Real-Time Optimization (RTO)

- In previous chapters we have emphasized control system performance for disturbance and set-point changes.
- Now we will be concerned with how the set points are specified.
- In *real-time optimization (RTO)*, the optimum values of the set points are re-calculated on a regular basis (e.g., every hour or every day).
- These repetitive calculations involve solving a constrained, steady-state optimization problem.
- **Necessary information:**
  1. Steady-state process model
  2. Economic information (e.g., prices, costs)
  3. A *performance Index* to be maximized (e.g., profit) or minimized (e.g., cost).

  Note: Items # 2 and 3 are sometimes referred to as an *economic model.*

Process Operating Situations That Are Relevant to Maximizing Operating Profits Include:

1. **Sales limited by production.**
2. **Sales limited by market.**
3. **Large throughput.**
4. **High raw material or energy consumption.**
5. **Product quality better than specification.**
6. **Losses of valuable or hazardous components through waste streams.**

Common Types of Optimization Problems

1. **Operating Conditions**
    - Distillation column reflux ratio
    - Reactor temperature
2. **Allocation**
    - Fuel use
    - Feedstock selection
3. **Scheduling**
    - Cleaning (e.g., heat exchangers)
    - Replacing catalysts
    - Batch processes

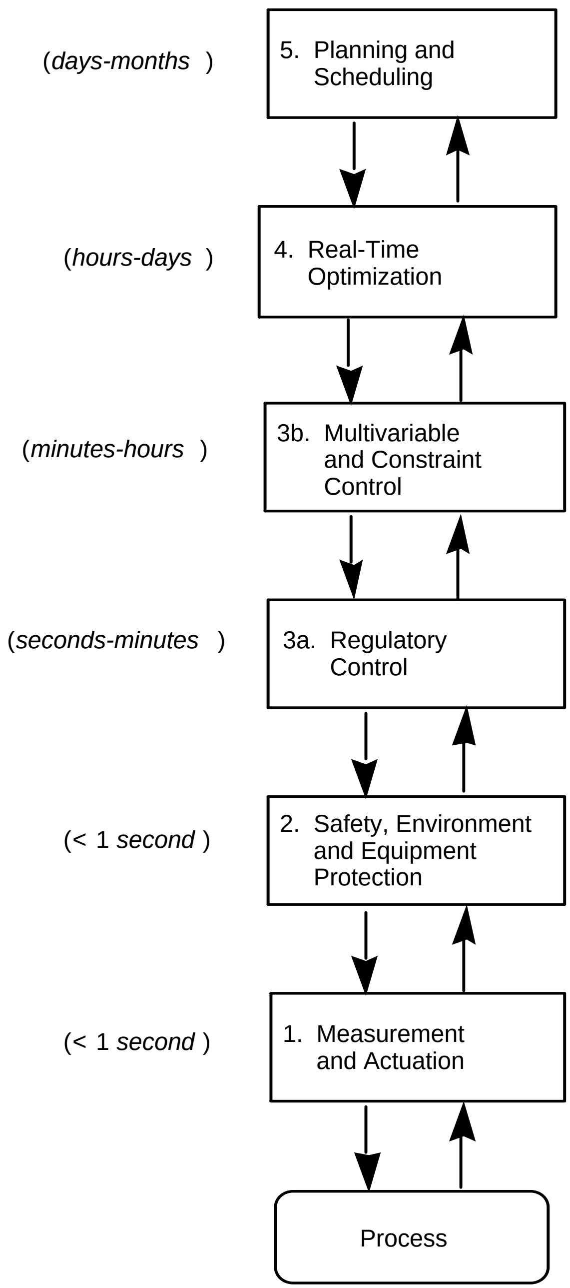

Figure 19.1 Hierarchy of process control activities.

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BASIC REQUIREMENTS IN REAL-TIME OPTIMIZATION

Objective Function:

$$P = \sum_s F_s V_s - \sum_r F_r C_r - OC \qquad (19\text{-}1)$$

where: P = operating profit/time

$\sum_s F_s V_s$ = sum of (product flow rate) x (product value)

$\sum_r F_r C_r$ = sum of (feed flow rate) x (unit cost)

OC = operating costs/time

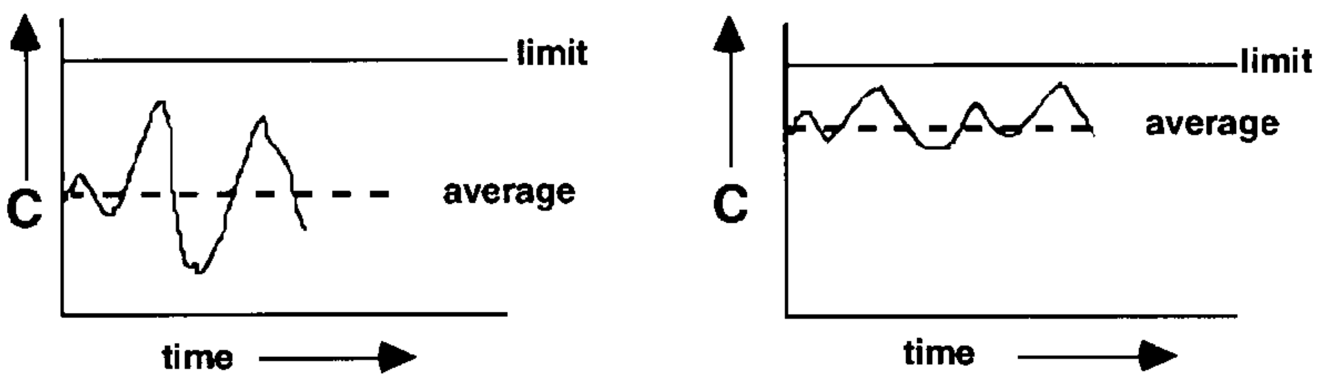
Both the operating and economic models typically will include constraints on:

1. Operating Conditions
2. Feed and Production Rates
3. Storage and Warehousing Capacities
4. Product Impurities

The Interaction Between Set-point Optimization and Process Control

Example: Reduce Process Variability

- Excursions in chemical composition => off-spec products and a need for larger storage capacities.
- Reduction in variability allows set points to be moved closer to a limiting constraint, e.g., product quality.



a) Before improved control

b) After improved control

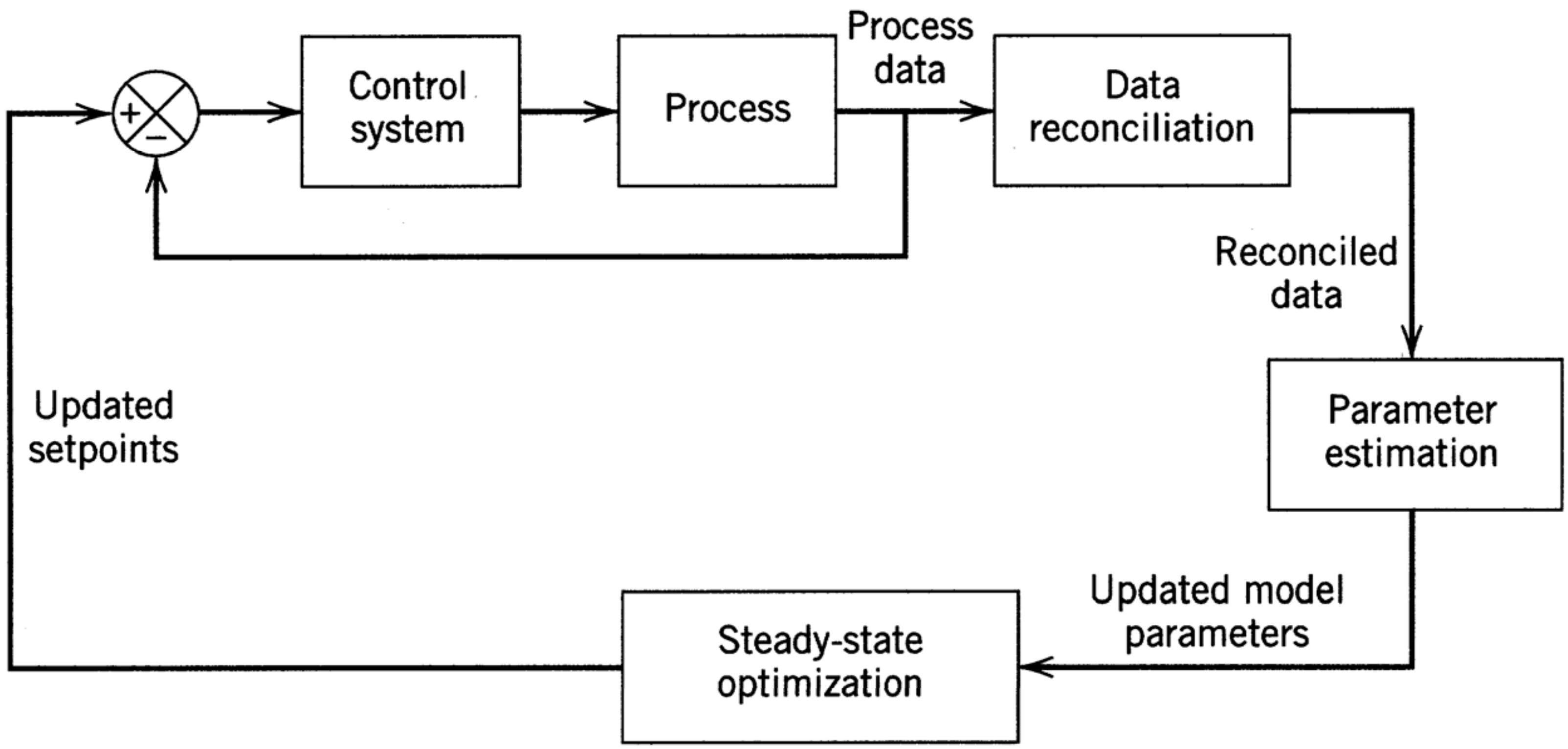


Figure 19.2 A block diagram for RTO and regulatory feedback control.

The Formulation and Solution of RTO Problems

1. ***The economic model*: An objective function to be maximized or minimized, that includes costs and product values.**
2. ***The operating model*: A steady-state process model and constraints on the process variables.**

The Formulation and Solution of RTO Problems

Table 19.1 Alternative Operating Objectives for a Fluidized Catalytic Cracker

1. Maximize gasoline yield subject to a specified feed rate.
2. Minimize feed rate subject to required gasoline production.
3. Maximize conversion to light products subject to load and compressor/regenerator constraints.
4. Optimize yields subject to fixed feed conditions.
5. Maximize gasoline production with specified cycle oil production.
6. Maximize feed with fixed product distribution.
7. Maximize FCC gasoline plus olefins for alkylate.

Selection of Processes for RTO

Sources of Information for the Analysis:

1. **Profit and loss statements for the plant**
   - Sales, prices
   - Manufacturing costs etc.
2. **Operating records**
   - Material and energy balances
   - Unit efficiencies, production rates, etc.

Categories of Interest:

1. **Sales limited by production**
   - Increases in throughput desirable
   - Incentives for improved operating conditions and schedules.
2. **Sales limited by market**
   - Seek improvements in efficiency.
   - Example: Reduction in manufacturing costs (utilities, feedstocks)
3. **Large throughput units**
   - Small savings in production costs per unit are greatly magnified.

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The Formulation and Solution of RTO Problems

- **Step 1. Identify the process variables.**
- **Step 2. Select the objective function.**
- **Step 3. Develop the process model and constraints.**
- **Step 4. Simplify the model and objective function.**
- **Step 5. Compute the optimum.**
- **Step 6. Perform sensitivity studies.**

Example 19.1

A section of a chemical plant makes two specialty products (E, F) from two raw materials (A, B) that are in limited supply. Each product is formed in a separate process as shown in Fig. 19.3. Raw materials A and B do not have to be totally consumed. The reactions involving A and B are as follows:

$$\text{Process 1:} \quad A + B \rightarrow E$$
$$\text{Process 2:} \quad A + 2B \rightarrow F$$

The processing cost includes the costs of utilities and supplies. Labor and other costs are \$200/day for process 1 and \$350/day for process 2. These costs occur even if the production of E or F is zero. Formulate the objective function as the total operating profit per day. List the equality and inequality constraints (Steps 1, 2, and 3).

Available Information

Raw Material	Maximum Available (lb/day)	Cost (¢/lb)
A	40,000	15
B	30,000	20

Process	Product	Reactant Requirements (lb) per lb Product	Processing Cost	Selling Price of Product	Maximum Production Level (lb/day)
1	E	2/3 A, 1/3 B	15 ¢/lb E	40 ¢/lb E	30,000
2	F	1/2 A, 1/2 B	5 ¢/lb F	33 ¢/lb F	30,000

SOLUTION The optimization problem is formulated using the first three steps delineated above.

Step 1. The relevant process variables are the mass flow rates of reactants and products (see Fig. 19.3):

$$x_1 = \text{lb/day A consumed}$$
$$x_2 = \text{lb/day B consumed}$$
$$x_3 = \text{lb/day E produced}$$
$$x_4 = \text{lb/day F produced}$$

Step 2. In order to use Eq. 19-1 to compute the operating product per day, we need to specify product sales income, feedstock costs, and operating costs:

$$\text{Sales income (\$/day)} = \sum_s F_s V_s = 0.4x_3 + 0.33x_4 \quad \textbf{(19-2)}$$

$$\text{Feedstock costs (\$/day)} = \sum_r F_r C_r = 0.15x_1 + 0.2x_2 \quad \textbf{(19-3)}$$

$$\text{Operating costs (\$/day)} = OC = 0.15x_3 + 0.05x_4 + 350 + 200 \quad \textbf{(19-4)}$$

Substituting into (19-1) yields the daily profit:

$$P = 0.4x_3 + 0.33x_4 - 0.15x_1 - 0.2x_2 - 0.15x_3 - 0.05x_4 - 350 - 200$$
$$= 0.25x_3 + 0.28x_4 - 0.15x_1 - 0.2x_2 - 550 \quad \textbf{(19-5)}$$

Step 3. Not all variables in this problem are unconstrained. First consider the material balance equations, obtained from the reactant requirements, which in this case comprise the process operating model:

$$x_1 = 0.667x_3 + 0.5x_4 \quad \textbf{(19-6a)}$$
$$x_2 = 0.333x_3 + 0.5x_4 \quad \textbf{(19-6b)}$$

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The limits on the feedstocks and production levels are:

$$0 \le x_1 \le 40{,}000 \quad \textbf{(19-7a)}$$

$$0 \le x_2 \le 30{,}000 \quad \textbf{(19-7b)}$$

$$0 \le x_3 \le 30{,}000 \quad \textbf{(19-7c)}$$

$$0 \le x_4 \le 30{,}000 \quad \textbf{(19-7d)}$$

Equations (19-5) through (19-7) constitute the optimization problem to be solved. Because the variables appear linearly in both the objective function and constraints, this formulation is referred to as a *linear programming problem*, which is discussed in Section 19.4. ■

UNCONSTRAINED OPTIMIZATION

- **The simplest type of problem**
- **No inequality constraints**
- **An equality constraint can be eliminated by variable substitution in the objective function.**

Single Variable Optimization

- **A single independent variable maximizes (or minimizes) an objective function.**
- **Examples:**

  1. Optimize the reflux ratio in a distillation column

  2. Optimize the air/fuel ratio in a furnace.

- **Typical Assumption: The objective function *f* (x) is *unimodal* with respect to *x* over the region of the search.**
  - **Unimodal Function: For a maximization (or minimization) problem, there is only a single maximum (or minimum) in the search region.**

Different Types of Objective Functions

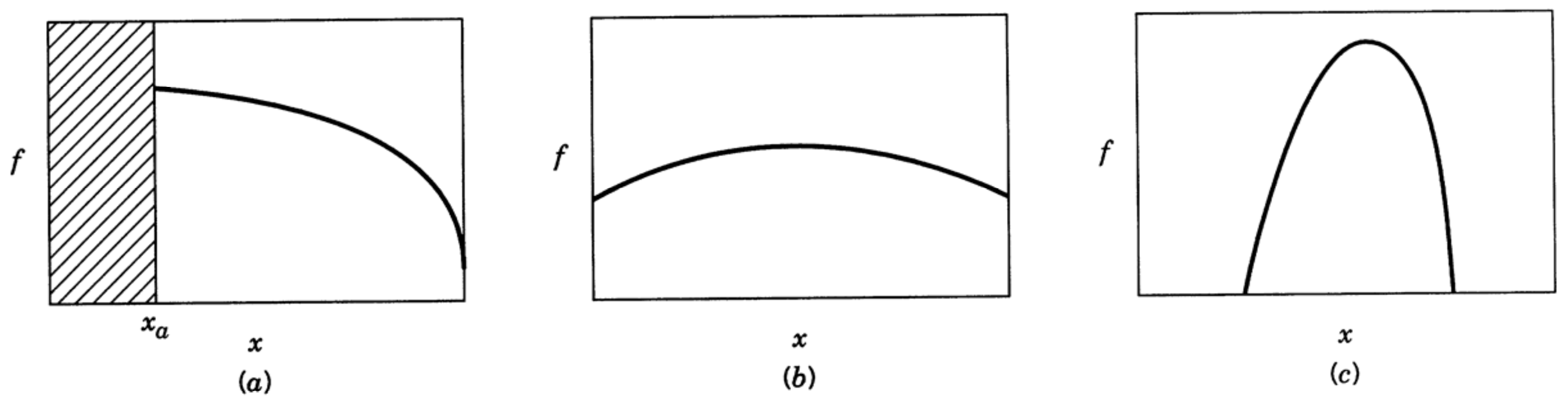

Figure 19.5 Three types of optimal operating conditions.

One Dimensional Search Techniques

Selection of a method involves a trade-off between the number of objective function evaluations (computer time) and complexity.

1. "Brute Force" Approach

Small grid spacing (Δx) and evaluate *f(x)* at each grid point $\Rightarrow$ can get close to the optimum but very inefficient.

2. Newton's Method

- **It is based on the necessary condion for optimality: $f'(x)=0$.**
- **Example: Find a minimum of $f(x)$. Newton's method gives,**

$$x^{k+1} = x^k - \frac{f'(x^k)}{f''(x^k)}$$

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3. Quadratic Polynomial fitting technique

1. **Fit a quadratic polynomial, *f (x)* = $a_0+a_1x+a_2x^2$, to three data points in the interval of uncertainty.**
   - Denote the three points by x_a, x_b, and x_c , and the corresponding values of the function as f_a, f_b, and f_c.
2. **Find the optimum value of *x* for this polynomial:**

$$x^* = \frac{1}{2}\frac{\left(x_b^2 - x_c^2\right) f_a + \left(x_c^2 - x_a^2\right) f_b + \left(x_a^2 - x_b^2\right) f_c}{\left(x_b - x_c\right) f_a + \left(x_c - x_a\right) f_b + \left(x_a - x_b\right) f_c} \qquad (19-8)$$

4. **Evaluate *f (x*)* and discard the *x value* that has the <u>worst</u> value of the objective function. (i.e., discard either x_a, x_b, or x_c).**
5. **Choose *x** to serve as the new, third point.**
6. **Repeat Steps 1 to 5 until no further improvement in *f (x*)* occurs.**

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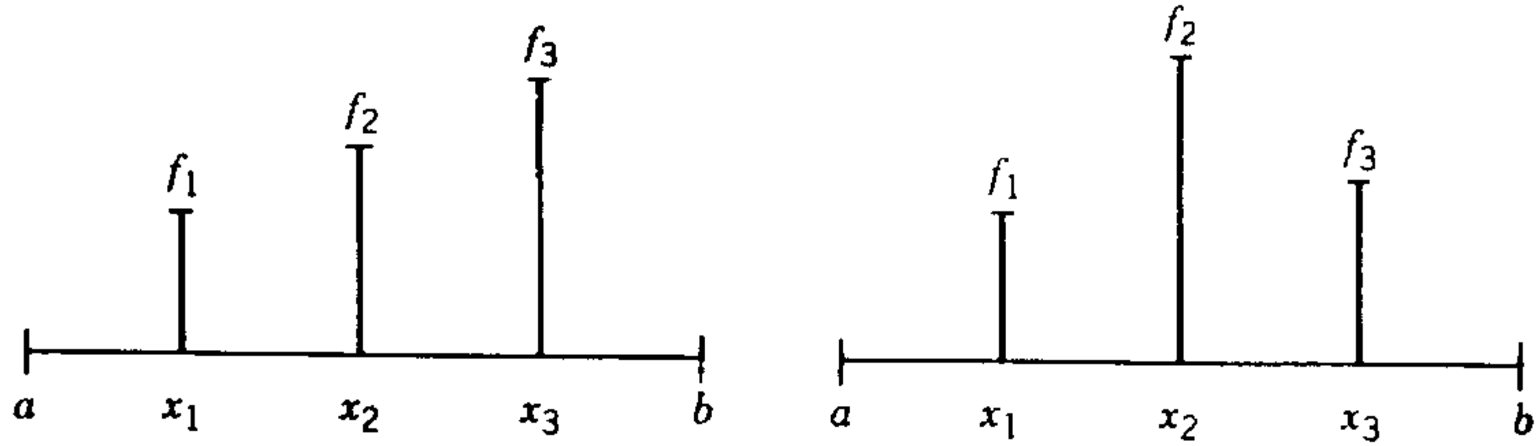
Equal Interval Search: Consider two cases



(1) $f_1 < f_2 < f_3$
$L_1 = [x_2, b]$

(2) $f_2 > f_3 > f_1$
$L_1 = [x_1, x_3]$

Figure 20.3. Two cases arising in a three-point equal-interval search.

Case 1: **The maximum lies in (x_2, b).**

Case 2: **The maximum lies in (x_1, x_3).**

Multivariable Unconstrained Optimization

$$f(\mathbf{x}) \quad f\left(x_1, x_2, ..., x_{N_v}\right)$$

- Computational efficiency is important when *N* is large.
- "Brute force" techniques are not practical for problems with more than 3 or 4 variables to be optimized.
- **Typical Approach:** Reduce the multivariable optimization problem to a series of one dimensional problems:

  (1) From a given starting point, specify a search direction.
  (2) Find the optimum along the search direction, i.e., a one-dimensional search.
  (3) Determine a new search direction.
  (4) Repeat steps (2) and (3) until the optimum is located

- **Two general categories for MV optimization techniques:**

  (1) Methods requiring derivatives of the objective function.
  (2) Methods that do not require derivatives.

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Constrained Optimization Problems

- **Optimization problems commonly involve equality and inequality constraints.**
- **Nonlinear Programming (NLP) Problems:**
  a. Involve nonlinear objective function (and possible nonlinear constraints).

  b. Efficient off-line optimization methods are available (e.g., conjugate gradient, variable metric).

  c. On-line use? May be limited by computer execution time and storage requirements.
- **Quadratic Programming (QP) Problems:**
  a. Quadratic objective function plus linear equality and inequality constraints.

  b. Computationally efficient methods are available.
- **Linear Programming (QP) Problems:**

  a. Both the objective function and constraints are

  b. Solutions are highly structured and can be rapidly obtai

LP Problems (continued)

- Most LP applications involve more than two variables and can involve 1000s of variables.
- So we need a more general computational approach, based on the Simplex method.
- There are many variations of the Simplex method.
- One that is readily available is the Excel Solver.

Recall the basic features of LP problems:

- Linear objective function
- Linear equality/inequality constraints

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Linear Programming (LP)

- **Has gained widespread industrial acceptance for on-line optimization, blending etc.**

- **Linear constraints can arise due to:**
  1. **Production limitation:** e.g. equipment limitations, storage limits, market constraints.
  2. **Raw material limitation**
  3. **Safety restrictions:** e.g. allowable operating ranges for temperature and pressures.
  4. **Physical property specifications:** e.g. product quality constraints when a blend property can be calculated as an average of pure component properties:

$$\overline{P} = \sum_{i=1}^{n} y_i P_i \leq \alpha$$

5. **Material and Energy Balances**
   - Tend to yield equality constraints.
   - Constraints can change frequently, e.g. daily or hourly.

- **Effect of Inequality Constraints**
  - Consider the linear and quadratic objective functions on the next page.
  - Note that for the LP problem, the optimum must lie on one or more constraints.

- **Solution of LP Problems**
  - Simplex Method
  - Examine only constraint boundaries
  - Very efficient, even for large problems

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Linear Programming Concepts

- For a linear process model,

$$y = Ku \tag{19-18}$$

The standard linear programming (LP) problem can be stated as follows:

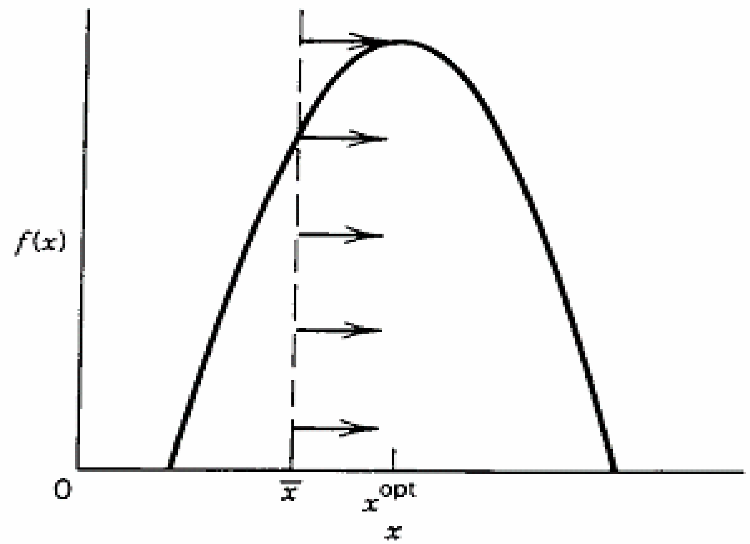
$$\text{minimize } f = \sum_{i=1}^{N_V} c_i x_i \tag{19-19}$$

subject to:

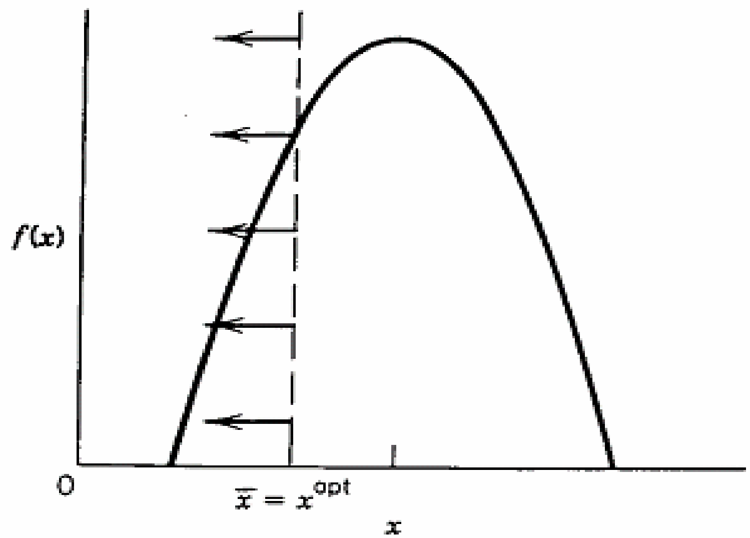
$$x_i \geq 0 \qquad i = 1, 2, \ldots N_V$$

$$\sum_{j=1}^{N_V} a_{ij} x_j \geq b_i \qquad i = 1, 2, \ldots N_I \tag{19-20}$$

$$\sum_{j=1}^{N_V} \tilde{a}_{ij} x_j = d_i \qquad i = 1, 2, \ldots N_E \tag{19-21}$$



(a) Constrained case $(x \geq \bar{x})$, $x^{opt} = \frac{-a_1}{2a_2}$



(b) Constrained case $(x \leq \bar{x})$, $x^{opt} = \bar{x}$

Figure The effect of an inequality constraint on the maximum of quadratic function, $f(x) = a_0 + a_1 + a_2x^2$. (The arrows indicate the allowable values of x.)

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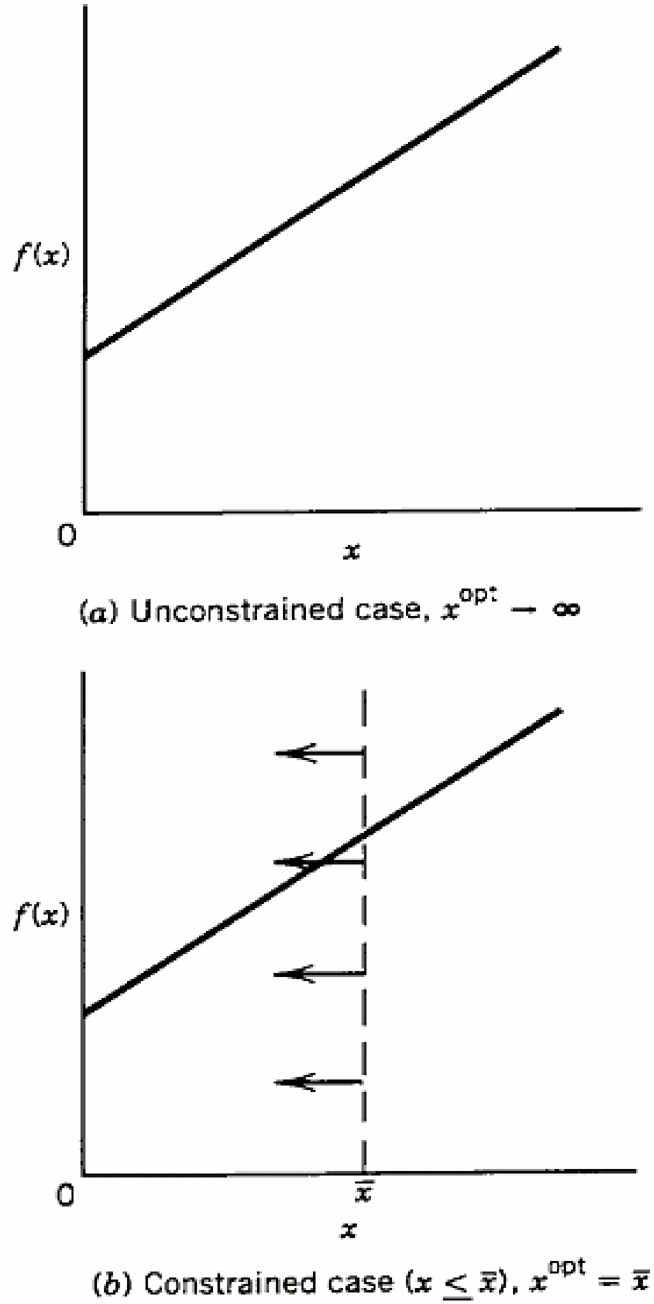

The effect of a linear constraint on the maximum of linear objective function, $f(x) = a_0 + a_1 x$.

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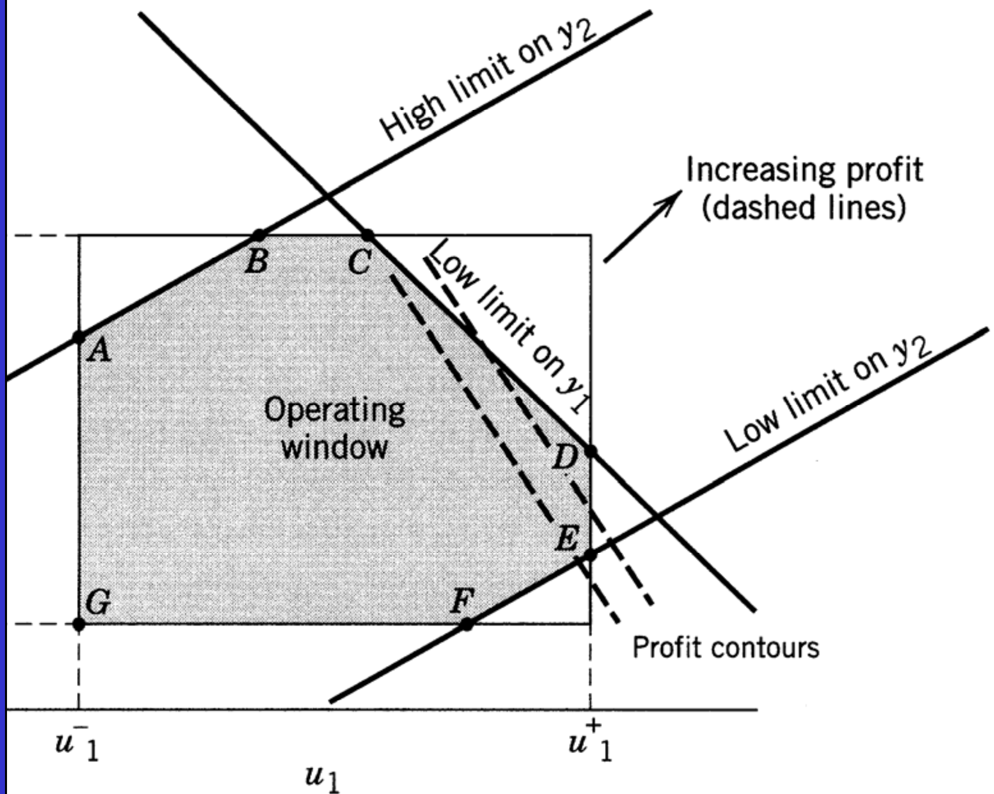

Figure 19.6 Operating window for a 2 x 2 optimization problem. The dashed lines are objective function contours, increasing from left to right. The maximum profit occurs where the profit line intersects the constraints at vertex *D*.

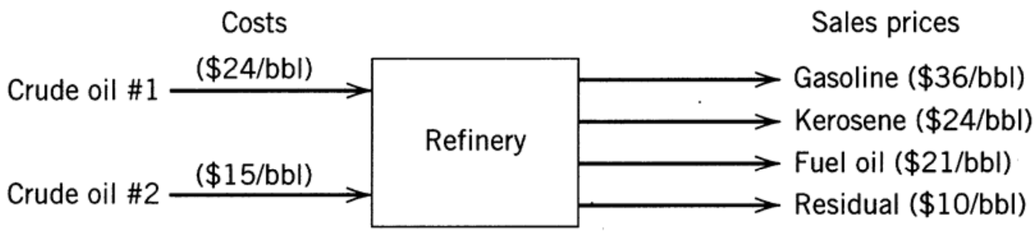

Figure 19.7 Refinery input and output schematic.

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Table 19.3 Data for the Refinery Feeds and Products

	Volume percent yield		Maximum allowable production (bbl/day)
	Crude #1	Crude #2	
Gasoline	80	44	24,000
Kerosene	5	10	2,000
Fuel oil	10	36	6,000
Processing cost ($/bbl)	0.50	1.00	

Solution

Let x_1 = crude #1 (bbl/day)
x_2 = crude #2 (bbl/day)

Maximize profit (minimize cost):

y = income - raw mat'l cost - proc.cost

Calculate amounts of each product produced:

gasoline = $0.80\ x_1 + 0.44\ x_2$
kerosene = $0.05\ x_1 + 0.10\ x_2$
fuel oil = $0.10\ x_1 + 0.36\ x_2$
residual = $0.05\ x_1 + 0.10\ x_2$

Income

gasoline $(36)(0.80\ x_1 + 0.44\ x_2)$
kerosene $(24)(0.05\ x_1 + 0.10\ x_2)$
fuel oil $(21)(0.10\ x_1 + 0.36\ x_2)$
residual $(10)(0.05\ x_1 + 0.10\ x_2)$

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So,

$$\text{Income} = 32.6\, x_1 + 26.8\, x_2$$

$$\text{Raw mat'l cost} = 24\, x_1 + 15\, x_2$$

$$\text{Processing cost} = 0.5\, x_1 + x_2$$

Then, the objective function is

$$\text{Profit} = y = 8.1\, x_1 + 10.8\, x_2$$

<u>Constraints</u>

Maximum allowable production:

$$0.80\, x_1 + 0.44\, x_2 \leq 24{,}000 \quad \text{(gasoline)}$$

$$0.05\, x_1 + 0.10\, x_2 \leq 2{,}000 \quad \text{(kerosene)}$$

$$0.10\, x_1 + 0.36\, x_2 \leq 6{,}000 \quad \text{(fuel oil)}$$

and, of course, $x_1 \geq 0, \quad x_2 \geq 0$

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Graphical Solution

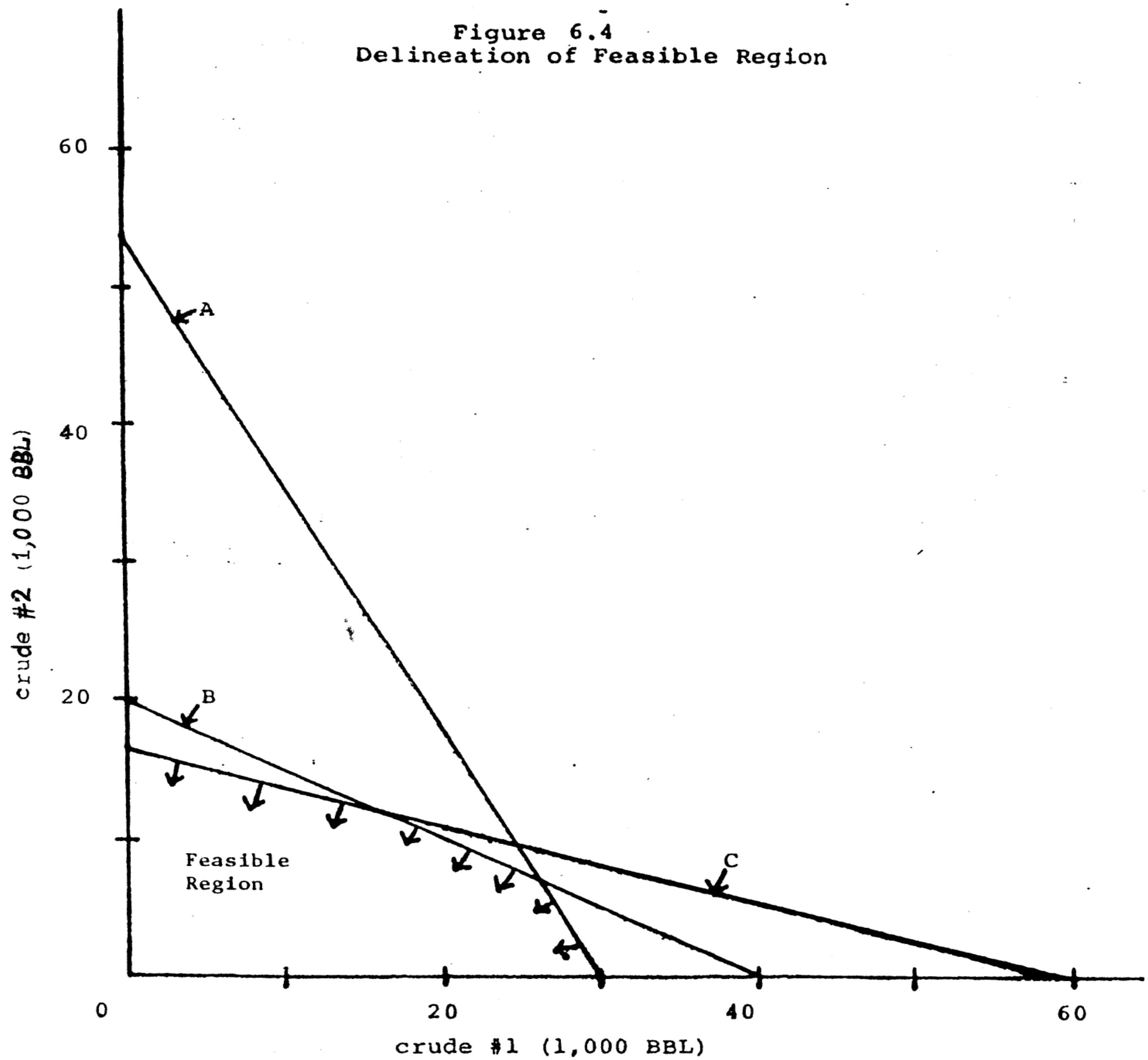
1. Plot constraint lines on x_1-x_2 plane.

2. Determine feasible region (those values of x_1 and x_2 that satisfy maximum allowable production constraints.

3. Find point or points in feasible region that maximize $y = 8.1\ x_1 + 10.8\ x_2$; this can be found by plotting the line $8.1\ x_1 + 10.8\ x_2 = P$, where P can vary, showing different profit levels.

$$.80x_1 + .44x_2 \leq 24{,}000 \quad (A)$$
$$.05x_1 + .10x_2 \leq 2{,}000 \quad (B)$$
$$.10x_1 + .36x_2 \leq 6{,}000 \quad (C)$$

Figure 6.4
Delineation of Feasible Region



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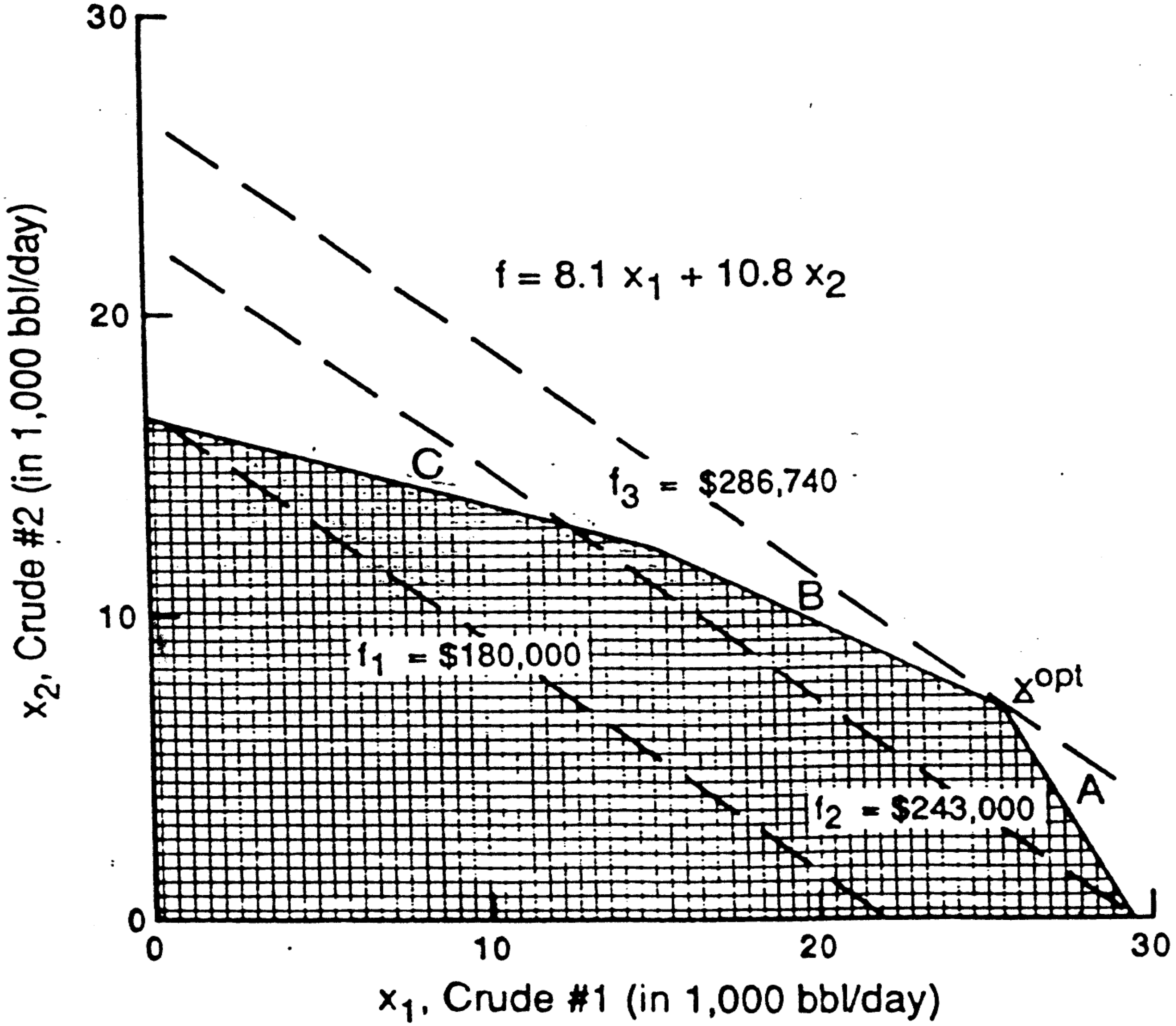

Figure 14

Feasible Region With Parameterization of Objective Function in Linear Programming

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From the graph,

$$x_1^{opt} \sim 26{,}000$$
$$x_2^{opt} \sim 7{,}000$$

More precisely, this is the intersection of the first two constraints, so x_1^{opt} and x_2^{opt} can be solved for simultaneously:

$$0.80\ x1 + 0.44\ x2 = 34{,}000$$
$$0.50\ x1 + 0.10\ x2 = 2{,}000$$

$$\Rightarrow\ x_1^{opt} = 26{,}200 \quad \text{and}\ x_2^{opt} = 6{,}900$$

with $P = \$\ 286{,}740/\text{day}$

As expected, optimum is at a corner of the feasible region.

Investigate the profit at the other corners:

(x_1, x_2)	Profit
(0,16667)	180,000
(15000,12500)	256,500
(30000,0)	243,000

QUADRATIC AND NONLINEAR PROGRAMMING

- The most general optimization problem occurs when both the objective function and constraints are nonlinear, a case referred to as nonlinear programming (NLP).

- **The leading constrained optimization methods include:**

1. Quadratic programming
2. Generalized reduced gradient
3. Successive quadratic programming (SQP)
4. Successive linear programming (SLP)

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Quadratic Programming

- A quadratic programming problem minimizes a quadratic function of *n* variables subject to *m* linear inequality or equality constraints.
- In compact notation, the quadratic programming problem is

$$\textbf{Minimize} \quad f(\boldsymbol{x}) = \boldsymbol{c}^{\boldsymbol{T}}\boldsymbol{x} + \frac{1}{2}\boldsymbol{x}^{\boldsymbol{T}}\boldsymbol{Q}\boldsymbol{x} \qquad (19-31)$$

$$\textbf{Subject to} \quad \boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$$

$$\boldsymbol{x} \geq 0 \qquad (19-32)$$

where ***c*** is a vector (n x 1), ***A*** is an m x n matrix, and ***Q*** is a symmetric n x n matrix.

Nonlinear Programming

$$\text{maximize} \quad f(x_1, x_2, \ldots, x_{N_V}) \qquad (19\text{-}13)$$

$$\text{subject to:} \quad h_i(x_1, x_2, \ldots, x_{N_V}) = 0 \quad (i = 1, \ldots, N_E) \qquad (19\text{-}14)$$

$$g_i(x_1, x_2, \ldots, x_{N_V}) \leq 0 \quad (i = 1, \ldots, N_I) \qquad (19\text{-}15)$$

a) **Constrained optimum:** The optimum value of the profit is obtained when $\boldsymbol{x}=\boldsymbol{x}_a$. Implementation of an active constraint is straight-forward; for example, it is easy to keep a valve closed.

b) **Unconstrained flat optimum:** In this case the profit is insensitive to the value of *x*, and small process changes or disturbances do not affect profitability very much.

c) **Unconstrained sharp optimum:** A more difficult problem for implementation occurs when the profit is sensitive to the value of *x*. If possible, we may want to select a different input variable for which the corresponding optimum is flatter so that the operating range can be wider.

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Nonlinear Programming (NLP) Example

- nonlinear objective function
- nonlinear constraints

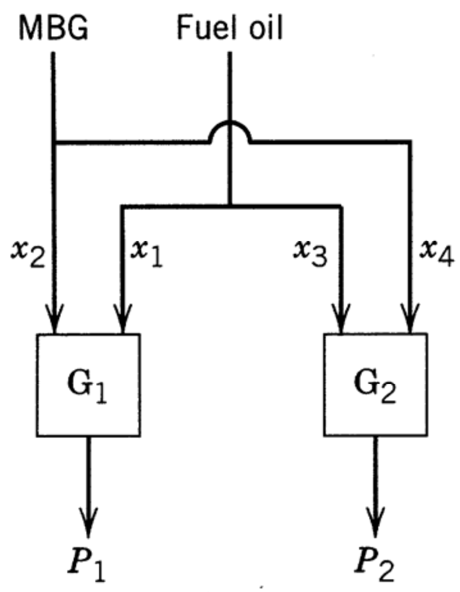

Figure 19.9 The allocation of two fuels in a boilerhouse with two turbine generators (G_1, G_2).