1 \ldots 1]^T$, and ε is an optimality tolerance (>0). Note that $\alpha<\varepsilon$ means that $\mathbf{x}$ is a feasible point at which the value of the objective function is lower than the previously found local minimum f^*. Implementation of this strategy is schematically described in Fig. 5.

3-2. Algorithm Modification

3-2-1. Decoding Strategy

Let us convert all inequality constraints $\mathbf{g}(x) \le \mathbf{0}$ in problem (P) into equality constraints $\mathbf{g}(x)+\mathbf{s}=\mathbf{0}$ where $\mathbf{s}$ is a vector of nonnegative slack variables. Then we have the following type of problem.

$$\min f(x, y) \qquad \text{(E)}$$

subject to

$$\mathbf{h}(x, y)=\mathbf{0}$$
$$\mathbf{a} \le x \le \mathbf{b}$$
$$\mathbf{c} \le y \le \mathbf{d}$$

where $\mathbf{x}$ represents n−m design (independent) variables, $\mathbf{y}$ represents m state (dependent) variables, and $\mathbf{h}$: $R^n \rightarrow R^m$ $(n>m)$. Assuming that $\mathbf{x}$ can be decoded to $\mathbf{y}$ by an equation solver, this problem can be viewed as follows.

$$\min f(x, y(x))$$

subject to

$$\mathbf{a} \le x \le \mathbf{b}$$

This type of problem is suitable for stochastic algorithms. Further-

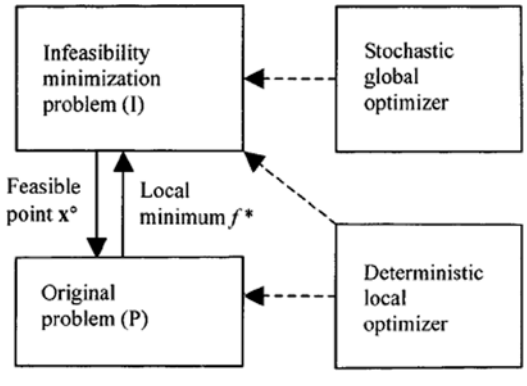

Fig. 5. A stochastic method based on feasible point strategy.

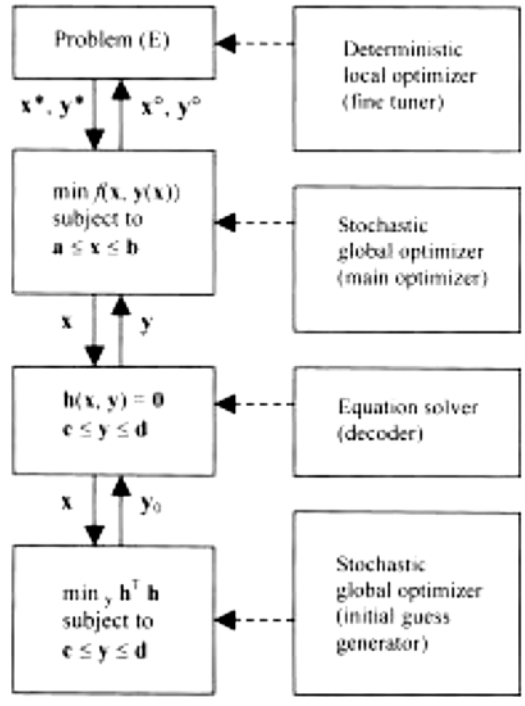

Fig. 6. A stochastic method based on decoding strategy.

more, chemical process design problems generally have small degrees of freedom, and thus the above problem is expected to be small in most cases. However, stochastic algorithms are inefficient for fine local tuning, and thus a deterministic local algorithm is to be incorporated.

The decoding strategy can easily be implemented when **h** is linear with respect to **y**, and is being widely used in algorithms devoted to specific problems. For general problems, a robust equation solver is required, and a Newton type algorithm can be used if a good initial guess generator is available. A rough solution to an infeasibility minimization problem can serve as a good initial guess, and a stochastic global optimizer can generate it with a large optimality tolerance. Note that decoding is valid even if there are multiple solutions for **y** at a given **x**, because the result is stochastic. Implementation of this strategy is schematically described in Fig. 6.

DISCUSSION AND CONCLUSION

Outer approximation and generalized Benders decomposition are suitable for low rank nonconvex problems only. Generally, however, chemical process optimization problems are high rank nonconvex problems. Therefore, branch and bound is the most efficient deterministic method currently available, especially when linear underestimators and interval analysis are incorporated to tighten the subproblem boxes. However, the guarantee of global optimality is still computationally too expensive.

Stochastic algorithms inevitably take forever to obtain a solution of which the global optimality is guaranteed. Therefore, we have to adopt and use the currently best solution at some stage of the procedure, and if necessary, keep the procedure running for a long time for a possibility of existence of a better solution. As mentioned before, the deterministic algorithms guarantee the global optimality of the obtained solution, but they don't give any useful information but the lower bound on the global minimum until the procedure converges and stops. Stochastic algorithms do not guarantee the global optimality of the obtained solution, but continually improve tentative solutions, and thus can give us useful results in a reasonable time span.

Studies on global optimization indicate that most chemical process design problems are still too tough targets. Deterministic algorithms take too much computation time even for moderately sized problems. Stochastic algorithms have difficulties in dealing with equality constraints. Therefore, stochastic methods based on the feasible point strategy or the decoding strategy are considered useful. Further research on feasible point finding and equation solving is suggested as future work.

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