Chapter 1

Introduction

1.1 Requirements for the Application of Optimization Methods

1.1.1 Defining the System Boundaries

- A system is the restricted portion of the universe under consideration.
- The system boundaries are simply the limits that separate the system from the remainder of the universe.

1.1.2 The Performance Criteria

- economic criteria: total capital cost, annual cost, annual net profit, return on investment, cost-benefit ratio, net present value
- technological factors: minimum production time, maximum production rate, minimum energy utilization, maximum torque, maximum weight

1.1.3 The Independent Variables

- distinguish variables whose values are amenable to change from
  - variables whose values are fixed by external forces
  - system parameters that can be treated as fixed and those that are subject to fluctuations influenced by external and uncontrollable factors
- include all the important variables that influence the operation of the system or affect the design definition
- another consideration in the selection of variables is the level of detail to which the system is considered

1.1.4 The System Model

The system model describes the manner in which the problem variables are related and the way in which the performance criterion is influenced by the independent variables.

- basic material and energy balances
- engineering design relations
- physical property equations that describes the physical phenomena tanking place in the system.

1.2 Application of Optimization in Engineering

1. Design of components or entire systems
2. Planning and analysis of existing operations
3. Engineering analysis and data reduction
4. Control of dynamic systems

1.2.1 Design Application

Example 1.1 (Design of an oxygen supply system) *The basic oxygen furnace (BOF) used in the production of steel is a large fed-batch chemical reactor that employs pure oxygen. The furnace is operated in a cyclical fashion. Ore and flux are charged to the unit, treated for a specified time period, and then discharged. The cyclical operation gives rise to a cyclically varying demand rate for oxygen. As shown in Figure 1.2(a), over each cycle there is a time interval of length* t_1 *of low demand rate* D_0 *and a time interval* $(t_2 - t_l)$ *of high demand rate* D_1*. The oxygen used in the BOF is produced in an oxygen plant, in a standard process in which oxygen is separated from air by using a combination of refrigeration and distillation. Oxygen plants are highly automated and are designed to deliver oxygen at a fixed rate. In order to mesh the continuous oxygen plant with the cyclically operating BOF, a simple inventory system shown in Figure 1.2(b), consisting of a compressor and a storage tank, must be designed. A number of desige possibilities can be considered. In the simplest case, the oxygen plant capacity could be selected to be equal to* D_1*, the high demand rate. During the low-demand interval the excess oxygen could just be vented to the air. At the other extreme, the oxygen plant capacity could be chosen to be just enough to produce the amount of oxygen required by the BOF over a cycle. During the low-demand interval, the excess oxygen produced would then be compressed and stored for use during the high-demand interval of the cycIe. Intermediate designs could use some combination of venting and storage of oxygen. The problem is to select the optimal design.*

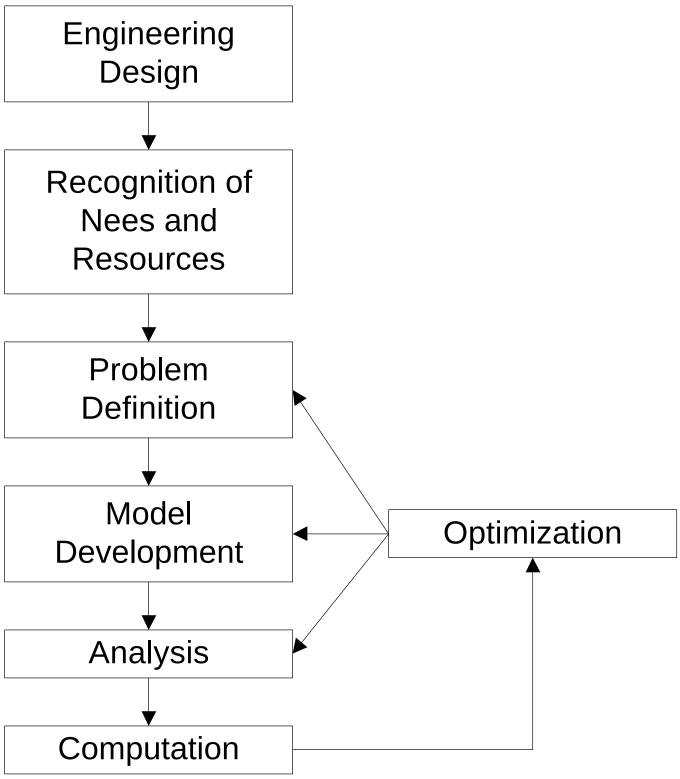
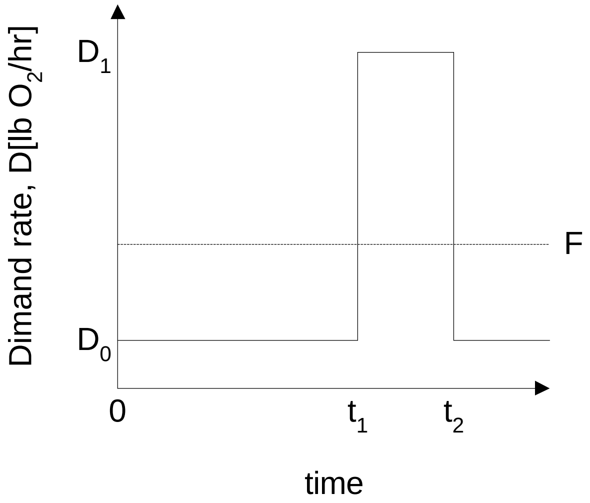
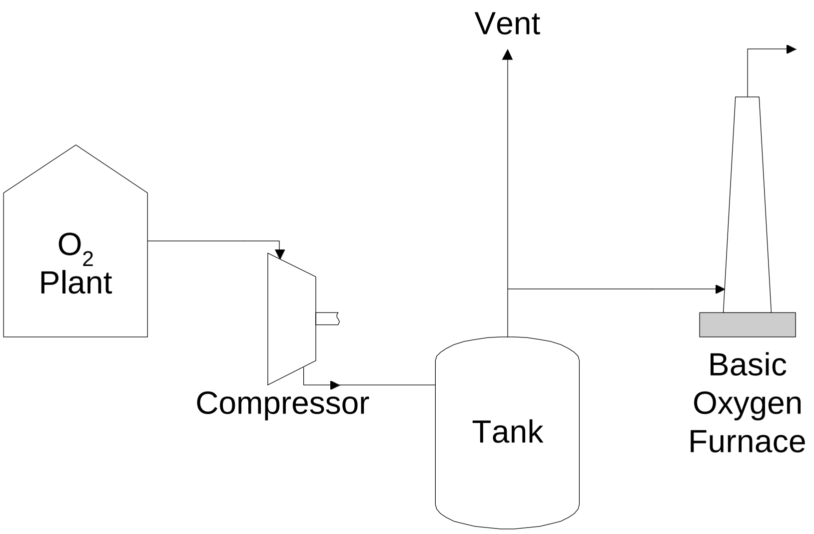


Figure 1.1: The engineering Design Process



(a) Oxygen demand cycle



(b) Oxygen production system

Figure 1.2: Design of an oxygen supply system, Example 1.1

System *consists of* O_2 *plant, compressor, and storage tank*

Performance index *total annual cost consists of*

- *oxygen production cost (fixed and variable)* $= a_1 + a_2F[\$/\mathrm{yr}]$
- *fixed costs of the storage vessel* $= b_1V^{b_2}[\$]$ *and compressor* $= b_3H^{b_4}[\$]$
- *compressor operating cost* $= b_5t_1H[\$/\mathrm{yr}]$

$$\textit{Annual cost} = a_1 + a_2F + d(b_1V^{b_2} + b_3H^{b_4}) + Nb_5t_1H[\$/\mathrm{yr}]$$

Independent variables

- F *is the oxygen plant production rate,* lb O_2/hr
- H *is the compressor capacity,* hp
- V *is the storage tank capacity,* ft^3
- p *is the maximum tank pressure,* psia

System model *Assume that*

- *the oxygen plant design is standard so that the production rate fully characterizes the plant, and*
- *the storage tank will be of a standard design approved for* O_2 *service.*

$$V = \frac{(D_1 - F)(t_2 - t_1)}{M}\frac{RT}{p}z = \frac{c_{11} - c_{12}F}{p}$$
$$H = \frac{(D_1 - F)(t_2 - t_1)}{t_1}\frac{RT}{k_1k_2}\ln\left(\frac{p}{p_0}\right) = (c_{21} - c_{22}F)\ln\left(\frac{p}{p_0}\right)$$
$$F \geq \frac{D_0t_1 + D_1(t_2 - t_1)}{t_2} = c_{31}$$
$$p \geq p_0$$

where

- k_1 *is a unit conversion factor*
- k_2 *is the compressor efficiency*
- M *is the molecular weight of* O_2
- p_0 *is the* O_2 *delivery pressure*
- R *is the gas constant*
- T *is the gas temperature (assumed to be fixed)*
- z *is the compressibility factor*

1.2.2 Operation and Planning Application

1. Accommodate increased production throughput
2. Adapt to different feedstocks or different product slate
3. Modify the operations because the initial design is itself inadequate or unreliable

Example 1.2 (Refinery Production Planning) *A refinery processes crude oils to produce a number of raw gasoline intermediates, which must subsequently be blended to make to grades of motor fuel, regular and premium. Each raw gasoline has a known performance rating, a maximum availability, and a fixed unit cost. The two motor fuels have a specified minimum performance rating and selling price, and their blending is achieved at a known unit cost. Contractual obligations impose minimum production requirements of both fuels. However, all excess fuel production or unused raw gasoline amounts can be sold in the open market at known prices. The optimal refinery production plan is to be determined over the next specified planning period.*

Independent variables *Let*

$$\begin{aligned} x_i &= \textit{amount used for regular}, \text{ Mbbl/period} \\ y_i &= \textit{amount used for premium}, \text{ Mbbl/period} \\ z_i &= \textit{amount sold directly}, \text{ Mbbl/period} \\ u_j &= \textit{amount allocated to contract}, \text{ Mbbl/period} \\ v_j &= \textit{amount sold in open market}, \text{ Mbbl/period} \end{aligned}$$

System model

1. *Material balances on each intermediate* $i = 1, \ldots, 5$*:*

$$x_i + y_i + z_i \leq \alpha_i$$

where α_i *is the availability if intermediate* i *in* Mbbl/period.

2. *Material balances on each product:*

$$\sum_i x_i = u_1 + v_1 \qquad \sum_i y_i = u_2 + v_2$$

3. *Blending constraints on each product*

$$\sum_i \beta_i x_i \geq \gamma_1(u_1 + v_1) \qquad \sum_i \beta_i y_i \geq \gamma_2(u_2 + v_2)$$

where β_i *is the performance rating of intermediate* i*, and* γ_j *is the minimum performance rating of product* j*.*

4. *Contract sales restrictions for each product* j*.*

$$u_j \geq \delta_j$$

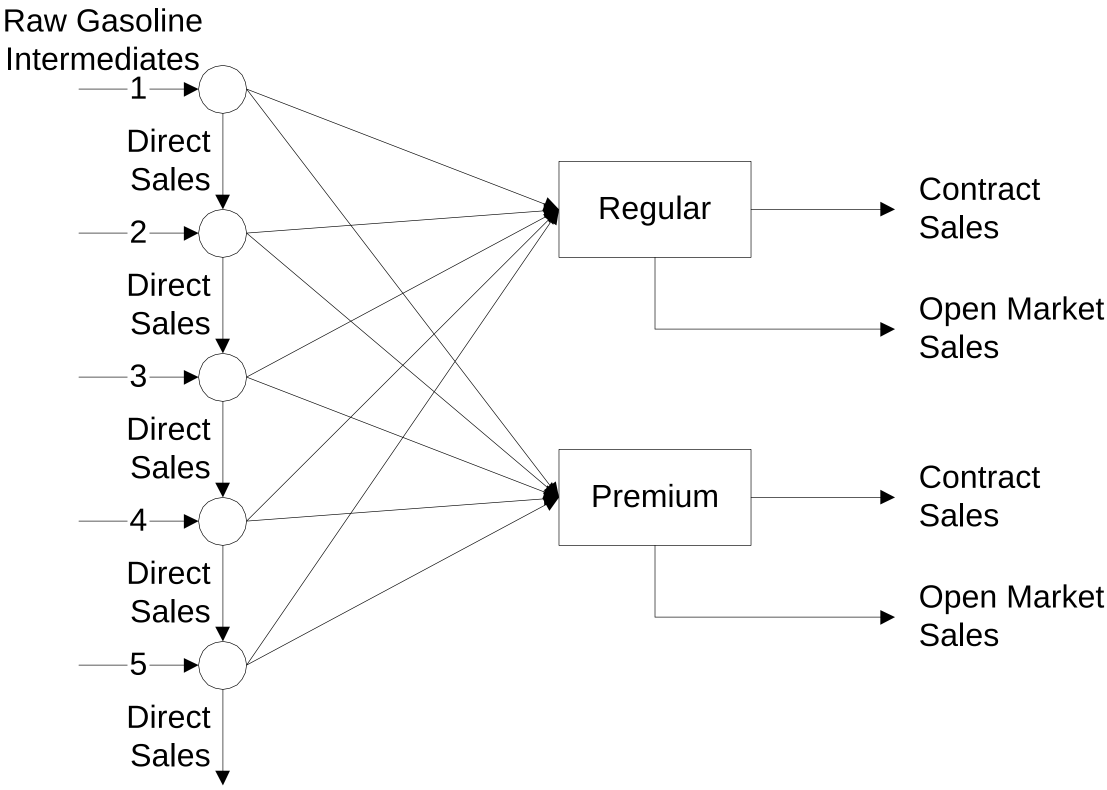


Figure 1.3: Schmatic of refinery planning problem, Example 1.2

Performance Criterion *(net profit) is given by*

$$Z = \sum_j c_j^{(1)} u_j + \sum_j c_j^{(2)} v_j + \sum_i c_i^{(3)} z_i - \sum_i c_i^{(4)} (x_i + y_i + z_i) - \sum_i c_i^{(5)} (x_i + y_i)$$

where

$$\begin{aligned} c_j^{(1)} &= \text{unit selling price for contract sales of } j \\ c_j^{(2)} &= \text{unit selling price for open market sales of } j \\ c_i^{(3)} &= \text{unit selling price of direct sales of intermediate } i \\ c_i^{(4)} &= \text{unit charge cost of intermediate } i \\ c_i^{(5)} &= \text{blending cost of intermediate } i \end{aligned}$$

Table 1.1: Data for Example 1.2

Raw Gasoline Intermediate	Availability α_i (bbl/period)	Performance Rating, β_i	Selling Price $c_i^{(3)}$	Charged Cost $c_i^{(4)}$	Blending Cost $c_i^{(5)}$
1	2×10^5	70	30.00	24.00	1.00
2	4×10^5	80	35.00	27.00	1.00
3	4×10^5	85	36.00	28.50	1.00
4	5×10^5	90	42.00	34.50	1.00
5	5×10^5	99	60.00	44.00	1.00
	Minimum	Minimum		Selling Price ($/bbl)	
Product Type	Contract Sales δ_j	Performance Rating		Contract $c_i^{(1)}$	Open Market $c_i^{(2)}$
Regular (1)	5×10^5	85		$40.00	$46.00
Premium (2)	4×10^5	95		$55.00	$60.00

Optimal solution $Z^* = \$28\text{M}$ *when*

$$\mathbf{x}^* = \begin{pmatrix} 0 \\ 0.4 \\ 0.4 \\ 1/6 \\ 1/12 \end{pmatrix} \quad \mathbf{y}^* = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1/3 \\ 5/12 \end{pmatrix} \quad \mathbf{z}^* = \begin{pmatrix} 0.2 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{u}^* = \begin{pmatrix} 0.5 \\ 0.4 \end{pmatrix} \quad \mathbf{v}^* = \begin{pmatrix} 0.55 \\ 0.35 \end{pmatrix}$$

1.2.3 Analysis and Data Reduction Applications

For a given system model

$$y = f(\mathbf{x}; \theta_1, \theta_2, \ldots)$$

the unknown parameters θ_1, θ_2, … can be determined if enough set of data (x_i, y_i), $i = 1, \ldots, n$ is given.

Least squares criterion

$$\min L(\theta_1, \theta_2, \ldots) = \sum_{i=1}^{n} [f(\mathbf{x}_i; \theta_1, \theta_2, \ldots) - y_i]^2$$

Example 1.3 (Nonlinear Curve Fitting) *Determine the parameters in the semiempirical Redlich-Kwong equation of state for a set of given PvT data.*

System model

$$P(v, T; a, b) = \frac{RT}{v - b} - \frac{a}{\sqrt{T} v(v + b)}$$

Independent variables a, b

Performance index

$$\min f(a, b) = \sum_{i=1}^{8} [P(v_i, T_i; a, b) - P_i]^2 = \sum_{i=1}^{8} \left[\frac{RT_i}{v_i - b} - \frac{a}{\sqrt{T_i} v_i (v_i + b)} - P_i \right]^2 \quad (1.1)$$

Table 1.2: PvT data for CO_2

Experiment Number	P atm	v cm^3/gmol	T K
1	33	500	273
2	43	500	323
3	45	600	373
4	26	700	273
5	37	600	323
6	39	700	373
7	38	400	273
8	63.6	400	373

1.2.4 Control of Dynamic Systems

Example 1.4 (Optimal Control of Batch Reactor) *A high-priced specialty chemicals is made in a batch reactor. The reactions of interest are*

$$R \xrightarrow{k_1} P$$

$$R \xrightarrow{k_2} W$$

where R is an expensive raw material, P is the product, and W is a waste byproduct. Both reactions are irreversible and first-order in species R.

System model *The velocity constants k_1 and k_2 are give by*

$$k_i = k_i^{\infty} e^{-E_i/RT(t)} \qquad i = 1,\ 2$$

Material balances on species R and P in the batch reactor are

$$\dot{R}(t) = -(k_1 + k_2)R(t)$$
$$\dot{P}(t) = k_1 R(t)$$
$$W(t) = R_0 - R(t) - P(t)$$
$$R(0) = R_0$$
$$P(0) = 0$$

Independent variable $T(t)$ *As a control engineer you have been asked to design a temperature control program for the batch reactor to be carried out over a given batch time, namely t_f, and which maximizes the amount of P produced at the end of the run.*

Performance index *the amount of P produced at $t = t_f$*

$$\max_{T(t)} P(t_f)$$

1.3 Structure of Optimization Problems

Optimization problem

$$\min(f_1(\mathbf{x}), \ldots, f_M(\mathbf{x}))$$

subject to

$$h_k(\mathbf{x}) = 0 \qquad k = 1, \ldots, K$$
$$g_j(\mathbf{x}) \geq 0 \qquad j = 1, \ldots, J$$
$$x_i^{(U)} \geq x_i \geq x_i^{(L)} \qquad i = 1, \ldots, N$$

where

- f_s, $s = 1, \ldots, M$ are objective functions
- $h_k = 0$ is equality constraint
- $g_j \geq 0$ and $x_i^{(U)} \geq x_i \geq x_i^{(L)}$ are inequality constraints

1.3.1 Classification of Optimization Problems

- If $M = 1$, the problem has single objective, and simply called optimization problem If $M \geq 2$ then the problem is called *multiobjective* optimization (MOO) problem.

- If $N = 1$ then the problem is called *single variable* optimization problem. If $N \geq 2$ then the problem is called *multivariable* optimization problem.

- If all x_i's are either 0 or 1 then the problem is called *binary* programming problem; if they are integers then *integer* programming (IP) problem; and if some of x_i's are integers and the rests are reals then the problem is called *mixed integer* programming (MIP) problem.

- If $J = K = 0$ and $x_i^{(U)} = -x_i^{(L)} = \infty$ for all $i = 1, \ldots, N$ the problem is called *unconstrained* problem, otherwise it is called *constrained* optimization problem.

- If all f, h_k's, and g_j's are linear w.r.t. $\mathbf{x}$ then the problem is called *linear* programming (LP) problem. If f is quadratic but all h_k's and g_j's are linear, then the problem is called *quadratic* programming (QP) problem. Otherwise it is called *nonlinear* programming (NLP) problem.

- If f is convex[1], all h_k's are linear, and all g_j's are concave[2], then the problem is *convex*, otherwise it is *nonconvex*.

1.3.2 Unsolvable or Trivial Problems

- For a constrained problem, there does not exist any $\mathbf{x}$ that satisfies all the constraints simultaneously, the the problem is said to be *infeasible*. If $K > N$ the problem has high chance of being infeasible.

- If the optimum is not bounded then the problem is said to be *unbounded*.

- If $K = N$, generally the solution is determined uniquely by the equality constraints.

1.4 Assignments

1.4.1 Reading Materials

- Reklaitis *et. al.*'s Chapter 1 [19]

- Edgar & Himmelblau's Part I [5]

- Rao's Chapter 1 [17]

[1] concave for maximization
[2] convex for $g_j \leq 0$

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Optimization Journals

- AIAA Journal
- ASCE Journal of Structural Engineering
- ASME Journal of Mechanical Design
- Computers and Chemical Engineering
- Computers and Operations Research
- Computers and Structures
- Engineering Optimization
- International Journal for Numerical Methods in Engineering
- Journal of Optimization Theory and Applications
- Management Sceience
- Operations Research
- SIAM Journal of Optimization
- Structural Optimization