Chapter

1

A Brief Discussion on Optimization

1.1 Introduction to Process Optimization

Optimization is a technique of obtaining the best available output for a system or process. The passion for optimality is inherent in human race. Knowingly or unknowingly, we are optimizing our efforts in daily life. This method is studied in every field of engineering, science, and economics. Optimization has been used from ancient times, mostly, by using analytical methods. There are many practical mathematical theories of optimization that have been developed since the sixties when computers become available. The main purpose of the theories is to develop reliable and fast methods to reach the optimum of a function by arranging its evaluations intelligently. Most of the modern engineering and planning applications incorporate optimization process at every step of their complex decision making process. Therefore, this optimization theory is significantly important for them. All of these fields have the same intention like maximization of profit or minimization of cost. As a process engineer, it is our primary concern to utilize resources carefully with minimum loss. An optimized process that use minimum input (raw material, energy, labor etc.) and gives maximum output (product quality and quantity, most environmental friendly) is always favorable. George E Davis extols, "The aim of all chemical procedures should be the utilization of everything and the avoidance of waste. It is often cheaper to prevent waste than to attempt to utilize a waste product." With proper design of optimized process, wastage of natural resources can be minimized. We can recall the famous quote by Dante *"All that is superfluous displeases God and Nature, All that displeases God and Nature is evil."* In nature, everything follows the optimized way to reach the destination. Heat, water etc. flow through the minimum resistance path.

Chemical process industries consist of several "unit operations" and "unit processes" e.g., heat exchanger, distillation column, batch reactor, packed bed reactor, etc. It is the responsibility of a process engineer to run the plant at an optimum condition to obtain the maximum profit with minimum environmental impact. The real driving force for process optimization is efficiency.

Chemical companies realize that if they can run the plant more efficiently, it will improve their bottom line. We can optimize the process by considering the individual unit one by one, or by considering many units at a time (e.g., water distribution system with pumps and pipe line, heat exchanger network, reactor network). Environmental pollution is also a crucial issue for process industries. Sometimes environmental issues are embedded with the objective function and solved as a multiobjective optimization problem. Process optimization involves the determination of process parameters (temperature, pressure, pH, time etc.) that provides us maximum output. In the chemical industry, proper selection of batch time gives the maximum selectivity for a batch reactor. Maximum amount of heat recovery is possible by the optimization of HEN.

1.2 Statement of an Optimization Problem

All optimization problems can be presented by some standard form. Each and every optimization problem contains objective function(s) $f(X)$ which we need to optimize. The general form of optimization problem is:

Min/Max $f(X)$

subject to $g(X) = 0$;

$h(X) \geq 0$

The solution $X = \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Bmatrix}$, which gives us the optimum value of $f(X)$.

Various terms are used for optimization problems, these are:

Decision variable During the optimization process, we have to formulate the objective function that depends on some variables. In real problem, there are many variables that control the output of any system. However, for optimization techniques, we consider few variables over which the decision maker has control. Decision variables are the variables within a model that one can control. Decision variables are usually input to the model that can be changed by the decision maker with the aim of revising the response of the system. For example, a decision variable might be operating temperature of a reactor, diameter of pipe, number of plates in a distillation column.

Identifying and prioritizing key decision variables Any variable that we need be controlled is a decision variable. However, all variables are not equally important during the optimization process. Based on the Pareto ranking of effects on objective function, the key decision variables are chosen. The sensitivity of the objective function to changes in the variables is the key factor for deciding important variables. Variables with high sensitivity may be considered as decision variables, whereas less sensitive variables may be ignored.

Limit of decision variables Every decision variables have some upper and lower limit. Say, mass/mole fraction of any component in a mixture must have the value $0 \leq X \leq 1$. Theoretically, some variable may reach infinity (e.g., time, length); however, in real life, we can allow them to certain practicable values. A first order irreversible reaction takes infinite time for 100 per cent conversion. However, we allow some limited time for practical application.

Objective function Objective function (also read as "cost function") is the mathematical expression that we need to optimize. This describes the correlation between the decision variables and process parameters. In most of the chemical engineering optimization, the objective functions are either profit from the process or cost of production. However, there are many types of objective functions like error during curve fitting/parameter estimation, minimization of environmental impact.

Constraint Constraints are additional relations between the decision variables and process parameters other than the objective function. For instance, during the optimization of any blending process, summation of all components should be equal to unity i.e., $\sum_{i=1}^{n} x_i = 1$. The limit of any variable can be incorporated as constraints i.e., $0 \le X \le 1$. As stated the constraints may be equality, inequality (reaction occurs at acidic condition, pH < 7; catalyst is active above certain temperature). Operation of chemical processes are also susceptible to market constraints; say, availability of raw materials and demand of products.

1.3 Classification of Optimization Problems

Classification of optimization methods into different categories has been made based on the physical structure of the problem, type of constraints, nature of design variables, nature of algorithms and area of applications. Optimization techniques are also classified based on the permissible value of the design variables, separability of the functions and number of objective functions. These classifications are briefly discussed in this book.

Topological optimization and parametric optimization

Topological optimization deals with the arrangement of the process equipments during the plant design. Topological optimization should be considered first because the topological changes usually have a large impact on the overall profitability of the plant. For instance, addition of one heat exchanger can change the scenario of the whole heat integration of the process plant. Parametric optimization is easier to interpret when the topology of the flow sheet is fixed. Combination of both types of optimization strategies may have to be employed simultaneously.

Topological arrangement like elimination of unwanted by-product, elimination/rearrangement of equipment, alternative separation methods, and alternative reactor configurations may be employed for the improvement of heat integration. Whereas, parametric optimization consists of the optimization of operating conditions like temperature, pressure, concentration, flow rate etc.

Unconstrained and constrained optimization

If we need to optimize the objective function without any additional constraints, then it is called unconstrained optimization.

e.g., find the minimum of the function $f(x) = x^2 - 2x - 3$.

Whenever, the objective function is accomplished with another correlation (constrained function), these optimization problems are called constrained optimization problems.

e.g., find the minimum of the function $f(x) = x^2 - 2x - 3$

subject to $x \geq 2$

For the unconstrained problem, the solution is $f_{\min} = -4$ whereas for the constrained problem the solution is $f_{\min} = -3$

Linear and nonlinear programming

This classification is done based on the structure of the equations involved in an optimization problem. If all the equations (objective function and constraints functions) involved in any optimization problem are linear, it is called linear programming.

e.g., minimize the function $f(X) = 2x_1 + 3x_2$

subject to $x_1 - x_2 = 2$

is a linear programming problem where both the objective function and constraint function are linear function of decision variables.

When any of these functions is nonlinear, then this class of optimization is termed as nonlinear programming.

e.g., minimize the function $f(X) = x_1^2 + 2x_2^2$

subject to $x_1 - x_2 = 2$

the aforesaid problem is a nonlinear programming as the objective function is nonlinear.

Convex function and concave function

The ease of optimization problem depends on the structure of the objective function and the constraints. A single-variable function can easily be solved if it is either a convex or a concave function.

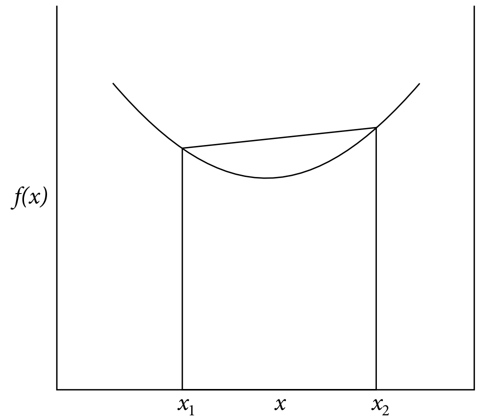

Fig. 1.1 Convex function

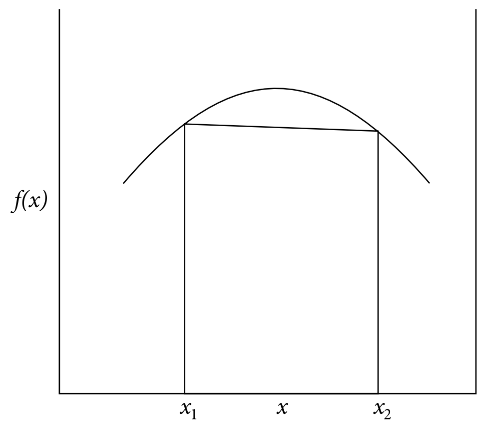

Fig. 1.2 Concave function

Draw a straight line between two points (x_1, x_2). If all point on the straight line x_1 x_2 lie above curve $f(x)$, then it is called convex function (Fig. 1.1). When all point on the straight line x_1 x_2 lie below curve $f(x)$, then it is called concave function (Fig. 1.2). The advantage of any convex or concave function is that it provides a single optimum point. Therefore, this optimum point is always a global optimum.

Continuous and discrete optimization

When the decision variables appear in any optimization problem are all real numbers (temperature, pressure, concentration, etc.) and the objective and constraint functions are continuous then these are called continuous optimization.

However, in some cases, we need to optimize an optimization problem where decision variables are discrete number these are termed as discrete optimization. Number of workers, number of batches per month, number of plate for distillation column etc., cannot be real numbers they are always integer, whereas the standard diameter of pipes are real numbers but, discrete in nature. The standard pipe available with OD (mm) of 10.3, 13.7, 17.1, 21.3, 26.7 etc. If we are interested to find the optimum pipe diameter, we have to perform a discrete optimization with these standard pipe diameters. Same heat exchanger can be used for both cooling and heating purpose: when we need to cool the process stream below the available temperature we have to use cooling water. On the other hand, if we need to heat the process stream we have to use hot water stream. For this situation, the presence of any stream (hot or cold) can be represented by binary variable 0–1.

Mixed integer optimization is another class of optimization method where both integer and real variables appear in the objective function (e.g., optimization of distillation column involves variables like temperature and number of tray/plate).

Single-objective and multi-objective optimization

When the optimization problem contains only one objective function it is known as single objective optimization. These types of problems are easy to solve. However, most of the chemical engineering problems involve more than one objective functions (e.g., optimization of yield and selectivity for a reactor). These problems need special consideration, as the objectives are conflicting.

Multi-objective optimization problem can be represented as

$$\min\left[F_1(X), F_2(X), \ldots, F_n(X)\right]$$

$$X \in R^m$$

$$h(X) = 0$$

$$g(X) \geq 0$$

The detail solution procedures are discussed in chapter 8.

Local and global search method

If the objective function possesses multiple stationary points, search algorithms have a tendency to find a stationary point nearer to the initial starting point. The algorithm is stuck in this local optimum point, they are not able to find the global optima. If the search process starts from point A, it will locate the point 1 as minimum (Fig. 1.3). Whereas, if it starts from point B, it will find point 2 as a minimum.

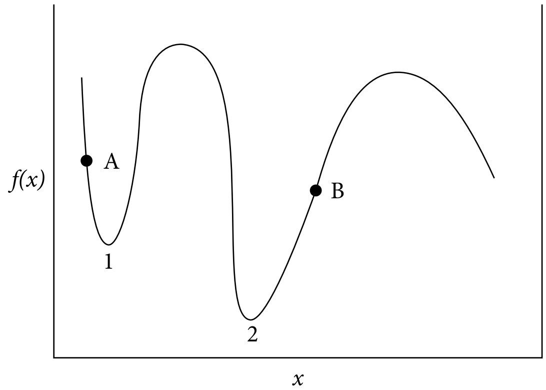

Fig. 1.3 Local and global optimum points

Global search algorithms are able to find the global optimum point. Global optimization algorithms are usually broadly classified into deterministic and stochastic methods.

Deterministic, stochastic and combinatorial optimization

Generally, optimization techniques fall into one of two categories, deterministic and stochastic. Deterministic methods use a simple algorithm, which start with some initial guess and then update iteratively to attain a solution. These techniques usually require the knowledge of the shape of the objective function. The examples of deterministic method are steepest descent method and

Powell's method (conjugate gradient method). Deterministic methods for optimization have primarily one strength and one weakness. The strength of deterministic optimization methods is that provided a good initial guess for an optimum solution they converge very quickly and with high precision. The weakness is that they have a tendency to get trapped in local minima if the initial guess is far from the optimum solution. On the other hand, stochastic optimization methods rely on randomness and retrials to better sample the parameter space in searching for an optimum solution. For these algorithms, search point moves randomly in the search space. The three most commonly used stochastic methods are Monte Carlo (MC), Simulated Annealing (SA), and the Genetic Algorithm (GA). Stochastic optimization problems are also used for optimization that attempt to model the process that has data with uncertainty by considering that the input is specified in terms of a probability distribution.

Combinatorial optimization is a topic that is discussed in applied mathematics and theoretical computer science. This technique consists of a finite set of objects from which we need to find an optimal object. Exhaustive search is not feasible for many such problems. This optimization technique works on the domain of those problems, in which the set of feasible solutions is either discrete or can be converted to discrete, and wherein the aim is to get the best solution. The traveling salesman problem (TSP) is the most common example of combinatorial optimization.

The following Fig. 1.4 shows the classification of optimization techniques.

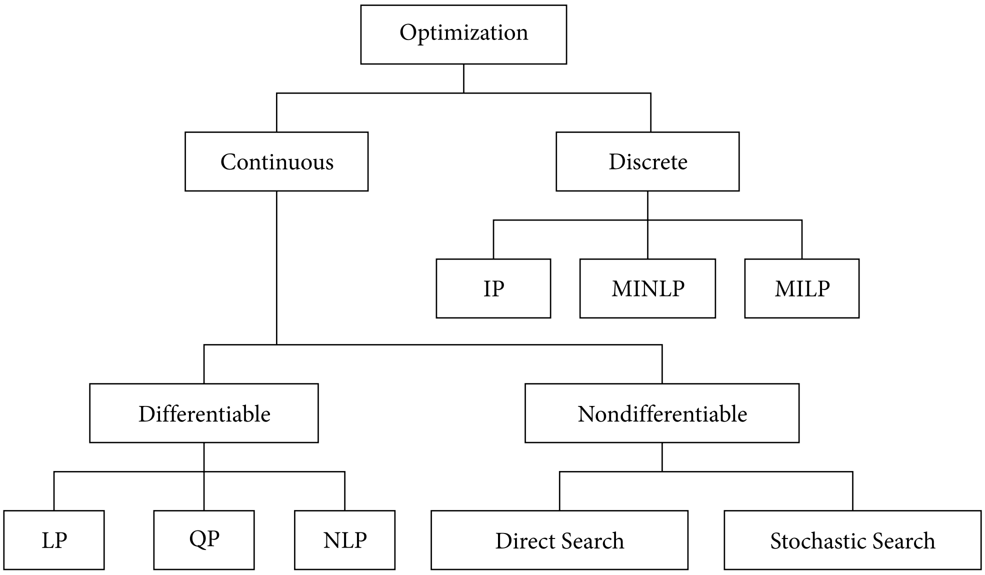

Fig. 1.4 Classification of optimization problem (IP: integer programming, MINLP: mixed integer non-linear programming, MILP: mixed integer linear programming, LP: linear programming, QP: quadratic programming, NLP: non-linear programming)

1.4 Salient Feature of Optimization

Optimization problem can be converted to a suitable form according to our convenience. The minimization of $f(X)$ can be transformed to maximization of $-f(X)$ as shown in Fig. 1.5.

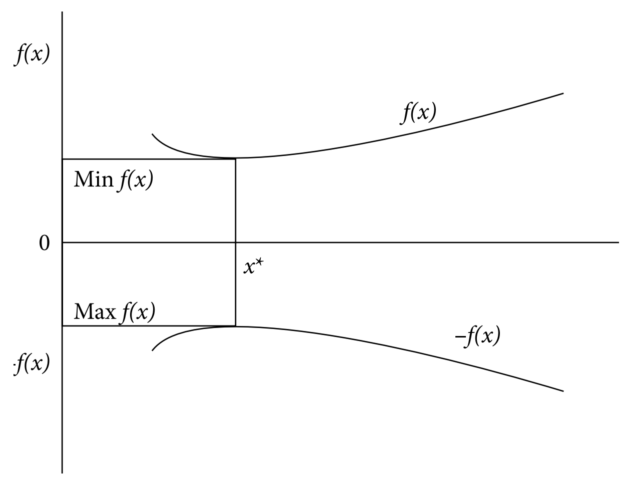

Fig. 1.5 Conversion of $f(x)$ to $-f(x)$

There is a common misconception that the first derivative of the objective function is zero at the optimum (minimum or maximum) point; this is not true for all cases. Consider an objective function as shown in Fig. 1.6. If we find the minimum and maximum values of that function within the range $[x_a, x_b]$, we will get the values f_a and f_b respectively. At these points x_a and x_b the value of the first derivative is not zero. Newton's method is not suitable for this situation as termination criteria does not work. This problem may be cursed with the entrapment at the local optimum point. Application of global optimization algorithm or multi-start algorithm may solve this problem. Solution of local search method may give us a wrong result. "Premature optimization is the root of all evil." Donald Ervin Knuth.

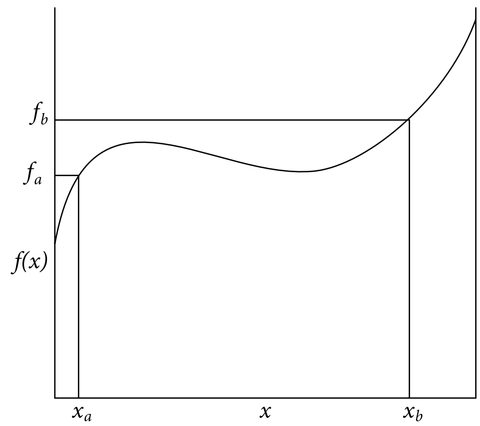

Fig. 1.6 Plot of objective function vs. decision variable

Several issues can make optimization problems practically complex and difficult to solve. Such complicating factors are the existence of multiple decision variables in the problem, multiple objective function in the problem. For solving any process optimization problem, we have to follow six important steps as described by Edger *et al.* These steps are:

1. Analyze the process properly to define the process variables and their characteristics. After that, prepare a list of all variables associated with the process.
2. Set the objective function in terms of the decision variables listed above along with coefficients involved with the process (heat conductivity, heat transfer coefficient, reaction rate constant etc.). Decide the criterion for optimization. This second step provides us the performance model; this model is also called the economic model when appropriate.
3. After developing the objective function, we need to check if any other process constraints are associated with this process. We have to include both equality and inequality constraints. For this purpose we generally use some well-known physical principles (conservation of mass and energy), empirical equations (Dittus–Boelter correlation for calculating heat transfer coefficient), implicit concepts (rules of thumb), and external restrictions. Identification of the independent and dependent variables has been done to determine the degrees of freedom.
4. When the formulated optimization problem is very large:

   (i) split the problem into small manageable parts or

   (ii) objective function and model equation can be simplified as per our convenience
5. Apply an appropriate optimization method to solve the problem. Selection of method depends on the structure of the problem. There is no such algorithm, which is suitable for all problems.
6. Check the sensitivity of the result to modify the coefficients in the problem

1.5 Applications of Optimization in Chemical Engineering

Optimization is an intrinsic part of design: the designer seeks the best, or optimum, solution of a problem [Coulson and Richardson]. The design of any chemical engineering systems can be formulated as optimization problems in which a measure of performance is to be optimized while satisfying all other constraints. In the field of chemical engineering, typical application of optimization problems arise in process identification, design and synthesis, model development, process control, and real-time optimization.

In this book, we have discussed many chemical engineering applications:

i. optimization of water storage tank
ii. optimization of water pumping network
iii. optimization of cost of an alloy
iv. optimization of heat exchanger network
v. optimization of chemical reactor and reactor network
vi. application of optimization in thermodynamics, determination of chemical equilibrium
vii. optimization of distillation system

viii. parameter estimation using least square/Levenberg–Marquardt method
ix. optimization of biological wastewater treatment plant
x. tuning of PID controller
xi. design of real-time controller
xii. optimization of air pollution control system
xiii. optimization of adsorption process
xiv. warehouse management
xv. optimization of blending process in petroleum refinery

1.6 Computer Application for Optimization Problems

In chemical engineering, optimization is a technique to find the most cost effective process under the given constraints. Most of the optimization problems in the chemical industry are very complicated in nature. There are a large number of variables with a large number of constraints involved in this process. Solving of these problems is difficult, sometimes impossible by hand. Numerical optimization helps us to solve these problems in an efficient way. There are many algorithms developed for solving complicated optimization problems. To execute these algorithms, we need the help of computer programming. Application of computer programming and software can solve these problems easily. However, the application of optimization is sometimes restricted by the lack of information as well as the lack of time to evaluate the problem. There are many commercial software available e.g., LINGO, MATLAB, MINITAB, GAMS etc. Chapter 12 discussed the detail of these software. Computer is also essential for real time optimization and controlling the process using advanced control systems (e.g., Model Predictive Control).

Summary

- This chapter explains different aspects of optimization methods. Classification of various algorithms has been made based on structure and application area of the optimization problem. There are six main steps for chemical process optimization. These steps of chemical process optimization have been discussed in this chapter. A list of chemical engineering application of optimization is given and the detail of those applications are discussed in the subsequent chapters.

Review Questions

1.1 Give a list of variables required to optimize a heat exchanger.
1.2 Why proper selection of decision variables is required for optimization process?
1.3 Devise a scheme for optimizing a reactor-separator process, which maximizes the yield.
1.4 How do you classify the optimization algorithms based on various aspects?
1.5 Define degree of freedom. What is the significance of degree of freedom during optimization of a chemical process?