

Chapter 1

INTRODUCTION

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1. Optimization in Chemical Engineering

Optimization is very important and relevant to practically all disciplines. It is being used both qualitatively and quantitatively to improve and enhance processes, products, materials, healthcare, and return on investments to name a few. In Chemical Engineering, optimization has been playing a key role in the design and operation of industrial reactors, separation processes, heat exchangers and complete plants, as well as in scheduling batch plants and managing supply chains of products across the world. In addition, optimization is useful in understanding and modeling physical phenomena and processes. Without the use of sophisticated optimization techniques, chemical and other manufacturing processes would not be as efficient as they are now. Even then, it is imperative to continually optimize the plant design and operation due to the ever changing technology, economics, energy availability and concerns on environmental impact. In short, optimization is essential for achieving sustainable processes and manufacturing.

In view of its importance and usefulness, optimization has attracted the interest of chemical engineers and researchers in both industry and academia, and these engineers and researchers have made significant

contributions to optimization and its applications in Chemical Engineering. This can be seen from the many optimization books written by Chemical Engineering academicians (e.g. Lapidus and Luus, 1967; Beveridge and Schechter, 1970; Himmelblau, 1972; Ray and Szekeley, 1973; Floudas, 1995 and 1999; Luus, 2000; Edgar *et al.*, 2001; Tawarmalani and Sahinidis, 2002; Diwekar, 2003; Ravindran *et al.*, 2006).

Optimization can be for minimization or maximization of the desired objective function with respect to (decision) variables subject to (process) constraints and bounds on the variables. An optimization problem can have a single optimum (i.e. minimum in the case of minimizing the objective function or maximum in the case of maximizing the objective function) or multiple optima (Fig. 1), one of which is the global optimum and the others are local optima. A global minimum has the lowest value of the objective function throughout the region of interest; that is, it is the best solution to the optimization problem. On the other hand, a local minimum has an objective function value lower than those of the points in its neighborhood but it is inferior to the global minimum. In some problems, there may be more than one global optimum with the same objective function value.

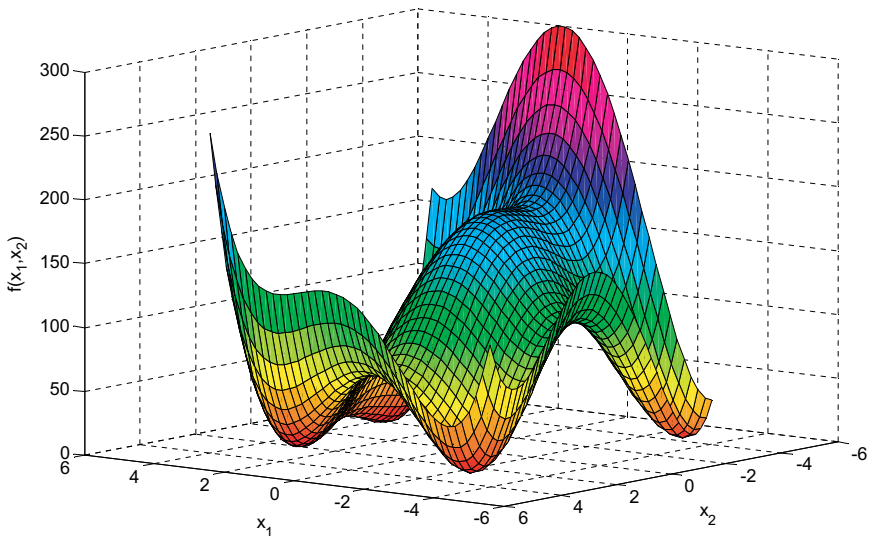


Figure 1. Three-dimensional plot of the modified Himmelblau function (Eq. (2)) showing four minima of which one is the global minimum.

In most applications, it is desirable to find the global optimum and not just the local optimum. Obviously, the global optimum is better than a local optimum in terms of the specified objective function. In some applications such as phase equilibrium, only the global optimum is the correct solution. Global optimization refers to finding the global optimum, and it encompasses the theory and techniques for finding the global optimum. As can be expected, finding the global optimum is more difficult than finding a local optimum. However, with the availability of cheap computational power, interest in global optimization has increased in the last two decades. Besides the need for global optimization, the application can involve two or more conflicting objectives, which will require multi-objective optimization (MOO). There has been increasing interest in MOO in the last two decades. This led to the first book on MOO techniques and its applications in Chemical Engineering (Rangaiah, 2009).

Many of the optimization books by chemical engineers cited above focus on optimization in general. Only two books: Floudas (1999) and Tawarmalani and Sahinidis (2002), are dedicated to global optimization, and they focus on deterministic methods. Besides these methods, however, many stochastic methods are available and attractive for finding the global optimum of application problems. Lack of a book on stochastic global optimization (SGO) techniques and applications in Chemical Engineering is the motivation for the book you are reading.

The rest of this chapter is organized as follows. The next section presents several examples having multiple minima, thus requiring global optimization. An overview of the global optimization methods is provided in Sec. 3. Scope and organization of the book are covered in the last section of this chapter.

2. Examples Requiring Global Optimization

2.1. Modified Himmelblau function

Consider the Himmelblau function (Ravindran *et al.*, 2006):

$$\text{Minimize } f(x_1, x_2) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2, \quad (1a)$$

with respect to x_1 and x_2 ,

$$\text{Subject to } -6 \leq x_1, x_2 \leq 6. \quad (1b)$$

Here, $f(x_1, x_2)$ is the objective (or performance) function to be minimized; it is a function of two (decision) variables: x_1 and x_2 . The feasible region is defined by the bounds on the variables (Eq. (1b)), and there are no other constraints in this problem. The above optimization problem has four minima with objective function value of 0 at $(x_1, x_2) = (3, 2)$, (3.584, -1.848), (-2.805, 3.131) and (-3.779, -3.283).

Himmelblau function has been modified by adding a quadratic term, in order to make one of these a global minimum and the rest local minima (Deb, 2002). The modified Himmelblau function is

$$\begin{aligned} \text{Minimize } & (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2 \\ & + 0.1[(x_1 - 3)^2 + (x_2 - 2)^2], \end{aligned} \quad (2a)$$

with respect to x_1 and x_2 ,

$$\text{Subject to } -6 \leq x_1, x_2 \leq 6. \quad (2b)$$

With the addition of the quadratic term, the minimum at $(x_1, x_2) = (3, 2)$ becomes the global minimum with objective value of 0 whereas the other minima have positive objective values (Table 1 and Fig. 1). Note that the locations of the local minima of the modified Himmelblau function have changed compared to the minima of the Himmelblau function in Eq. (1).

2.2. Ellipsoid and hyperboloid intersection

Consider an ellipsoid and a hyperboloid in three dimensions. There can be four intersection points between these surfaces, one of which will be the farthest from the origin. Luus (1974) formulated a global optimization problem for finding this particular intersection, which is also considered in

Table 1. Multiple minima of the modified Himmelblau function (Eq. (2)).

No.	Objective function	Decision variables: x_1 and x_2
1	0.0	3.0, 2.0
2	1.5044	3.5815, -1.8208
3	3.4871	-2.7871, 3.1282
4	7.3673	-3.7634, -3.2661

Chapter 2 of this book. The global optimization problem can be expressed mathematically as:

$$\text{Maximize } x_1^2 + x_2^2 + x_3^2, \quad (3a)$$

with respect to x_1, x_2 and x_3 ,

$$\begin{aligned} \text{Subject to: } & 4(x_1 - 0.5)^2 + 2(x_2 - 0.2)^2 + x_3^2 + 0.1x_1x_2 \\ & + 0.2x_2x_3 = 16, \end{aligned} \quad (3b)$$

$$2x_1^2 + x_2^2 - 2x_3^2 = 2. \quad (3c)$$

Here, the objective function (Eq. (3a)) is the square of the distance of a point (x_1, x_2 and x_3 in the three-dimensional space) from the origin, and Eqs. (3b) and (3c) are the equality constraints. Since Eqs. (3b) and (3c) represent respectively an ellipsoid and a hyperboloid in the three-dimensional space, any point satisfying these constraints corresponds to an intersection of the two surfaces. The global optimization problem (Eq. (3)) for finding the farthest intersection between the two surfaces has four maxima as shown in Table 2, of which only one is the global maximum and also the correct solution.

2.3. Reactor design example

We now consider a reactor design example that has two minima. In this problem, it is desired to find the optimal design of three continuous stirred tank reactors (CSTRs) wherein the following series-parallel reactions take place.

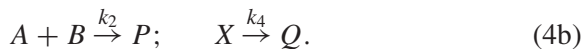
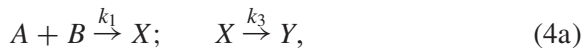


Table 2. Multiple optima for the optimization problem in Eq. (3).

No.	Objective function	Decision variables: x_1, x_2, x_3
1	8.7823	1.5682, -1.8007, -1.7551
2	9.5691	1.3763, -2.1262, 1.7761
3	10.473	1.0396, 2.4915, 1.7846
4	11.677	0.9884, 2.6737, -1.8845

Here, reactant *A* is expensive whereas reactant *B* is available in excess amount for reaction. The desired product is *Y* via the intermediate *X*, whereas *P* and *Q* are the products of side reactions. The above reactions are taken to be first order with respect to concentration of *A* (for the first two reactions) and *X* (for the last two reactions). The specific reaction rates are given by (Denbigh, 1958):

$$k_2/k_1 = 10,000 e^{-3000/T}, \quad (5a)$$

$$k_3/k_1 = 0.01, \quad (5b)$$

$$k_4/k_1 = 0.0001 e^{3000/T}, \quad (5c)$$

where *T* is the reaction temperature.

Component mass balances for *A*, *X* and *Y* around the *n*th reactor are:

$$C_A^{n-1} = C_A^n + (k_1^n + k_2^n)C_A^n \theta^n, \quad (6a)$$

$$C_X^{n-1} = -k_1^n C_A^n \theta^n + C_X^n + (k_3^n + k_4^n)C_X^n \theta^n, \quad (6b)$$

$$C_Y^{n-1} = -k_3^n C_X^n \theta^n + C_Y^n, \quad (6c)$$

where *C* is the concentration of a component (*A*, *X* and *Y* as indicated by the subscript), θ is the residence time in the CSTR and superscript *n* refers to the reactor number. Assume that concentrations in the feed to the first reactor are $C_A^0 = 1$, $C_X^0 = 0$ and $C_Y^0 = 0$. Optimal design of the three CSTRs is to find the values of *T* (involved in the rate coefficients) and θ for each reactor in order to maximize the concentration of the desired product *Y* from the last CSTR. In effect, the problem involves 6 design variables. For simplicity, the optimization problem is formulated in the dimensionless variables:

$$\alpha = \theta k_1 \quad \text{and} \quad \tau = k_2/k_1 = 10,000 e^{-3000/T} \quad (7)$$

The mathematical problem for the optimal design of the three CSTRs is:

$$\begin{aligned} \text{Minimize} \quad & -0.01x_1x_4 - 0.01x_5x_8 - 0.01x_9 \\ & \times \frac{[x_8 + x_7x_9/(1 + x_9 + x_9x_{10})]}{(1 + 0.01x_9 + 0.01x_9/x_{10})}, \end{aligned} \quad (8a)$$

with respect to x_1, x_2, \dots, x_{10} ,

$$\text{Subject to} \quad x_3 = 1/(1 + x_1 + x_1x_2), \quad (8b)$$

$$x_4 = x_1x_3/(1 + 0.01x_1 + 0.01x_1/x_2), \quad (8c)$$

$$x_7 = x_3 / (1 + x_5 + x_5 x_6), \quad (8d)$$

$$x_8 = (x_4 + x_5 x_7) / (1 + 0.01 x_5 + 0.01 x_5 / x_6), \quad (8e)$$

$$0 \leq x_i \leq 2100 \quad \text{for } i = 1, 5, 9, \quad (8f)$$

$$0 \leq x_i \leq 4.934 \quad \text{for } i = 2, 6, 10, \quad (8g)$$

$$0 \leq x_i \leq 1.0 \quad \text{for } i = 3, 4, 7, 8, \quad (8h)$$

Here, the objective function is $[-C_Y^3]$, whose minimization is equivalent to maximizing C_Y^3 (i.e. concentration of the desired product Y in the last CSTR). Variables: x_1, x_5 and x_9 correspond to α^1, α^2 and α^3 (i.e. residence time multiplied by the rate coefficient k_1 in each of the three reactors); x_2, x_6 and x_{10} are the temperature as given by τ in each CSTR; x_3 and x_7 are the concentration of A in reactor 1 and 2 respectively; and x_4 and x_8 are the concentration of X in reactor 1 and 2 respectively.

The above problem for the CSTRs design is a constrained problem with 10 decision variables and 4 equality constraints besides bounds on variables. Alternatively, the equality constraints can be used to eliminate 4 decision variables (x_3, x_4, x_7 and x_8) and then treat the problem as having only 6 decision variables with bounds and inequality constraints. One solution to the design optimization problem is -0.50852 at $(3.7944, 0.2087, 0.1790, 0.5569, 2100, 4.934, 0.00001436, 0.02236, 2100, 4.934)$, and another solution is -0.54897 at $(1.3800, 0.1233, 0.3921, 0.4807, 2.3793, 0.3343, 0.09393, 0.6431, 2100, 4.934)$ (Rangaiah, 1985). The latter solution is the global solution and also better with higher concentration of the desired product in the stream leaving the third CSTR.

2.4. Stepped paraboloid function

Consider the two-variable, stepped paraboloid function synthesized by Ingram and Zhang (2009):

$$\begin{aligned} \text{Minimize } & 0.2(\lfloor x_1 \rfloor + \lfloor x_2 \rfloor) + [\text{mod}(x_1, 1) - 0.5]^2 \\ & + [\text{mod}(x_2, 1) - 0.5]^2, \end{aligned} \quad (9a)$$

with respect to x_1 and x_2 ,

$$\text{Subject to } \quad -5 \leq x_1, x_2 \leq 5. \quad (9b)$$

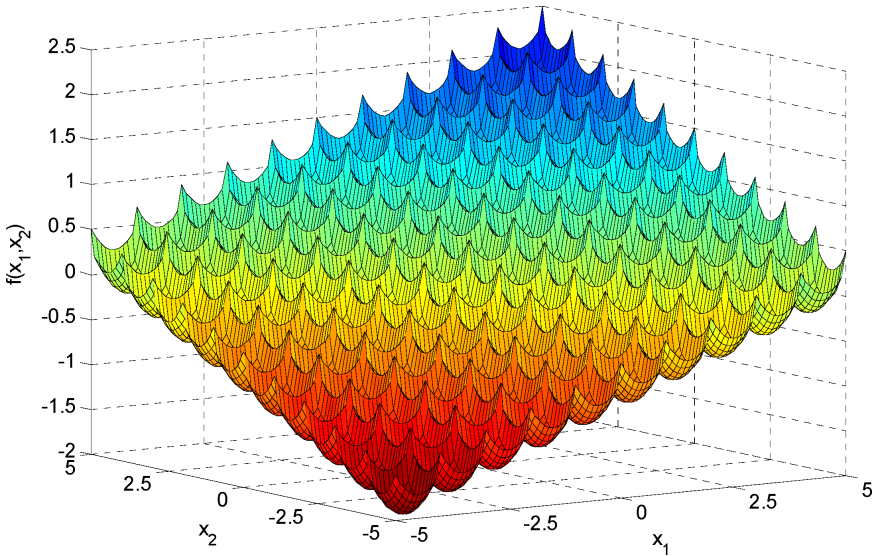


Figure 2. Three-dimensional plot of the discontinuous stepped paraboloid function (Eq. (9)) showing 100 minima of which one is the global minimum.

The notation $\lfloor x \rfloor$ denotes the floor function, which returns the largest integer less than or equal to x , and $\text{mod}(x, y)$ is the remainder resulting from the division of x by y . Equation (9) contains 100 minima within the search domain, which are located at $(x_1, x_2) = (-4.5 + i, -4.5 + j)$ for i and $j = 0, 1, \dots, 9$ (Fig. 2). In contrast to the examples considered thus far, there are discontinuities in both the function value and the function's derivative within the solution domain, specifically at $x_1 = -5, -4, \dots, 4, 5$ and at $x_2 = -5, -4, \dots, 4, 5$. The global minimum is located at $(x_1, x_2) = (-4.5, -4.5)$ and has an objective function value of -2 . The problem can be extended to any number of variables and also can be made more challenging by decreasing the coefficient (0.2) in the first term of Eq. (9a), thus making the global minimum comparable to a local minimum.

The examples considered above have relatively simple functions, a few variables and constraints but still finding their global optimum is not easy. In general, optimization problems for many Chemical Engineering applications involve complex algebraic and/or differential equations in the constraints and/or for computing the objective function as well as numerous decision variables. Objective function and/or constraints

in the application problems may not be continuous. Chemical Engineering problems generally involve continuous variables with or without integer variables. All these characteristics make finding the global optimum challenging. SGO techniques are well-suited for such problems. Hence, this book focuses on SGO techniques and their applications in Chemical Engineering.

3. Global Optimization Techniques

The goal of global optimization techniques is to find reliably and accurately the global minimum of the given problem. Many methods have been proposed and investigated for global optimization, and they can be divided into two main groups: deterministic and stochastic (or probabilistic) techniques. Deterministic methods utilize analytical properties (e.g. convexity) of the optimization problem to generate a deterministic sequence of points (i.e. trial solutions) in the search space that converge to a global optimum. However, they require some assumption (e.g. continuity of functions in the problem) for their success and provide convergence guarantee for problems satisfying the underlying assumptions. Deterministic methods include branch and bound methods, outer approximation methods, Lipschitz optimization and interval methods (e.g. see Floudas, 1999; Horst *et al.*, 2000; Edgar *et al.*, 2001; Biegler and Grossman, 2004; Hansen and Walster, 2004).

Stochastic global optimization (SGO) techniques, the subject of this book, involve probabilistic elements and consequently use random numbers in the search for the global optimum. Thus, the sequence of points depends on the seed used for random number generation. In theory, SGO techniques need infinite iterations to guarantee convergence to the global optimum. However, in practice, they often converge quickly to an acceptable global optimal solution. SGO techniques can be divided into four groups: (1) random search techniques, (2) evolutionary methods, (3) swarm intelligence methods and (4) other methods (Fig. 3).

Random search methods include pure random search, adaptive random search (ARS), two-phase methods, simulated annealing (SA) and tabu search (TS). ARS methods incorporate some form of adaptation including region reduction into random search for computational efficiency. Two-phase methods, as the name indicates, have a global and a local phase.

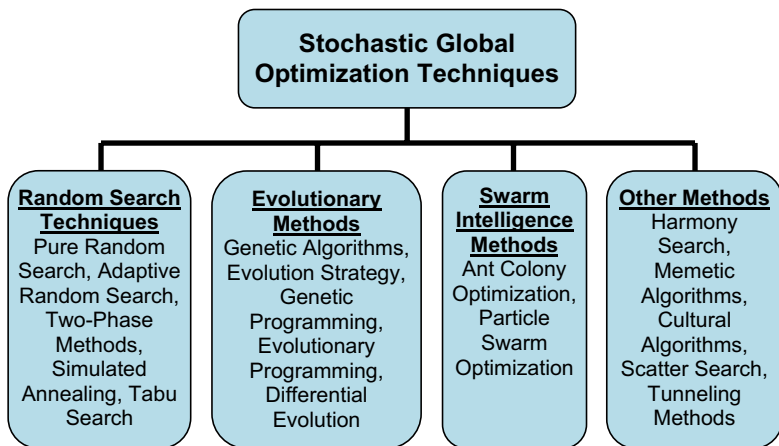


Figure 3. Classification of stochastic global optimization techniques.

Multi-start algorithms and their variants such as multi-level single-linkage algorithm belong to two-phase methods. SA is motivated by the physical process of annealing (i.e. very slow cooling) of molten metals in order to achieve the desired crystalline structure with the lowest energy. TS is derived from principles of intelligent problem solving such as tabu (i.e. prohibited) steps and memory. In this book, ARS methods are covered in Chapters 2, 3, 12 and 15, SA is presented in Chapter 3, and TS is described in Chapters 5 and 19.

Evolutionary methods/algorithms are population-based search methods inspired by features and processes of biological evolution. They have found many applications in Chemical Engineering. Genetic algorithms (GA), evolution strategy (ES), genetic programming, evolutionary programming and differential evolution (DE) belong to evolutionary methods. GA and ES are now quite similar although the former was originally based on binary coding compared to real coding used in ES. GA and its applications are discussed in Chapters 4, 16 and 18, and DE and its variants are the subject of Chapters 6, 13 and 14.

Ant colony optimization (ACO) covered in Chapter 7 and particle swarm optimization (PSO) presented in Chapter 8 are motivated by the *swarm intelligence* or social behavior. An application of ACO is described in Chapter 17. *Other SGO methods* include harmony search (HS, introduced

in Chapter 9), memetic algorithms, cultural algorithms, scatter search and random tunneling methods. This book covers many SGO methods which have found applications in Chemical Engineering.

Many SGO techniques (such as SA, TS, GA, DE, PSO, ACO, HS, memetic algorithms, cultural algorithms and scatter search) are also known as meta-heuristic methods. A meta-heuristic guides a heuristic-based search in order to find the global optimum. On the other hand, a heuristic-based search such as a descent method is likely to converge to a local optimum.

SGO techniques have a number of attractive features. First, they are simple to understand and program. Second, they require no assumption on the optimization problem (e.g. continuity of the objective function and constraints), and hence can be used for any type of problem. Third, SGO methods are robust for highly nonlinear problems even with large number of variables. Fourth, they often converge to (near) global optimal solution quickly. Finally, they can be adapted for non-conventional optimization problems. For example, several SGO techniques have been modified for multi-objective optimization (Rangaiah, 2009).

Significant progress has been made in SGO techniques and their applications in the last two decades. However, further research is needed to improve their computational efficiency, to establish their relative performance, on handling constraints and for solving large application problems. More theoretical analysis of SGO techniques is also required for better understanding and for improving them.

4. Scope and Organization of the Book

The broad objective of this book is to provide an overview of a number of SGO techniques and their applications to Chemical Engineering. Accordingly, there are two parts in the book. The first part, Chapters 2 to 11, includes description of the SGO techniques and review of their recent modifications and Chemical Engineering applications. The second part, Chapters 12 to 19, focuses on Chemical Engineering applications of SGO techniques in detail. Each of these chapters is on one or more applications of Chemical Engineering using the SGO techniques described earlier. Each chapter in the book is contributed by well-known and active researcher(s) in the area.

Luus presents a simple and effective random search with systematic region reduction, known as Luus-Jaakola (LJ) optimization procedure in Chapter 2. He illustrates its application to several Chemical Engineering problems and mathematical functions, and discusses the effect of two parameters in the algorithm on a design problem. He also describes a way for handling difficult equality constraints, with examples.

In Chapter 3, Jeżowski *et al.*, describe in detail two SGO techniques, namely, a modified version of LJ algorithm and simulated annealing combined with simplex method of Nelder and Mead. They investigate the performance of these techniques on many benchmark and application problems as well as the effect of parameters in the techniques.

Chapter 4 deals with genetic algorithms (GAs) and their applications in Chemical Engineering. After reviewing the Chemical Engineering applications of GAs, Younes *et al.*, explain the main components of GAs and discuss implementation issues. Finally, they outline some modifications to improve the performance of GAs.

Tabu (or taboo) search (TS) for global optimization of problems having continuous variables is presented in Chapter 5 by Sim *et al.* After describing the algorithm with an illustrative example, they review TS methods for continuous problems, Chemical Engineering applications of TS and available software for TS. They also briefly describe TS features that can be exploited for global optimization of continuous problems.

In Chapter 6, Chen *et al.*, describe differential evolution (DE) including its parameter values. They summarize the proposed modifications to various components of DE and provide an overview of Chemical Engineering applications of DE reported in the literature. In particular, DE has found many applications for parameter estimation and modeling in addition to process design and operation.

Ant colony optimization (ACO) for continuous optimization problems is illustrated with an example, by Shelokar *et al.* in Chapter 7. They also review ACO for combinatorial optimization, multi-objective optimization and data clustering. Performance of ACO for test and application problems is presented and discussed in the later sections of the chapter.

Particle swarm optimization (PSO) motivated by the social behavior of birds and fishes, is the subject of Chapter 8. Jarboui *et al.* describe

a basic PSO algorithm and its modifications that include global best and local best algorithms. They evaluate the performance of six PSO algorithms for solving nonlinear and mixed-integer nonlinear programming problems.

In Chapter 9, Ingram and Zhang introduce harmony search (HS), which is motivated by the improvisation process of musicians, describe its basic algorithm for global optimization and summarize many modifications to the basic algorithm. They also review HS applications, mention the available software and provide an illustrative example and programs for the HS algorithm.

Younes *et al.*, discuss many issues in the evaluation and reporting of SGO techniques, in Chapter 10. These include performance measures (of solution quality, efficiency and robustness), test problems, experiment design, parameter tuning, presentation and discussion of performance results.

Constraints are common in Chemical Engineering applications, and need to be tackled in solving the optimization problems by SGO techniques. In Chapter 11, Durand *et al.* present an overview of five approaches for handling constraints. Then, they describe a hybrid strategy involving Karush-Kuhn-Tucker conditions for optimality, for handling constraints in SGO techniques, and evaluate its performance on selected nonlinear and mixed-integer nonlinear programming problems.

In Chapter 12, Luus illustrates the use of LJ procedure to model reduction, parameter estimation and optimal control applications, and also investigates the potential of line search in the LJ procedure.

Bonilla-Petriciolet *et al.*, in Chapter 13, apply DE and TS, each in conjunction with a local optimizer, to phase stability and equilibrium calculations in reactive systems, which are formulated using transformed composition variables.

Srinivas and Rangaiah describe two versions of DE with tabu list in Chapter 14. They demonstrate their performance and compare them with DE and TS on benchmark and phase stability problems.

In Chapter 15, Poplewski and Jeżowski describe industrial water (usage) networks and the formulation of optimization problems for them. They then solve three water network problems with equality constraints and numerous binaries, by the modified LJ algorithm described in Chapter 3.

Bochenek and Jeżowski consider the difficult and yet important problem of heat exchanger network retrofitting in Chapter 16. They employ a two-level optimization with GA in both outer level (for structural optimization) and inner level (for parameter optimization) for solving two retrofitting problems.

Finding classification rules in measured data by ACO is described in Chapter 17 by Shelokar *et al.* One ACO algorithm for classification and another for feature selection are presented. The former was tested on a number of data sets, and the two algorithms together were used on two data sets for simultaneous classification and feature selection.

In the pen-ultimate Chapter 18, Kotecha *et al.*, apply GA and Constraint Programming (CP) for a job scheduling problem and a sensor network design problem, and compare the performance of the two techniques. Prior to the application, they describe CP that reduces the search domain for optimization, mainly based on constraint propagation.

Lin and Miller, in the last Chapter 19, describe schemes for developing parallel SGO algorithms and illustrate them for solving heat exchanger network synthesis and computer aided molecular design problems using parallel TS. The fully documented code for the first example is provided on the CD accompanying the book.

Each chapter in this book is comprehensive and can be read by itself with little reference to other chapters. Introduction to, description, algorithm, illustrative examples and programs of the SGO techniques given in the first part of this book are useful to senior undergraduates and post-graduates doing courses and projects related to optimization. Reviews of modifications and Chemical Engineering applications of the techniques in a number of chapters are of particular interest to researchers and engineers. Applications covered in the second part of this book and programs/files on the accompanying CD are valuable to many readers of this book.

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Exercises

- (1) Find the global optimum of the modified Himmelblau function (Eq. (2)) and the geometric problem (Eq. (3)) using a local optimizer and/or programs provided on the attached CD. Try different initial estimates for

- the decision variables and/or parameters in the optimization program. Is it easy to find the global optimum of these two problems?
- (2) Develop the optimization problem (Eq. (8)) for the design of CSTRs based on the description and equations provided in this chapter. Note that this requires Chemical Engineering background.
 - (3) Solve the optimization problem (Eq. (8)) for the design of CSTRs using a local optimizer and/or programs provided on the attached CD. Try different initial estimates for the decision variables and/or parameters in the optimization program. Is it easy to find the global optimum of this problem?
 - (4) Find the global optimum of the stepped, paraboloid function (Eq. (9)) using a local optimizer and/or programs provided on the attached CD. Ensure that the floor and mod functions in Eq. (9) are correctly implemented in your program. Try different initial estimates for the decision variables and/or parameters in the optimization program. Present and discuss the results obtained.