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978-1-107-10683-3 — Optimization for Chemical and Biochemical Engineering
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PART I

Overview of Optimization

Applications and Problem Formulations

1

Introduction to Optimization

1.1 STATEMENT OF GENERAL MATHEMATICAL PROGRAMMING (MP) (OPTIMIZATION) PROBLEM

A general optimization problem statement is presented in this section. The general form is that of the selection of an optimal set of system variables satisfying the modeling equations of the system considered.

The objective function is given by

$$\min_{x} \text{ or } \max_{x} \ f(x), \tag{1.1a}$$

where $x \in \mathbb{R}^n$ is a real-valued n-dimensional vector of system variables that have to be chosen optimally, and $f(x) : \mathbb{R}^n \mapsto \mathbb{R}^1$ is a scalar function we wish to either minimize or maximize. For example, we might wish to

- minimize production cost and
- maximize the profit of a process.

subject to the following equality constraint:

$$h(x) = 0, \tag{1.1b}$$

where $h(x) : \mathbb{R}^n \mapsto \mathbb{R}^{m_h}$ is a vector of m_h functions that have to be satisfied at the solution of the optimization problem. For example,

- Material and energy balances
- Equilibrium relations
- Physicochemical property estimators

The inequality constraint is given by

$$g(x) \ \leq \text{or} \geq 0, \tag{1.1c}$$

where $g(x) : \mathbb{R}^n \mapsto \mathbb{R}^{m_g}$ is a vector of m_g functions that have to be satisfied at the solution of the optimization problem. For example,

- Quality constraints, concentration limitations of by-products and pollutants
- Operating condition limitations, *e.g.* pressure and temperature bounds
- Availability of raw materials

Often, we may have simple bounds explicitly imposed on the system variables x:

$$x^L \leq x \leq x^U. \tag{1.1d}$$

Variations of the general optimization problem presented in Equations (1.1a)–(1.1d) are presented in the next few subsections.

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1.1.1 Unimodal vs Multimodal Objective Functions

We consider the case here of minimizing some objective function $f(x)$ without any constraints within a region of the variables x. Unimodal functions exhibit one extremum (either maximum or minimum), whereas multimodal functions have many extrema.

The case of one-dimensional functions is given in Figures 1.1 and 1.2.

The case of two-dimensional functions is given in Figures 1.3 and 1.4.

We will deal with such cases and learn to distinguish the type of functions when we discuss convexity in Chapter 3.

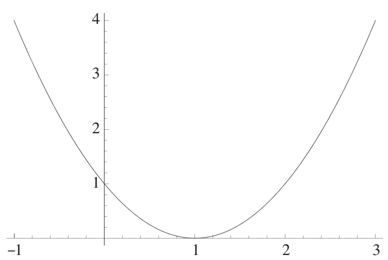

Figure 1.1 Unimodal function in one dimension.

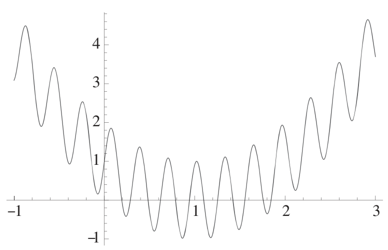

Figure 1.2 Multimodal function in one dimension.

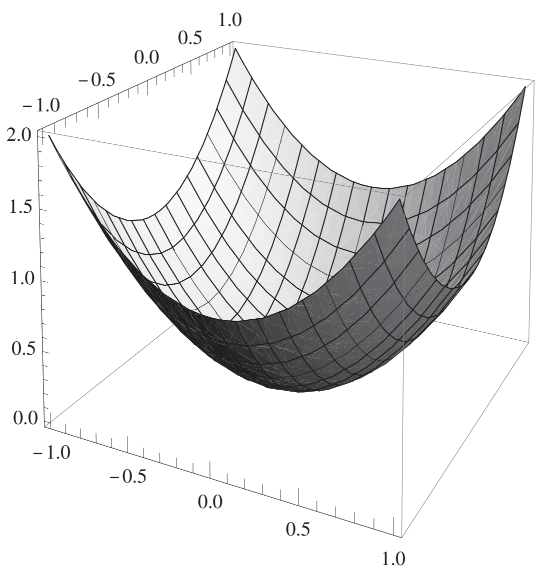

Figure 1.3 Unimodal function in two dimensions.

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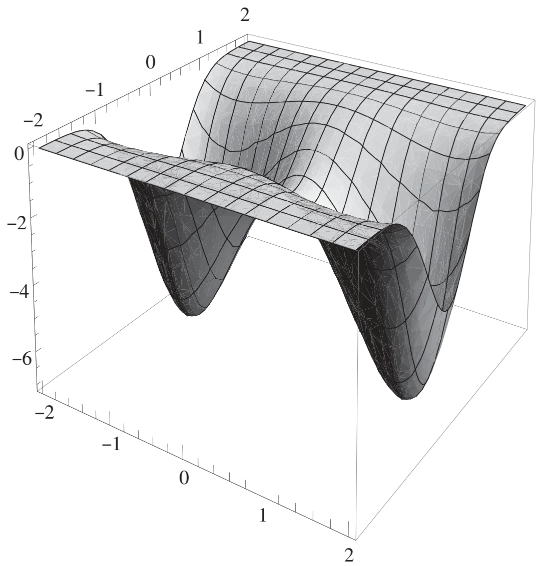

Figure 1.4 Multimodal function in two dimensions.

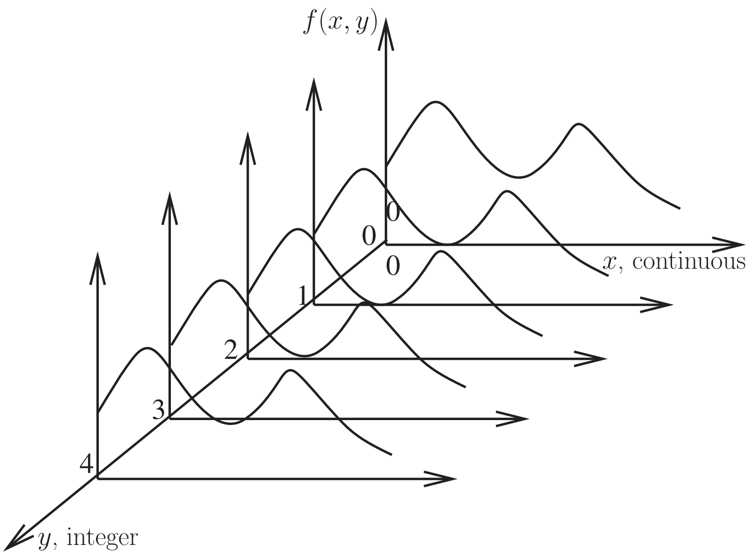

Figure 1.5 Mixed Integer function example.

1.1.2 Variable Types: Continuous, Integer, and Binary

In many real-world applications, we may wish to model systems for which the variables are not all continuous. Integer variables might be used to

- Count indivisible numbers of quantities, such as
  - number of people in a shift
  - the number of trays in a distillation column
  - the number of heat exchangers, *etc.*

- In the simplest integer form the variables might be binary
  - to reflect the presence of a unit or not
  - to reflect logic constraints (0/1 operations)

This type of variables results in *discrete optimization problems,* which need special techniques to be solved. In effect, the problems become discontinuous, as shown for the case of one variable being continuous and one being an integer in Figure 1.5.

1.2 APPLICATIONS IN TECHNOLOGICAL AND SCIENTIFIC PROBLEMS

Optimization is a very widely used tool for many real-world applications and in cutting-edge technologies. Some examples of such applications are given in the next few subsections.

1.2.1 Predicting the 3D Structures of Complex Molecules: Molecular Conformation and the Protein Folding Problem

The protein folding problem is set out here:

- Determine the 3D structure of the protein, given its linear sequence of amino acids
- Variables are the relative locations of the amino acids (angles, distances)
- Objective is the total energy of the conformation
  1. bending energy,
  2. bond stretching energy,
  3. bond torsion energy,
  4. electrostatic energies on amino acids.
- Constraints are the sequence and distance metrics of the amino acids

The characteristic of these problems is that their complexity grows quickly, in particular

- The problem is multimodal, *i.e.* there are multiple local minima of the energy objective function
- The number of local minima grows exponentially with the problem size

The solution of these problems falls within the category of global optimization methods, which are specially designed to guarantee the global optimality.

Global optimization, see Chapter 27, with rigorous guarantees of optimality is difficult – otherwise the formulation is fine and we would be able to predict *ab initio*[1] the structure of any given protein, and to design *de novo*[2] arbitrary proteins with prespecified functionality!

1.2.2 Designing Simpler Molecules: Organic Solvents and Refrigerants

The task here is to design organic molecules such that

- they have thermodynamic properties within specified tolerance margins

[1] *I.e.,* using basic micro-scale mechanisms *to predict* the larger-scale properties.
[2] "*from the start; new; not present previously;*" *i.e.* using fundamental microscale mechanisms to design *a given* larger-scale structure.

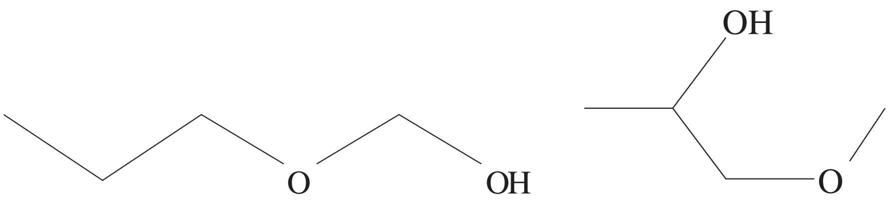

Figure 1.6 Skeletal formulae for propoxymethanol and 1-methoxy-2-propanol.

- they obey certain structural constraints (*e.g.* exclusion of given groups or types of bonds)
- they involve about 16 carbon atoms
- the applications are
  - new solvent design
  - new refrigerant design,
  - new monomers to produce polymers with desired properties
- the design is based on the selection of functional groups to include in the new molecules, such as CH3-, -CH2-, -OH, halogens, aromatic rings, *etc*.

The optimization problem formulations also involve continuous and binary variables. The following is an example of replacing an old solvent with new molecules:

- Ethyl glycol: CH3-CH2-O-CH2-CH2-OH
  - Environmentally problematic
  - Safety and health issues in the working environment of paint and ink industries
  - Toxic substance; serious health hazard
    - Respiratory problems
    - Infiltration into the blood stream can lead to liver problems
- New molecules obtained with optimization method, trying to match a list of thermodynamic properties are shown in Figure 1.6

Although this problem is also of combinatorial nature, the formulation results in an optimization problem with a smaller number of variables and it can be solved very efficiently, which will be considered in Chapter 21.

1.2.3 Refinery Operations: The Case of Pooling-Blending Problems

The blending problem is a typical case of refinery decision-making problem, as set out here:

- A number of r streams of distillate products (from crude oil distillation; raw materials to be blended)
- A number of p pools where the raw materials will be "pooled"
- A number of b blends (the final products)
- Target is to minimize cost of blends produced
- while satisfying blending constraints on concentrations (minimum octane number, maximum concentration of impurities, *e.g.* sulphur)
- and satisfying market demand (minimum production level)

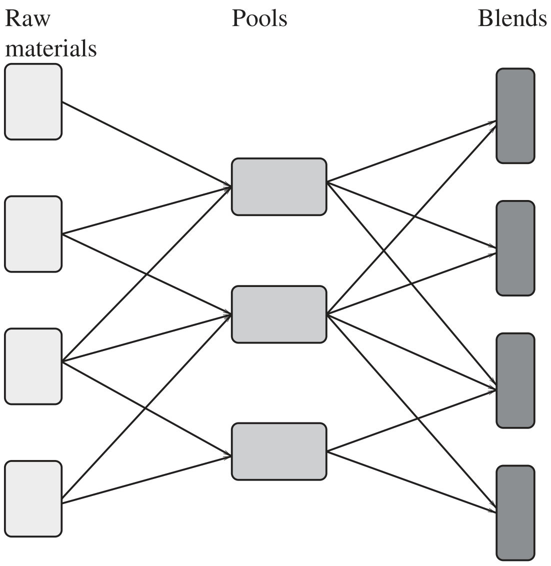

Figure 1.7 Sample pooling-blending flow chart.

A typical flow sheet of a pooling-blending problem is shown in Figure 1.7.

The model equations of this system are,

- Component-wise balances over the pools and blends
- Total flow balances over pools and blends
- Typical network flow problem, to be covered in Chapter 15

A simpler form, the pure blending problem, will be examined in Chapter 13.

The pooling-blending problem

- Is nonlinear, involving *bilinear terms, i.e.* product forms between two unknowns in the component balances,
- hence it belongs to the class of multimodal optimization problems
- and to guarantee its global optimality special solution procedures must be used

1.2.4 Parameter Estimation Problems (Model Fitting to Experimental or Plant Data)

Parameter estimation is a very important area of application of optimization methods. A number of uses are

- Fit a theoretical model to experimental data
- Fit a large nonlinear model to plant data for
  - simulation purposes
  - online optimizing control systems

The typical fitting criterion is the minimization of the sum of squares of the perpendicular distances of experimental data-points from the fitted model line, in one dimension, or the response “hypersurface” of a multidimensional model.

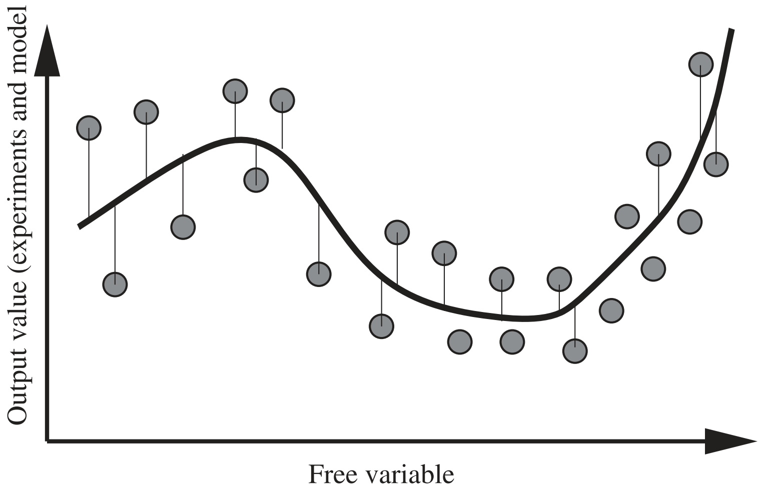

Figure 1.8 One-dimensional model fitting example.

The 1-D case is shown in Figure 1.8.

We shall examine a special case of fitting in detail in Chapter 4, the case of a linear model and least squares error minimization. A more general form of fitting, again with linear models, will be examined in Chapter 14.

1.2.5 Model Predictive Control (MPC) and Optimizing Control

Model Predictive Control (MPC) is the solution of Optimal Control problems in a continuous matter.

The key characteristics of this area of applications are the following,

- Identify the process model (by parameter estimation as in the previous section)
  - a process "drifts" with time (the process changes always), so there is a need to monitor the model's predictive ability and to reestimate its parameters
- Use an optimizer to predict a sequence of future control actions to regulate a process
- Implement the first period control actions predicted by the optimizer

Schematically, MPC is shown in Figure 1.9.

1.2.6 Process Design: The Case of the Synthesis of Binary Distillation Column Sequences

The design of separation sequences, for multicomponent mixtures, is a combinatorial optimization problem. Such problems can be formulated as optimization problems with both continuous and binary variables (logic variables).

Consider the case of a ternary mixture, of three components A, B, and C, listed in order of decreasing volatility. The possible sequences for the separation of the three components are given in Figure 1.10.

For a five-component mixture, Figure 1.11 shows the number of sequences and separations for the mixture A, B, C, D, and E, listed in order of decreasing volatility.

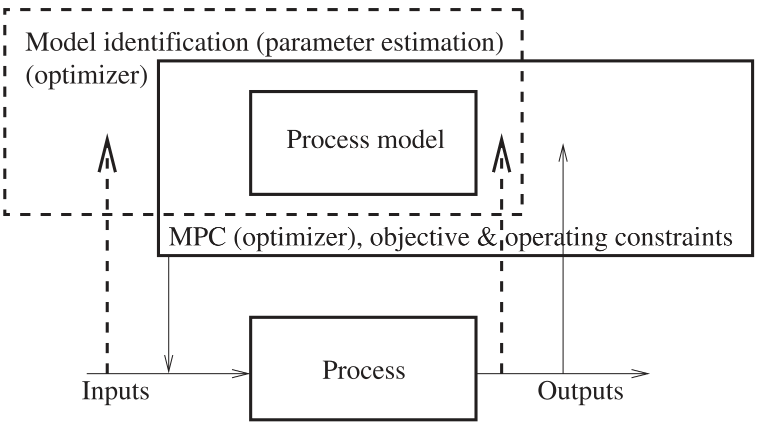

Figure 1.9 Schematic of an MPC algorithm.

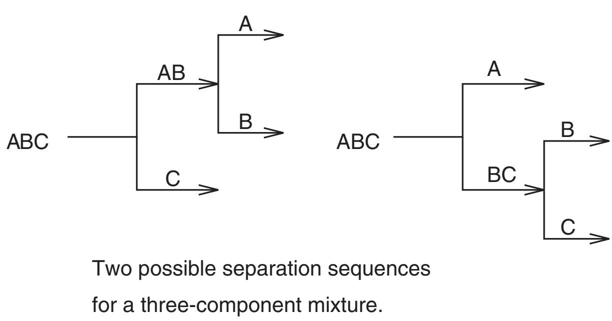

Figure 1.10 Two possible separation sequences for a three-component mixture.

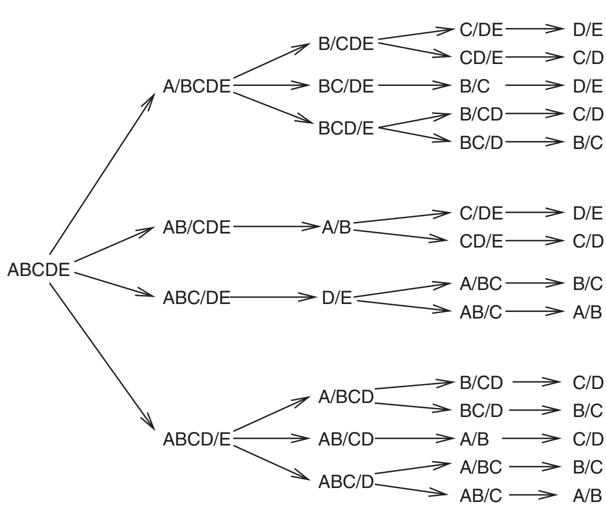

Figure 1.11 Possible separation sequences for a five-component mixture.