

## **Chapter 6**

# **Optimization**

### **Introductory Example**

Consider the problem of choosing the diameter of a pipe to convey a fluid from one process to another. In general, the larger the pipe diameter used, the lower the pressure drop requirements, and therefore, the lower the cost of pumping (operating costs). Larger pipe diameters require greater capital investment for the pipe and, to a much lesser extent, lower capital costs for the pump. These competing factors (operating costs and capital costs) make it possible for there to be an optimum pipe size for which the overall cost is minimized. That is, neither very small nor very large pipe diameters are economically efficient.

Let us find the optimum pipe diameter to be used to transport 50 gallons per minute of water 500 feet with no net elevation changes, using the following economic factors:

- Yearly capital charges are 20% of original purchase price.
- System is in use 90% of the time.
- Pump efficiency is 80%.
- Cost of electricity is \$.06/kW-hr.
- Schedule 40 carbon steel pipes are used.
- Cost of one inch diameter pipe is \$.70/ft.
- Spare pump is used to ensure continuous operation.

**Table 6.1** shows a comparison of yearly capital charges and yearly operating costs for five different pipe sizes. Note that the 2-inch pipe diameter case resulted in the lowest overall cost, representing the best compromise between capital and operating costs.

**Table 6.1** Economic Comparison of Cost (\$/yr) for Different Pipe Diameters\*

Costs	Pipe Diameter (inches)				
	1	1.25	1.5	2	2.5
Operating Costs	4697	660	312	164	75
Pipe Capital Costs	350	400	446	530	636
Pump Capital Costs	401	192	150	150	150
Total	5448	1210	908	844	861

\*Based upon the method presented by Peters and Timmerhaus [1] with pump capital costs included.

## Introduction

Optimization can be defined in a general sense as the method of identifying the best way to do something. In the introductory example, the best pipe size for a particular application was considered. Following are several other types of optimization problems:

- Find the best route to drive to work.
- Schedule construction in the most efficient manner.
- Design a particular chemical plant to be as profitable for a company as possible.

Let us consider the first problem. The *best* route to drive to work is usually the shortest route. But what if another route is actually quicker, e.g., a route involving travel on a freeway. Additional considerations might include traffic, scenery, and safety. Clearly, best in this case would mean different things to different people. Therefore, in order to solve the first problem, one must clearly and explicitly define what best means, i.e., minimum driving time, shortest route, or an explicit combination of several factors.

The second problem also suffers from the lack of explicitness associated with the terms "most efficient manner." For example, one schedule might minimize the time of construction but require higher rates of wages (due to overtime) and the more costly use of more contractors. On the other hand, if the cost of construction were minimized, the time of construction could be excessive. In this case, both factors must be put on the same basis: economic. That is, the time of construction must be converted into a cost figure.

The third problem is more clearly defined but still has considerable ambiguity associated with it. Obviously, a company is not interested in an investment that maximizes net profit without regard to the capital investment requirements. Depending upon a company's current financial situation, there are a number of possible methods for analyzing the economic viability of a project. Among these are the

internal rate of return, payback method, and present value to capital investment ratio [2]. Each one of these methods places a different emphasis upon the capital expenditures and cash flows of the project. In addition, the application of each one of these methods is highly dependent upon the interest rate assumed (i.e., a company's cost of capital), which can change significantly from one company to another and even during a project.

The point of this discussion is to emphasize a basic principle:

**The objective function must be explicitly defined before a meaningful optimization can be performed.**

Almost all optimization studies performed use an economic objective function, since the monetary value of a project is the easiest and most relevant basis of comparison. An example of a noneconomic optimization would be the optimization of the accuracy of a particular experimental measurement.

Another important consideration in an optimization study is the constraints on the problem. For example, in the best route problem, if the objective were to minimize travel time, the speed limit on the route would be a constraint on the problem. Also, when a stop sign is encountered, the resumption of speed would not be instantaneous. **Table 6.2** lists some of the engineering constraints that are commonly encountered when performing an optimization study.

There is a temptation when performing an optimization study to find the optimum set of conditions to a high degree of accuracy. It is highly unlikely that the mathematical description of the objective function and the set of constraints are nearly as accurate. As a result, one should be aware of the accuracy of the model or experimental measurements when selecting the optimum set of independent variables for the solution. In other words, an optimization study is no better than the description of the objective function and constraints. In addition, the sensitivity of the optimum

**Table 6.2** Commonly Encountered Constraints

- Environmental factors
- Safety considerations
- Availability of utilities
- Corrosion considerations
- Space limitations
- Availability and characteristics of feed stocks
- Manpower availability
- Market demand for the product
- An upper limit on the capital investment
- Maximum conversion limitations
- Strength of materials
- Maximum process temperature
- Product purity
- Maximum flow rate limitations

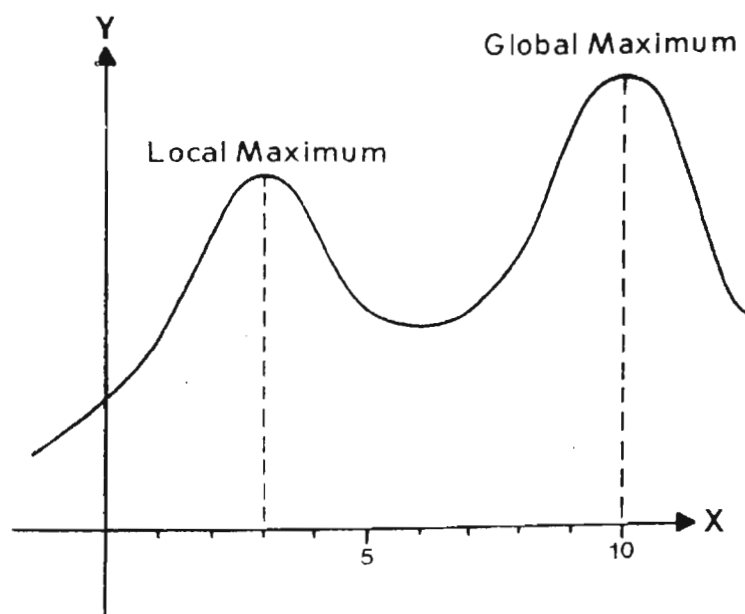


Figure 6.1 Example function.

to the uncertainty in the process model and the parameters of the problem should also be assessed.

Finally, most numerical optimizers assume that the objective function is unimodal over the range of interest of the independent variables. A unimodal function is shown in **Figure 6.1** for  $0 < x < 5$ . A unimodal function has either one *hump* or one *valley*. Note that in **Figure 6.1**, for  $0 < x < 5$ , the objective function has a local maximum; i.e., the objective function has a hump. The global maximum (the largest value) of the objective function for this problem occurs at  $x = 10$ . This function is not unimodal for  $0 < x < 10$ .

This chapter is intended to be an introduction to the subject of optimization. A more complete handling of the subject can be found in texts by Beveridge and Schechter [3] and by Edgar and Himmelblau [4].

## 6.1 One-Dimensional Optimization Problems

This section considers both analytical and numerical methods for the solution of one-dimensional optimization problems. A one-dimensional optimization problem can be represented by

$$y = f(x)$$

subject to

$$a \leq x \leq b$$

where  $y$  is the value of the objective function,  $x$  is the independent variable, and  $a \leq x \leq b$  is the constrained range of  $x$  for the problem.

### 6.1.1 Analytical Methods

An example of a one-dimensional analytical optimization problem would be to find the global minimum of

$$y = x^4 - 4x^3 + 12x^2 - 16x + 16$$

subject to

$$0 \leq x \leq 5$$

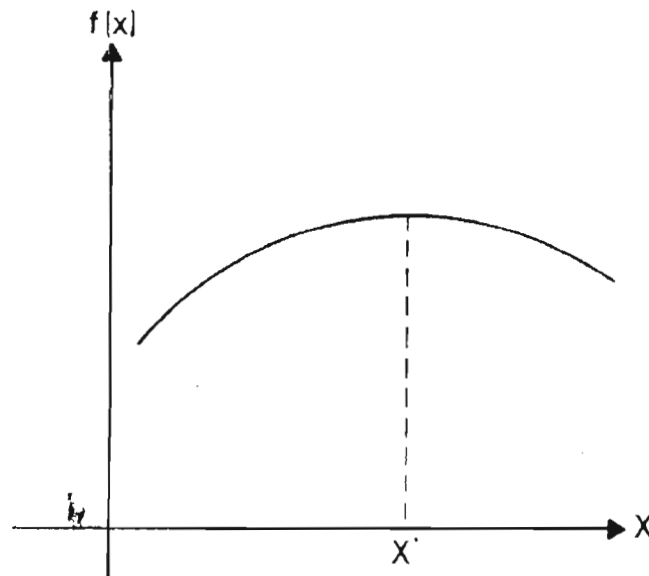
In this case,  $y$  is the objective function and  $x$  is the independent variable. Note that the constraint limits the permissible values of  $x$  for the problem. This type of problem results when a closed-form expression for the objective function can be written containing only one independent variable. The global maximum and minimum of such a problem are located at one of three possible locations:

- At a stationary point (local maximum or local minimum)
- At a boundary formed by the constraints of the problem
- At a discontinuity in the objective function or the first derivative of the function

That is, in order to locate the global maximum or minimum, it is necessary to compare function values at stationary points, at boundaries, and at discontinuities. This statement is true for one-dimensional or multidimensional optimization problems and for analytical or numerical approaches.

Consider the local maximum of  $f(x)$  shown in **Figure 6.2**. Applying the Taylor series expansion (**Section 3.1**) at the local maximum ( $x^*$ ) yields

$$f(x^* + h) = f(x^*) + hf'(x^*) + \frac{h^2}{2}f''(x^*) + \cdots$$



**Figure 6.2** Function with a local maximum.

where  $h$  is the distance away from the local maximum. On rearranging,

$$f(x^* + h) - f(x^*) = hf'(x^*) + \frac{h^2}{2}f''(x^*) + \dots$$

For a local maximum, the left-hand side of this equation must be less than zero for all  $h$ , positive or negative, since  $f(x^*)$  is the largest value of  $f(x)$  near  $x = x^*$ . Therefore,  $f'(x^*)$  must be zero since  $h$  can be arbitrarily chosen to be positive or negative. This is the *necessary condition* for a local maximum: any point  $x$  which satisfies

$$f'(x) = 0$$

is called a stationary point.

Using the necessary condition for a local maximum converts the earlier equation into

$$f(x^* + h) - f(x^*) = \frac{h^2}{2}f''(x^*) + \dots$$

which we noted must be negative for a local maximum. For the right-hand side of the equation to be negative,

$$f''(x^*) < 0$$

which is the *sufficiency condition* for a local maximum.

Similar arguments can be made for a local minimum. A summary of the necessary and sufficient conditions for local maximum and minimum follows:

	Maximum	Minimum
Necessary Condition	$y'(x^*) = 0$	$y'(x^*) = 0$
Sufficiency Condition	$y''(x^*) < 0$	$y''(x^*) > 0$

### Example 6.1 Unconstrained One-Dimensional Optimization

#### Problem Statement

Find the local maximum and minimum of

$$f(x) = 2x^3 - 15x^2 + 36x + 7$$

#### Solution

Application of the necessary conditions yield

$$f'(x) = 6x^2 - 30x + 36 = 0$$

There are two roots to this equation:  $x^* = 2$  and  $x^* = 3$ . The sufficiency condition indicates the character of these stationary points; i.e.,

$$f''(x) = 12x - 30$$

Then  $f''(2) = -6$ , which indicates  $x^* = 2$  is a local maximum. For  $x^* = 3$ ,  $f''(x^*) = +6$ , indicating a local minimum.

When  $f''(x^*)$  is equal to zero, the stationary point may be a saddle point (Figure 6.3). Note that a saddle point satisfies the necessary conditions for a local maximum.

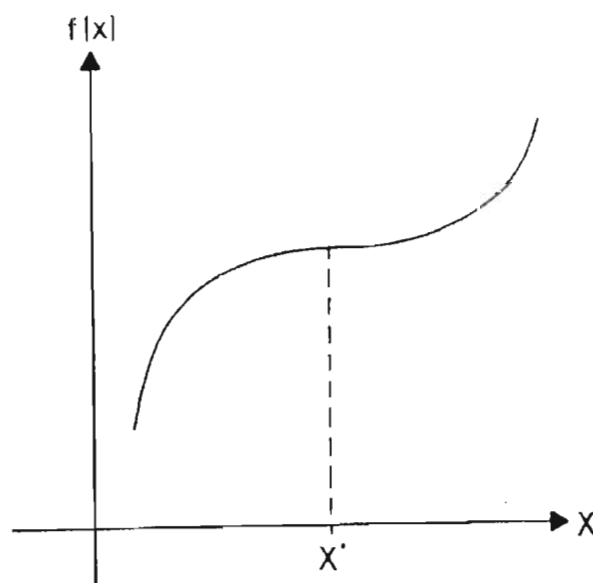
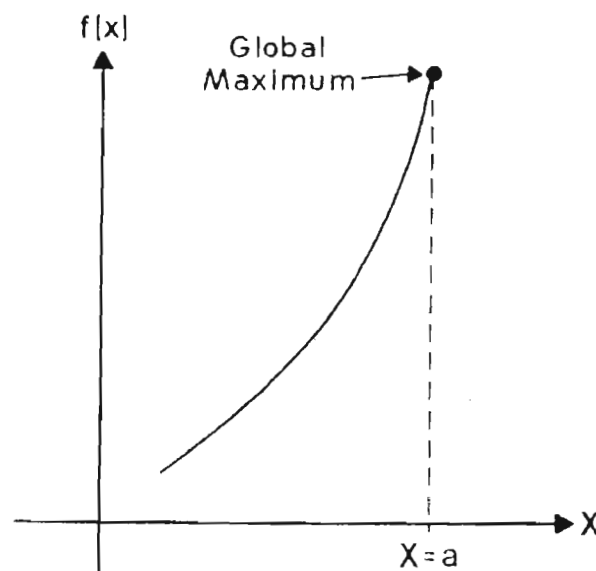


Figure 6.3 Function with a saddle point at  $x = x^*$ .



**Figure 6.4** Function with a maximum at a boundary formed by a constraint.

or minimum but does not satisfy the sufficiency conditions. When  $f''(x^*) = 0$ , the stationary point can be a local maximum, local minimum, or a saddle point. A complete analysis of this problem is presented by Beveridge and Schechter [3], who outline a procedure for identifying the character of such a stationary point.

**Figure 6.4** shows a case in which the global maximum occurs at a boundary formed by a constraint. For this case,  $x$  is constrained to be less than or equal to  $a$ . In order to determine if a global maximum or minimum occurs at a boundary, simply evaluate the function at the boundary and compare that value with others at stationary points and discontinuities.

### Example 6.2 Constrained One-Dimensional Optimization

#### Problem Statement

Consider the previous example,

$$f(x) = 2x^3 - 15x^2 + 36x + 7$$

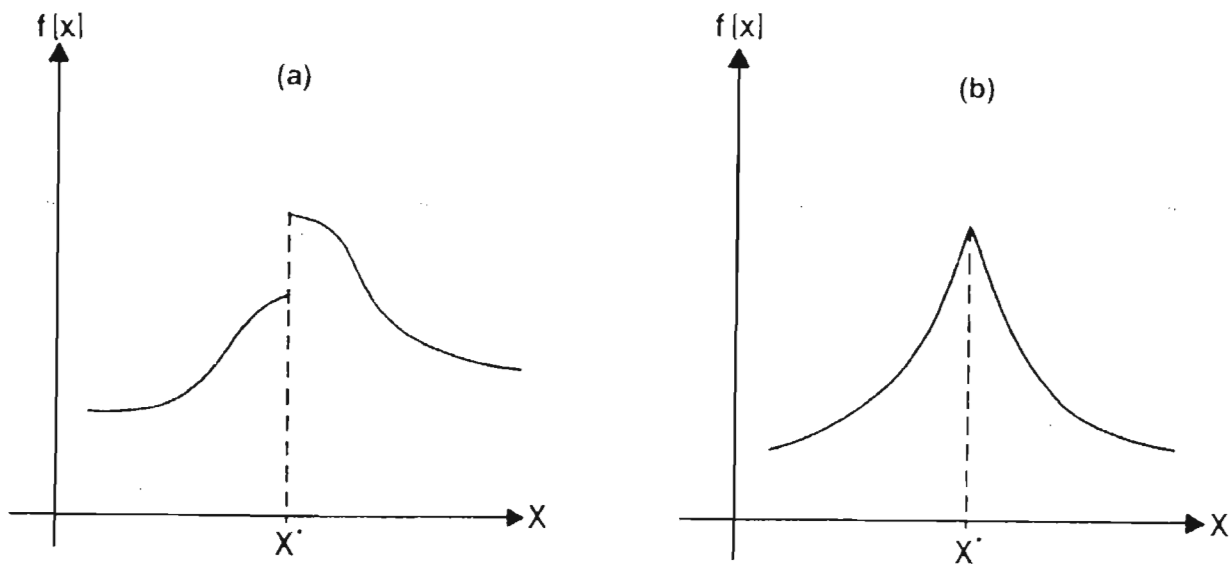
with the following constraints:

$$x \geq -2$$

and

$$x \leq 4$$





**Figure 6.5** (a) Optimum at a discontinuity in the function (b) optimum at a discontinuity in the derivative of the function.

### Solution

Evaluating  $f(x)$  at both boundaries yields

$$f(-2) = -141$$

$$f(4) = 39$$

Comparing these results with the values of the local maximum and local minimum shows that the global maximum is at the right-hand side constraint ( $x = 4$ ) and the global minimum is at the other constraint ( $x = -2$ ).

An optimum can also exist at a discontinuity in the function or a discontinuity in the first derivative of the function. These two cases are shown in **Figure 6.5a** and **b**, respectively. Usually, discontinuities can be identified by examination of the objective function. Then function values at the discontinuity can be evaluated and compared with function values at stationary points and boundaries in order to determine the global maximum and minimum. When dealing with discontinuities in the objective function, evaluate the function at both sides of the discontinuity in order to locate extreme values of the objective function.

### Example 6.3 Optimum at a Discontinuity in the Function Value

#### Problem Statement

Find the global maximum of the following objective function:

$$f(x) = \frac{x^2}{1+x}$$

subject to

$$x \geq -5$$

$$x \leq 10$$

### Solution

Differentiating  $f(x)$  yields

$$f'(x) = \frac{x}{1+x} \left( 2 - \frac{x}{1+x} \right)$$

Therefore, there is a stationary point at  $x = 0$  and  $x = -2$ . For  $x = -2$ ,  $f''(-2)$  is negative; therefore, this stationary point is a local maximum. For  $x = 0$ , it may be a saddle point since  $f''(0) = 0$ . By checking the function values at  $x = \pm 0.1$ , it shows that this stationary point is actually a local minimum. Now check the boundaries

$$f(-5) = -6.25$$

and

$$f(10) = 9.09$$

Next we should check for a discontinuity in  $f(x)$  or  $f'(x)$ . There is a discontinuity in both at  $x = -1$ . As  $x$  approaches  $-1$  from the positive side,  $f(x) \rightarrow +\infty$ . And as  $x$  approaches  $-1$  from the negative side,  $f(x) \rightarrow -\infty$ , as is evident in the following summary.

<u>Stationary Points</u>	<u><math>f(x)</math></u>	<u>Comments</u>
$x = 0$	0	local minimum
	-2	local minimum
<u>Boundary Points</u>		
$x = -5$	-6.25	
$x = 10$	9.09	
<u>Discontinuities</u>		
$x = -1^+$	$\rightarrow +\infty$	global maximum
$x = -1^-$	$\rightarrow -\infty$	global minimum

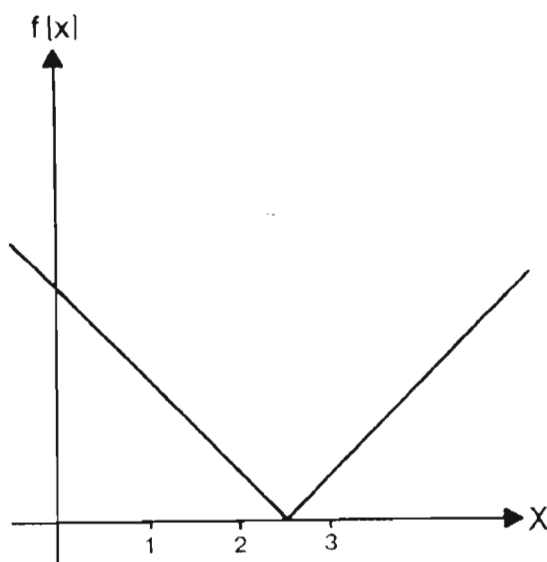


Figure 6.6 Plot of Example 6.4.

### Example 6.4 Optimum at a Discontinuity in the Slope of the Function

#### Problem Statement

Find the global minimum of

$$y = |2x - 5|$$

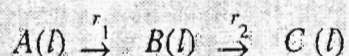
#### Solution

There are no stationary points for this function and there are no constraints. Also, the function is continuous but the first derivative is not continuous at  $x = 2.5$ . This point is also the global minimum as shown in Figure 6.6.

### Example 6.5 Optimization of a Series Reaction

#### Problem Statement

Consider the following reaction system:



where

$$r_1 = k_1 C_A$$

$$r_2 = k_2 C_B$$



For a batch reactor, an unsteady-state mole balance yields

$$\begin{aligned}\frac{dC_A}{dt} &= -k_1 C_A \\ \frac{dC_B}{dt} &= k_1 C_A - k_2 C_B\end{aligned}$$

where

$$\begin{aligned}C_A &= C_{A_0} \quad \text{at } t = 0 \\ C_B &= C_{B_0} \quad \text{at } t = 0\end{aligned}$$

The first ODE can be integrated by separation of variables, yielding

$$C_A = C_{A_0} \exp(-k_1 t)$$

Substituting this result into the second ODE yields

$$\frac{dC_B}{dt} = k_1 C_{A_0} \exp(-k_1 t) - k_2 C_B$$

Solving this ODE using an integrating factor yields

$$C_B = C_{B_0} \exp(-k_2 t) + \frac{k_1 C_{A_0}}{k_2 - k_1} [\exp(-k_1 t) - \exp(-k_2 t)]$$

Find the reaction time that yields the maximum concentration of  $B$ .

### Solution

First, check the stationary points; i.e.,

$$\frac{dC_B}{dt} = 0 = -C_{B_0} k_2 \exp(-k_2 t^*) + \frac{k_1 C_{A_0}}{k_2 - k_1} [-k_1 \exp(-k_1 t^*) + k_2 \exp(-k_2 t^*)]$$

Rearranging gives

$$\exp(-k_2 t^*) \left( \frac{k_1 k_2 C_{A_0}}{k_2 - k_1} - C_{B_0} k_2 \right) = \frac{k_1^2 C_{A_0} \exp(-k_1 t^*)}{k_2 - k_1}$$

Collecting the exponential terms yields

$$\exp[(k_2 - k_1)t^*] = \frac{\frac{k_1 k_2 C_{A_0}}{k_2 - k_1} - C_{B_0} k_2}{\frac{k_1^2 C_{A_0}}{k_2 - k_1}}$$

Finally,

$$t^* = \frac{1}{k_2 - k_1} \ln \left[ \frac{k_2}{k_1} - \frac{C_{B_0} k_2 (k_2 - k_1)}{k_1^2 C_{A_0}} \right]$$

There are no discontinuities, but there is an implied constraint that  $t \geq 0$ . At this constraint,  $C_B = C_{B_0}$ . This point could be the maximum value of  $C_B$  if  $C_{B_0}$  were large enough. In that case,  $r_2 > r_1$  and  $C_B$  would continuously decrease. This point can also be seen from the analysis of the equation for the stationary point. Assume that  $k_2 = 2k_1$  and  $C_{B_0} / C_{A_0}$  is equal to 0.8. Then the argument of the logarithm term would be 0.4, yielding a negative value for  $t^*$ . For this case, what happens when  $C_{B_0} / C_{A_0} > 1$ ?

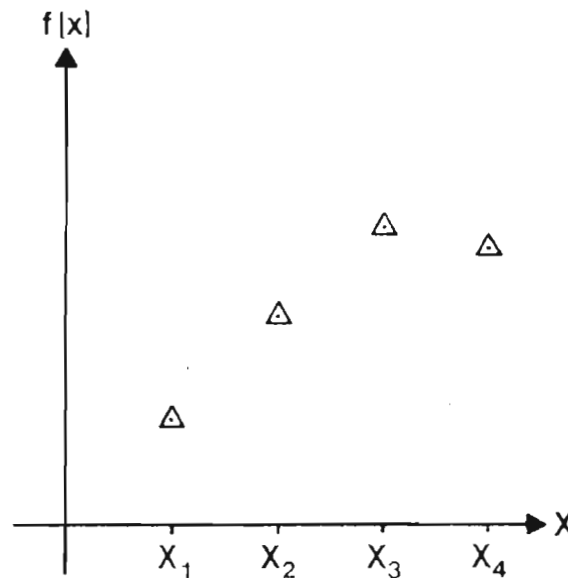
### 6.1.2 One-Dimensional Numerical Methods

In most cases, the analytical formulation of the objective function of a one-dimensional optimization problem will not be available. Many times, a complex model of a system will be used to calculate the value of the objective function. As a result, one must find the optimum using only the value of the objective function at discrete values of the independent variable. The same situation exists when trying to optimize an existing process by adjusting a single independent variable. In these cases, a numerical optimization technique is required.

Most one-dimensional optimization techniques are based upon a problem with a bounded range for the independent variable. That is, they assume that the independent variable is less than some specified maximum value and greater than a specified minimum. Also, these numerical techniques assume that the objective function is unimodal over the bounded range of the independent variable.

Some one-dimensional optimization problems are unbounded. For these cases the first step is to bound the optimum. For example, searching for a maximum, one moves from the starting point in the direction in which the objective function increases. This search direction is maintained until a decrease in the value of the objective function is obtained. Assuming that the objective function is unimodal, the global maximum has then been bounded. **Figure 6.7** shows such a procedure. Note that the maximum lies between  $x_2$  and  $x_4$ ; i.e.,

$$x_2 < x^* < x_4$$



**Figure 6.7** Bounding an optimum using a constant step size.

Then the resulting region of uncertainty is equal to  $2\Delta x$ .

In certain cases, using a fixed step size,  $\Delta x$ , to bound the optimum will lead to an excessive number of function evaluations, especially if the starting point is a poor initial guess. For such cases, it can be more efficient to use an increasing step size. For example, the step size could be doubled after each step. That is,

$$\Delta x_{i+1} = 2\Delta x_i$$

In this manner, larger and larger step sizes would be used until the optimum is bounded. A graphical example of this approach is shown in **Figure 6.8**. In this case, the maximum was bounded such that

$$x_3 < x^* < x_5$$

assuming a unimodal objective function.

### Example 6.6 Bounding a One-Dimensional Optimum

#### Problem Statement

Consider the following objective function:

$$y = (x - 200)^2$$

with a starting point of  $x = 0$ . Search for a minimum. How many function evaluations and what region of uncertainty would result if:

- A fixed step size of 1.0 were used?
- The step size were doubled after each step using an initial step size of 1.0?

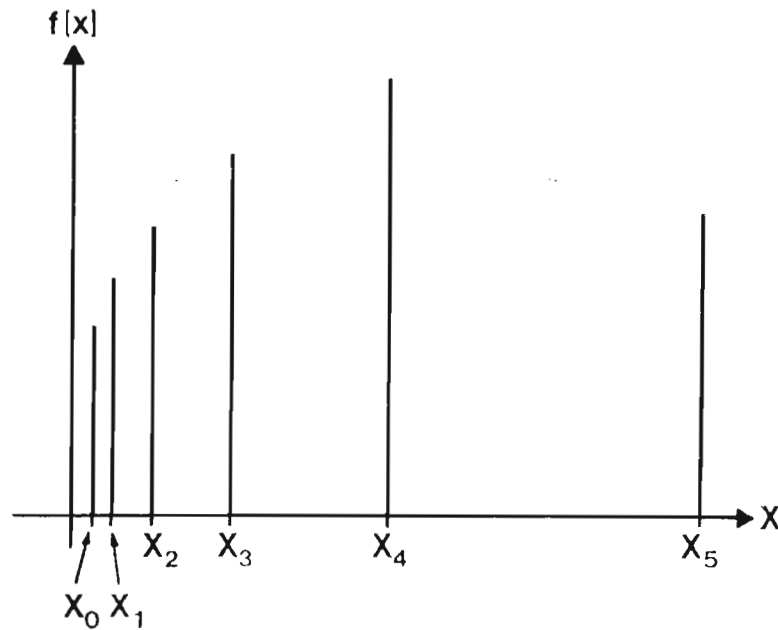


Figure 6.8 Bounding the optimum using an accelerating step size.

### Solution

- a. It would require 202 function evaluations and the region of uncertainty would be  $199 < x^* < 201$ .
- b. It would require only 9 function evaluations but the region of uncertainty would be  $127 \leq x^* < 255$ .

Case b would be preferred even though the region of uncertainty is greater. It will be shown later that only 10 additional function evaluations would be required to reduce the region of uncertainty to less than that of case a. Therefore, if the starting point is likely to be a poor initial guess, use an accelerating step size bounding method.

Once an optimum has been bounded, a one-dimensional optimization method can be applied. The dichotomous method and the modified Fibonacci method are presented next for numerically solving bounded one-dimensional optimization problems.

**Dichotomous Search Method.** The dichotomous method uses two closely spaced objective function evaluations in order to estimate the slope of the objective function and thereby reduce a portion of the region of uncertainty. One pair of function evaluations is used “per cycle”<sup>1</sup> and the function evaluations are placed symmetrically about the center of the search region and close to each other. The two function evaluations should thus be located at

$$x_1 = \frac{a+b}{2} - \frac{\delta}{2}$$

$$x_2 = \frac{a+b}{2} + \frac{\delta}{2}$$

1. Each time a portion of the region of uncertainty is eliminated, a new cycle begins.



where the region of uncertainty is  $a < x < b$  and  $\delta$  is a small number. Then after the evaluation of the function at  $x_1$  and  $x_2$ , the width of the region of uncertainty would be

$$\frac{a+b}{2} + \frac{\delta}{2}$$

Therefore, in the limit of  $\delta$  approaching zero, the region of uncertainty is reduced by a factor of 2 for each cycle (i.e., for each two objective function evaluations). But care should be taken that  $\delta$  is not so small that the difference in the function evaluations is less than the accuracy of the function evaluation.

### Example 6.7 Dichotomous Search

#### Problem Statement

Consider

$$y = (x - 200)^2$$

where

$$127 < x^* < 255$$

Conduct 3 cycles of search for the dichotomous method using  $\delta = 0.2$  while seeking a minimum.

#### Solution

For this case

$$x_1 = 191 - 0.1 = 190.9$$

$$x_2 = 191 + 0.1 = 191.1$$

then

$$y(x_1) = 82.81$$

$$y(x_2) = 79.21$$



Therefore, the minimum lies between  $190.9 < x^* < 255$ . Now

$$x_1 = 222.95 - 0.1 = 222.85$$

$$x_2 = 222.95 + 0.1 = 223.05$$

$$y(x_1) = 522.12$$

$$y(x_2) = 531.30$$

Therefore,

$$190.9 < x^* < 223.05$$

Next,

$$x_1 = 206.975 - .1 = 206.875$$

$$x_2 = 206.975 + .1 = 207.075$$

$$y(x_1) = 47.27$$

$$y(x_2) = 50.05$$

Therefore, after 3 cycles of search,

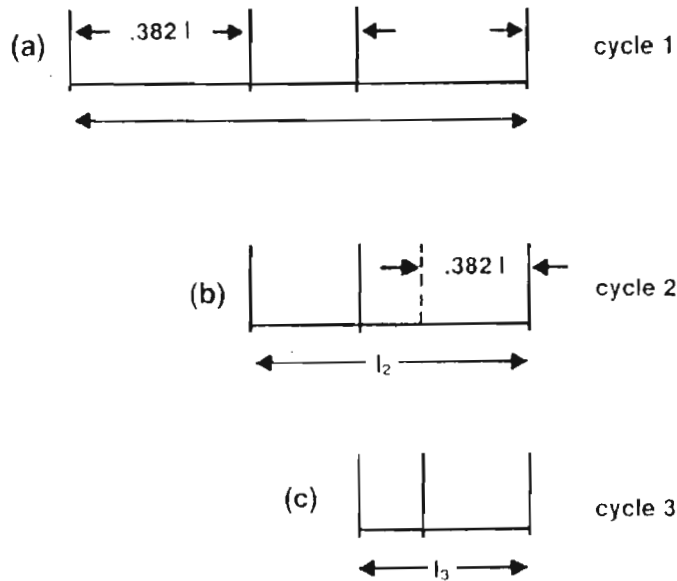
$$190.9 < x^* < 207.075$$

and the region of uncertainty has a width of 16.175. Assuming that the search region was reduced by a factor of 2 after each cycle would have predicted that the search region after 3 cycles would have been

$$128/2^3 = 16.000$$

**Modified Fibonacci Method.** The Fibonacci method is the most efficient one-dimensional search method considered here. Once initiated, it requires only one objective function evaluation per cycle and usually reduces the region of uncertainty by 38.2% each cycle. In addition, the last 2 objective function evaluations are done using the dichotomous method. But when using the Fibonacci method, the number of objective function evaluations must be set at the beginning of the search. The modified Fibonacci method (also known as the *golden section method*) is very nearly as efficient as the Fibonacci method, but is applied in the same fashion regardless of the number of experiments used.

The modified Fibonacci method is shown graphically in **Figure 6.9**. In order to initiate the search, objective function evaluations are performed at 38.2% of the length of the search region from both boundary points. In **Figure 6.9a**, the left-hand region can be discarded, leaving the search region shown in **Figure 6.9b**. Notice that now the second objective function evaluation from cycle 1 is located  $0.382 l_2$  from



**Figure 6.9** Three cycles of search using the modified Fibonacci method.

the left-hand boundary of cycle 2. It can be seen in **Figure 6.9b** that the separation between the two objective function evaluations ( $0.236l_1$ ) is equal to  $0.382l_2$ .

Only one additional objective function evaluation is required at  $0.382l_2$  from the right boundary. Once again, only one objective function evaluation is required in order to reduce the search region by 38.2%. In this manner, the region of uncertainty is reduced by 38.2% with each additional function evaluation.

The rationale for this approach can be seen by the following derivation. Define  $x$  as the fraction of the region of uncertainty that locates the two objective function evaluations. We want to choose  $x$  such that after a region is discarded, one of the objective function evaluations is located  $x$  from a boundary of the next cycle, i.e.,

$$(1 - 2x) l_i = x l_{i+1}$$

But

$$l_{i+1} = (1 - x) l_i$$

Substituting and solving

$$x^2 - 3x + 1 = 0$$

yields  $x = 0.38197, 2.61803$ . The second root is extraneous, and therefore the 38.2% factor used by the modified Fibonacci method results.

**Example 6.8 Procedure for the Modified Fibonacci Method****Problem Statement**

Apply 3 cycles of search using the modified Fibonacci method to the following problem seeking a minimum:

$$y = (x - 200)^2$$

$$127 < x^* < 255$$

**Solution**

Evaluate the function at  $0.382l_1$  from both boundaries. Here,  $l_1 = 255 - 127 = 128$ . Then

$$\begin{aligned} x_1 &= 175.896 & y(x_1) &= 581.00 \\ x_2 &= 206.104 & y(x_2) &= 37.26 \end{aligned}$$

From the function evaluations, the region  $127 < x < 175.896$  can be discarded; therefore, after cycle 1, the optimum is given by  $175.896 < x^* < 255$ .

The next objective function evaluation is located at  $0.382l_2$  from the right boundary, or

$$x_3 = 224.78 \quad y(x_3) = 616.16$$

Now the region  $224.78 < x < 255$  can be discarded, leaving after cycle 2

$$175.896 < x^* < 224.78$$

The three function values for this region are

$$\begin{aligned} x_1 &= 175.896 & y(x_1) &= 581.00 \\ x_2 &= 206.104 & y(x_2) &= 37.26 \\ x_3 &= 224.780 & y(x_3) &= 616.16 \end{aligned}$$

The next objective function evaluation would be placed at

$$x_4 = 194.57 \quad y(x_4) = 29.49$$

leaving the following region of uncertainty after 3 cycles:

$$175.896 < x^* < 206.104$$



### Example 6.9 Computer Version of the Modified Fibonacci Method

#### Problem Statement

Find the maximum value of

$$y = -3x^2 + 10x + 5$$

where

$$-10 \leq x \leq 10$$

to a region of uncertainty of less than 0.01.

#### Solution

First determine the number of function evaluations required. Each cycle of search reduces the region of uncertainty by 38.2%. After  $n$  cycles, the region of uncertainty is given as

$$L_n = L_0 (1 - 0.382)^n$$

For this problem,

$$L_n = 0.01$$

and

$$L_0 = 20$$

Solving for  $n$  yields

$$n = 15.79 \text{ cycles}$$

That is, 16 cycles are required. Only the first cycle requires two function evaluations and the remainder of cycles require only one objective function evaluation.

Following is a program which applies the modified Fibonacci method to this problem.

#### PROGRAM LISTING FOR EXAMPLE 6.9

```

C
C ***** ABSTRACT *****
C
C   THIS PROGRAM CALLS SUBROUTINE MODFIB IN ORDER TO FIND THE MAXIMUM
C   OF A FUNCTION. SUBROUTINE MODFIB USES THE MODIFIED FIBONACCI METHOD
C   TO FIND THE OPTIMUM OF A BOUNDED ONE-DIMENSIONAL OPTIMIZATION
C   PROBLEM TO A RESOLUTION XMIN.
C
C ***** NOMENCLATURE *****
C
C   XMIN- THE DESIRED ACCURACY IN THE OPTIMUM VALUE OF X
C   TYPE- +1 PROGRAM SEEKS A MAXIMUM; -1 PROGRAM SEEKS A MINIMUM
C   XLB- THE LEFT BOUNDARY OF THE REGION OF UNCERTAINTY
C   XRB- THE RIGHT BOUNDARY OF THE REGION OF UNCERTAINTY
C   YLB- VALUE OF Y AT X=XLB

```

```

C   YRB- VALUE OF Y AT X=XRB
C
C*****
1   IMPLICIT REAL*8(A-H,O-Z)
2   EXTERNAL F
C   INPUT INITIAL PROBLEM PARAMETERS
3   TYPE=1.
4   XMIN=1.E-3
5   XLB=-10.
6   XRB=10.
C
C   CALL MODFIB
C
7   CALL MODFIB(F,XLB,XRB,XMIN,TYPE,YLB,YRB)
C
C   PRINT OUT RESULTS
C
8   10 WRITE(6,20)XLB,XRB
9   20 FORMAT( 26H THE OPTIMUM X IS BETWEEN ,D13.6,4H AND,D13.6)
10  30 FORMAT( 26H THE OPTIMUM Y IS BETWEEN ,D13.6,4H AND,D13.6)
11  WRITE(6,30)YLB,YRB
12  STOP
13  END

C
C***** ABSTRACT *****
C
C   THIS SUBROUTINE CALCULATES THE OPTIMUM OF A BOUNDED, ONE-DIMENSIONAL
C   OBJECTIVE FUNCTION USING THE MODIFIED FIBONACCI METHOD.  WHEN TYPE
C   IS EQUAL TO +1, THE PROGRAM SEEKS A MAXIMUM.  WHEN TYPE IS EQUAL TO
C   -1, THE PROGRAM SEEKS A MINIMUM.
C
C***** NOMENCLATURE *****
C
C   XL- THE LENGTH OF THE REGION OF UNCERTAINTY
C   XMIN- THE DESIRED ACCURACY IN THE OPTIMUM VALUE OF X
C   TYPE- +1 PROGRAM SEEKS A MAXIMUM; -1 PROGRAM SEEKS A MINIMUM
C   XLB- THE LEFT BOUNDARY OF THE REGION OF UNCERTAINTY
C   XRB- THE RIGHT BOUNDARY OF THE REGION OF UNCERTAINTY
C   X1- VALUE OF X AT (XLB+.382*L)
C   X2- VALUE OF X AT (XRB-.382*L)
C   YLB- VALUE OF Y AT X=XLB
C   YRB- VALUE OF Y AT X=XRB
C   Y1- VALUE OF Y AT X=X1
C   Y2- VALUE OF Y AT X=X2
C
C*****
1   SUBROUTINE MODFIB(F,XLB,XRB,XMIN,TYPE,YLB,YRB)
2   IMPLICIT REAL*8(A-H,O-Z)
3   EXTERNAL F
C   EVALUATE Y AT THE BOUNDARIES
4   CALL F(XLB,YLB)
5   CALL F(XRB,YRB)
C   INITIATE THE MODIFIED FIBONACCI SEARCH
6   XL=XRB-XLB
7   X1=XLB+.382*XL

```

```

8      CALL F(X1,Y1)
9      X2=XRB-.382*XL
10     CALL F(X2,Y2)
11     1 CONTINUE
12     IF(TYPE*Y2.GT.TYPE*Y1)GO TO 2
C     DISCARD THE RIGHT SIDE OF THE REGION OF UNCERTAINTY
13     XRB=X2
14     YRB=Y2
15     X2=X1
16     Y2=Y1
17     XL=XRB-XLB
18     IF(XL.LT.XMIN) GO TO 10
19     X1=XLB+.382*XL
20     CALL F(X1,Y1)
21     GO TO 1
C     DISCARD THE LEFT SIDE OF THE REGION OF UNCERTAINTY
22     2 XLB=X1
23     YLB=Y1
24     X1=X2
25     Y1=Y2
26     XL=XRB-XLB
27     IF(XL.LT.XMIN)GO TO 10
28     X2=XRB-.382*XL
29     CALL F(X2,Y2)
30     GO TO 1
C     RETURN TO CALLING PROGRAM
31 10  RETURN
32     END

```

```

C
C
C***** ABSTRACT *****
C
C     THIS SUBROUTINE CALCULATES THE VALUE OF THE OBJECTIVE FUNCTION Y
C     GIVEN THE VALUE OF X.
C
C*****
C
1      SUBROUTINE F(X,FV)
2      IMPLICIT REAL*8(A-H,O-Z)
3      FV=-3.0*X*X+10.*X+5.
4      RETURN
5      END

```

```

THE OPTIMUM X IS BETWEEN      .166657D+01 AND  .166720D+01
THE OPTIMUM Y IS BETWEEN      .133333D+02 AND  .133333D+02

```

## Section Summary

The optimum will lie at one of these possible locations: (1) at a stationary point; (2) at a boundary formed by the constraints of the problem; or (3) at a discontinuity in the objective function or the first derivative of the objective function. A stationary point is located at a point where the slope of the objective function is zero. The

character of the stationary point (local maximum, local minimum, or saddle point) can usually be determined by the value of the second derivative of the objective function at the stationary point. When seeking a global optimum, compare the function values of the stationary points, the boundaries, and points of discontinuity.

The first step in the numerical solution of a one-dimensional optimization problem is developing limits on the range of the independent variable (bounding the problem). If the location of the optimum is fairly well known, a constant step size search can be used. If not, an accelerating step size should be used.

Once the problem has been bounded, the modified Fibonacci method can be used to efficiently locate the optimum, assuming that the function is unimodal over the bounded region.

## 6.2 Multidimensional Optimization Problems

In this section, optimization methods applied to multidimensional problems are considered. Analytical multidimensional methods are considered first. Then numerical methods for unconstrained problems are presented. Next, linear programming is considered. Finally, several methods are presented for optimization of industrial scale problems.

### 6.2.1 Analytical Methods

Analytical methods applied to multidimensional optimization problems are not practical in most cases because (1) if there are more than two independent variables, the methods become excessively cumbersome, and (2) the objective function and all constraints must be expressed in closed-form expressions. Even when an optimization problem contains only two independent variables and analytical expressions for the problem are available, it is usually easier to use a numerical solution procedure. But the understanding of analytical methods provides insight into the problem of multidimensional optimization, as well as background for the understanding of certain numerical multidimensional optimizers.

**Unconstrained Problems.** For multidimensional problems without constraints, there are necessary conditions to determine stationary points as well as sufficiency conditions which can be used to determine the character of the stationary points. Consider an objective function,

$$y = f(x)$$

where  $x = (x_1, x_2, \dots, x_n)$  is a vector of the independent variables of the problem. The necessary conditions for a stationary point are simply

$$\frac{dy}{dx_i} = 0 \quad i = 1, 2, \dots, n$$

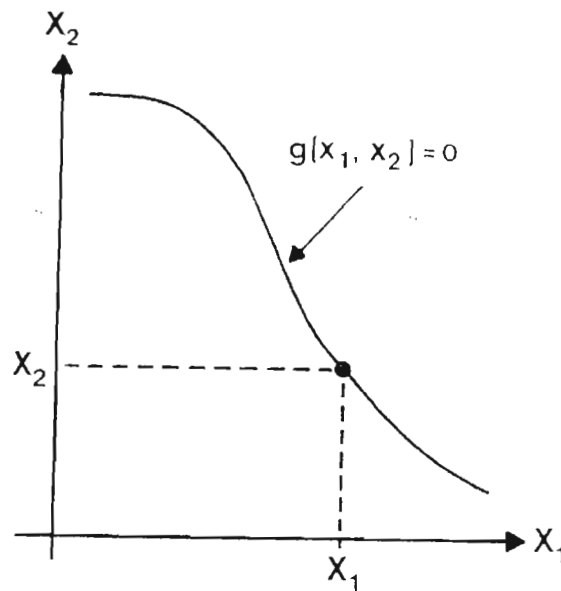
The necessary conditions will produce a system of  $n$  equations with  $n$  unknowns ( $x$ ). There can be multiple roots of this system of equations which would mean that there are multiple stationary points.

The sufficiency conditions are determined by the calculation of a series of determinants whose elements are the second derivatives of the objective function with respect to the independent variables. Listing of the sufficiency conditions is beyond the scope of the presentation here, but can be found elsewhere [3]. It should also be pointed out for multidimensional problems that if the sufficiency conditions are not met, the stationary point could still be a global optimum. That is, if the sufficiency conditions are satisfied, then the character of the stationary point is clearly defined; if not, the character of the stationary point is undetermined.

**Problems with Equality Constraints.** Again consider a multidimensional objective function,

$$y = f(x)$$





**Figure 6.10** An example of an equality constraint.

which is to be optimized subject to the following set of equality constraints:

$$g_k(x) = 0 \quad k = 1, 2, \dots, m$$

That is, the value of  $f(x)$  is optimized while choosing  $x$  such that all the equality constraints are satisfied. Two methods of solving such problems will be outlined.

In order to illustrate the method of constrained variation, consider a two-dimensional optimization problem subject to one equality constraint:

Optimize

$$y = f(x_1, x_2)$$

subject to

$$g_1(x_1, x_2) = 0$$

**Figure 6.10** plots  $x_2$  as a function of  $x_1$  such that

$$g_1(x_1, x_2) = 0$$

If  $x_1$  is specified, then from the equality constraint,  $x_2$  is automatically set. So in effect, there is only one degree of freedom left in the problem. In multidimensional problems with a number of equality constraints, the number of degrees of freedom is reduced by one for each equality constraint.

For the two-dimensional example shown in **Figure 6.10**, the optimization problem is one of searching the range of  $x_1$  while using the corresponding value of  $x_2$  that satisfies  $g_1(x_1, x_2) = 0$ , or searching the range of  $x_2$  while using the appropriate value of  $x_1$ . Note that in certain cases when  $g_1(x_1, x_2)$  allows,  $g_1(x_1, x_2)$  can be substituted directly into  $y(x)$  to eliminate  $x_1$  or  $x_2$  and convert the problem to an unconstrained one-dimensional problem.

The method of constrained variation takes into account the degree-of-freedom reduction and provides a set of necessary and sufficient conditions for a local optimum of an equality constrained multidimensional optimization problem. The stationary points are determined by the solution of a set of equations where  $m$  equations are the equality constraints and  $(n - m)$  equations result from the determinants of the Jacobians formed by the partial derivatives of  $y$  and  $g_k$  with respect to the independent variables. The sufficiency conditions are quite tedious.

One feature of the method of constrained variation is that in certain cases, difficulties can result due to the unnatural distinction between independent variables. From the degree-of-freedom analysis, the first  $m$  variables are treated differently in the analysis than the remaining  $(n - m)$  variables. This limitation of the method of constrained variation is overcome by the method of Lagrangian multipliers.

For the method of Lagrangian multipliers, a modified objective function is defined as

$$F = f(x) + \sum_{k=1}^m \lambda_k g_k(x)$$

where the  $\lambda_k$ 's are the Lagrangian multipliers. The necessary conditions for a stationary point are

$$\begin{aligned} \frac{\partial F}{\partial x_i} &= 0 & i = 1, 2, \dots, n \\ \frac{\partial F}{\partial \lambda_k} &= 0 & k = 1, 2, \dots, m \end{aligned}$$

Note that the second condition simply reduces to the constraints of the problem, i.e.,  $g_k(x) = 0$ . The necessary conditions will generate a system of  $(n + m)$  equations containing  $(n + m)$  unknowns (i.e.,  $x, \lambda$ 's). The roots ( $x$ ) of this system of equations will be the locations of the stationary points.

It is important to note that the modified objective function  $F$  cannot be treated as an unconstrained optimization problem. That is, the sufficiency conditions for an unconstrained problem cannot be applied to the modified objective function to determine the character of the stationary points. The value of the method of Lagrangian multipliers is that it is relatively easy to use to find the stationary points and that it offers significant advantages when applied to problems which have inequality constraints.

**Inequality Constrained Problems.** Consider the following multidimensional optimization problem:

Optimize

$$y = f(x)$$

subject to

$$g_k(\mathbf{x}) < 0 \quad k = 1, 2, \dots, l$$

and

$$g_k(\mathbf{x}) = 0 \quad k = l + 1, l + 2, \dots, m$$

The inequality constraints can be converted to equality constraints by the addition of slack variables,  $s_k$ :

$$g_k(\mathbf{x}) + s_k = 0 \quad k = 1, 2, \dots, l$$

where  $s_k \geq 0$ . Note that  $s_k = 0$  when  $\mathbf{x}$  lies on the boundary formed by the  $k$ th constraint. In addition, the value of  $s_k$  is a qualitative measure of how close  $\mathbf{x}$  is to the boundary formed by the constraint. That is, as  $s_k$  is reduced,  $\mathbf{x}$  will move closer to the boundary formed by  $g_k(\mathbf{x})$ .

A convenient form for  $s_k$  is

$$s_k = x_{n+k}^2 \quad k = 1, 2, \dots, l$$

since  $s_k$  would always be positive definite (i.e., nonnegative). With this addition, there are now  $(n + l)$  independent variables ( $n$  for  $\mathbf{x}$ , and  $l$  slack variables) and the problem has been converted into a multidimensional problem with equality constraints.

The application of the method of constrained variables would be similar to the procedure presented earlier in this section for equality constrained problems. With the addition of the slack variables, the dimensionality of the problem must be revised. The number of constraint equations would be  $m$  and the number of Jacobian type equations would be  $(n + l - m)$ .

Now consider the application of Lagrangian multipliers. The locations of the stationary points are determined as before:

$$F = f(\mathbf{x}) + \sum_{k=1}^m \lambda_k g_k(\mathbf{x})$$

$$\frac{\partial F}{\partial x_i} = 0 \quad i = 1, 2, \dots, n + l$$

$$\frac{\partial F}{\partial \lambda_k} = 0 \quad k = 1, 2, \dots, m$$

When  $n + 1 \leq i \leq n + l$  (i.e.,  $x_i$  is a slack variable for the  $i$ th inequality constraint),

$$\frac{\partial F}{\partial x_i} = 2 x_i \lambda_{i-n} = 0$$

for  $s_i = x_{m+i}^2$ . This means that if a slack variable is nonzero, the Lagrangian multiplier for that constraint must be zero, or vice versa. In other words, if  $\lambda_i$  is not equal to zero, the stationary point is located on the  $i$ th inequality constraint. But if  $\lambda_i$  is zero, the stationary point may lie on the boundary or inside the constraint. Then the slack variables may be eliminated from the problem since the necessary conditions resulting from the slack variables add no additional information about the stationary point.

Then

$$F = f(x) + \sum_{k=1}^m \lambda_k g_k(x)$$

and the necessary conditions for a stationary point are

$$\begin{aligned} \frac{\partial F}{\partial x_i} &= 0 & i = 1, 2, \dots, n \\ \frac{\partial F}{\partial \lambda_k} &= 0 & k = 1, 2, \dots, m \end{aligned}$$

Further, for a stationary point, the sign of the  $\lambda$ 's for the inequality constraints provide information about the character of the stationary point. Kuhn and Tucker [5] concluded if the  $\lambda$ 's for all the inequality constraints were nonzero and positive, the stationary point would *not* be a maximum (i.e., it could be a minimum or a saddle point). Likewise, if the  $\lambda$ 's for all the inequality constraints were nonzero and negative, the stationary point would *not* be a minimum (i.e., it could be a maximum or a saddle point). If the  $\lambda$ 's for all the inequality constraints are zero, the stationary point can be a maximum, a minimum, or a saddle point. These statements are known as the *Kuhn-Tucker conditions* and are summarized in **Table 6.3**.

### 6.2.2 Multidimensional Numerical Methods

This section is concerned with unconstrained multidimensional optimization, while a later section on industrial practice will consider large multidimensional optimization problems with constraints.

**Table 6.3** Kuhn-Tucker Conditions [5]

Sign of $\lambda$ 's for Inequality Constraints	Nature of the Stationary Point
All negative, nonzero	Not a minimum
All positive, nonzero	Not a maximum
All zero	A maximum, a minimum, or a saddle point

It is important to note that multidimensional optimization problems with equality and inequality constraints can be converted into unconstrained optimization problems using penalty functions. As an example, consider the following simple example:

Minimize

$$y = x_1^2 + x_2^2$$

subject to

$$2x_1 + 3x_2^2 + 5x_1 x_2 = 0$$

and

$$3x_1 + 2x_2 \geq 0$$

First, the inequality constraint must be converted into an equality constraint using a slack variable,  $x_3$ ; i.e.,

$$-3x_1 - 2x_2 + x_3^2 = 0$$

Now a new function  $F$  can be defined as

$$F = y + P (g_1^2 + g_2^2)$$

or

$$F = x_1^2 + x_2^2 + P \left[ (2x_1 + 3x_2^2 + 5x_1 x_2)^2 + (-3x_1 - 2x_2 + x_3^2)^2 \right]$$

where  $P$  is chosen as a large positive number in order to “force” the constraints to be satisfied. When the constraints are not satisfied,  $F$  will have a larger value than  $y$ . Note that when the constraints are satisfied, the coefficient of  $P$  is zero. Also, since a minimum is required, the term containing the constraints is added to the original objective function. Likewise, when seeking a maximum, this term would be subtracted from the original objective function.

This approach is usually applied in stages: an initial value of  $P$  is chosen and the problem is solved numerically. Then, using the values of the independent variables just determined as the initial guesses, increase the value of  $P$  and solve the problem again. This procedure is continued until the values of the independent variables approach constant values. Therefore, for large values of  $P$ , all the constraints will be satisfied. This approach can be effectively applied to certain small-scale multidimensional problems with constraints, but it usually becomes difficult to obtain a solution for large scale problems due to the sharp “ridges” created (**Figure 6.11**) by the penalty portion of the new function and the size of the problem.

There are two general classes of unconstrained multidimensional numerical optimizers: those that use only function evaluations (nongradient methods), and those

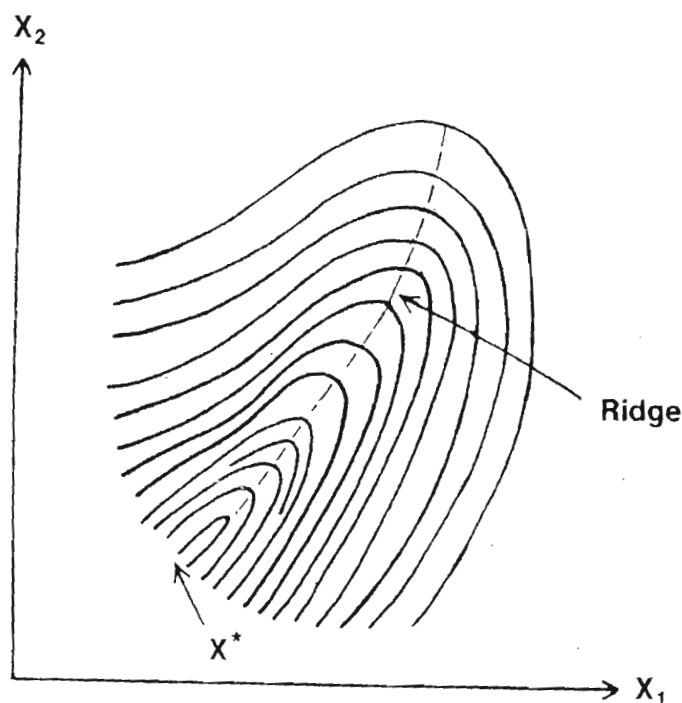


Figure 6.11 Two-dimensional optimization problem with a ridge.

that use both function evaluations and the gradient of the objective function (gradient methods). The gradient is a vector that indicates the local slope of the function (Section 1.2). The components of this vector are the partial derivatives of  $y$  with respect to each independent variable, i.e.,  $\partial y / \partial x_i$ . For gradient methods, the partial derivatives can be calculated analytically or numerically.

**Nongradient Methods.** There are two general classes of nongradient methods: pattern search methods and methods that use changing step sizes and/or changing directions of search.

Pattern search methods usually use a standard geometric configuration in searching for the optimum. One pattern search method is the sequential simplex method. A two-dimensional representation of this method is shown in Figure 6.12. For the two-dimensional case, the method uses three function values which form an equilat-

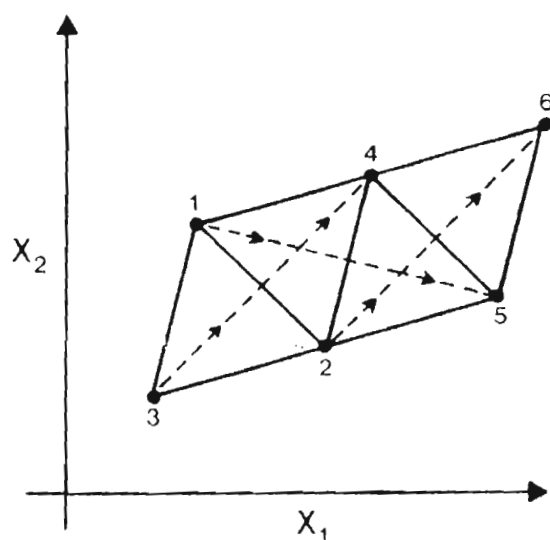


Figure 6.12 Several cycles of the sequential simplex method.

eral triangle. The worst function value (point 3) is discarded and projected through the center of mass of the two remaining points (1 and 2). The projection locates a new point (point 4). Next, the function values of points 1, 2, and 4 are compared. Point 1 is discarded and point 5 is located. Next, point 2 is found to have the worst function value when compared with points 4 and 5. In this manner, the triangular shape is maintained while proceeding toward the optimum. There are also other rules for this method which are designed to overcome some localized difficulties of this technique. In addition, this method can easily be extended to higher order problems. In general, the method is easy to implement and works well for functions that change gradually with changes in the independent variables. But when the function changes rapidly with some independent variables and gradually for others (i.e., a problem with a steep ridge), this method is not very reliable. **Figure 6.11** shows a two-dimensional problem with a ridge.

The Nelder-Mead simplex method [6] is similar to the sequential simplex except that with the Nelder-Mead method the shape of the simplex changes during the course of the search. The Nelder-Mead method uses a general triangular shape, not an equilateral triangle. That is, the simplex expands in a certain direction when repeated improvements are obtained and contracts after failures to improve. In fact, the simplex of the Nelder-Mead method will elongate down long inclined planes, change direction when encountering ridges, and contract in the neighborhood of the optimum. Since the Nelder-Mead simplex method has reasonable convergence speed and is highly reliable, it is one method used to solve unconstrained optimization problems in this section (see **Example 6.10**).

The Hookes-Jeeves method (a nongradient method) starts with small step sizes about the starting point in order to find a preferred direction of search. The step size used along the preferred direction of search increases with repeated improvement in the objective function. The accelerating step size is used until a move is encountered which does not provide an improvement in the objective function. At this point, the method reverts back to small step sizes. Although the Hookes-Jeeves method works better than the sequential simplex method for problems with ridges, it is not very efficient for problems with sharp ridges or with curved ridges.

Two other popular nongradient search methods are the Powell method and the Rosenbrock method. The Powell method is based upon using a quadratic approximation of the objective function and using a series of one-dimensional searches in order to find the best search direction. The Rosenbrock method uses both an accelerating step size and the best search direction. More details on the implementation of nongradient optimizers is provided by Beveridge and Schechter [3].

**Gradient Methods.** The simplest gradient method is the method of steepest ascent. For this method, the search direction is chosen as the gradient at the starting point and a one-dimensional search is performed along that direction. The optimum of the one-dimensional search is the starting point for the next cycle of search. Once again, the search direction is along the gradient at the new point. This procedure is continued until adequate approach to the optimum is obtained. **Figure 6.13** shows two cycles of search for a two-dimensional problem. The method is simple to

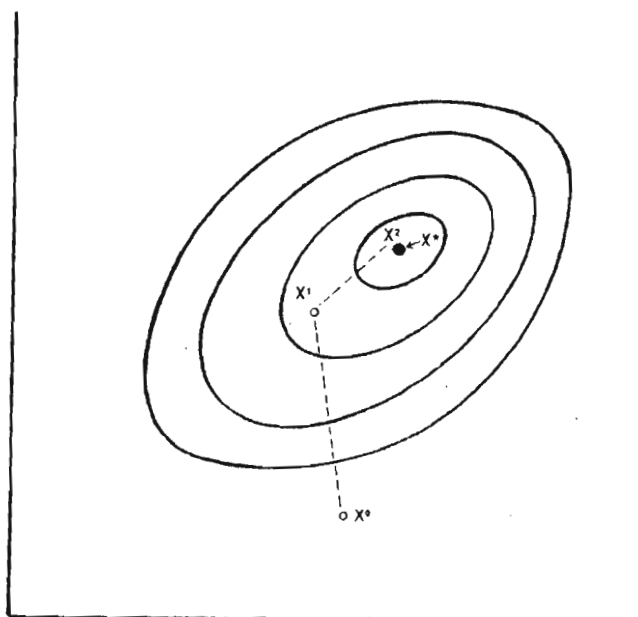


Figure 6.13 Two cycles of a gradient search.

implement but sometimes zigzags along ridges (**Figure 6.14**). Also, steepest ascent methods can tend to oscillate about the optimum.

Another gradient method, the method of conjugate directions [3], overcomes these problems (**Example 6.11**). A property of conjugate directions is that they will converge to the optimum of a quadratic objective function in  $n$  searches where  $n$  is the number of independent variables. Near the optimum, the objective function is well represented as a quadratic function; therefore, conjugate direction methods provide rapid, reliable convergence near the optimum.

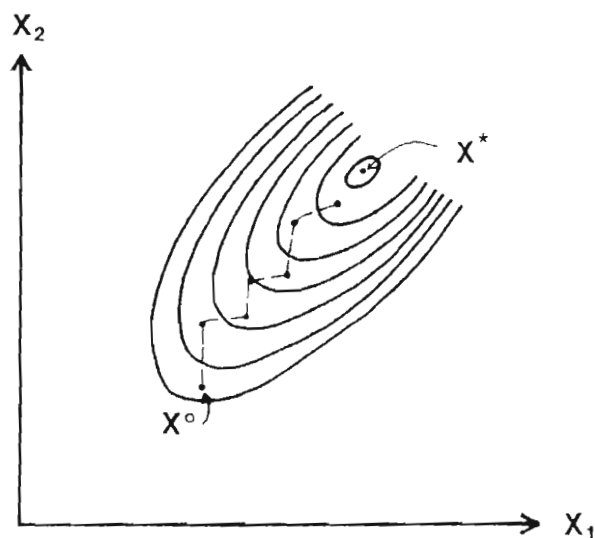


Figure 6.14 Gradient search on a ridge.



**Example 6.10 Nelder-Mead Method****Problem Statement**

Find the optimum of

$$y = 10(x_2 - x_1^2)^2 + (1 - x_1)^2$$

using the library routine NMEAD with an initial value of  $x_1 = x_2 = 10$ . This function is a form of the well-known Rosenbrock function [3], which has been used to compare the efficiency of various search methods.

**Solution**

Following is a listing of the program used to solve this problem using the library subroutine NMEAD, as well as results for this problem.

**PROGRAM LISTING FOR EXAMPLE 6.10**

```

C
C***** ABSTRACT *****
C
C   THIS PROGRAM USES THE LIBRARY ROUTINE NMEAD TO OPTIMIZE A FORM OF
C   THE ROSENBROCK FUNCTION.  SINCE THE NELDER-MEAD SIMPLEX METHOD IS
C   A PATTERN SEARCH METHOD, IT REQUIRES ONLY FUNCTION VALUES WHICH ARE
C   SUPPLIED BY SUBROUTINE NSOLV.
C
C***** NOMENCLATURE *****
C
C   IPRINT- THE PRINT OPTION FOR THE NELDER-MEAD METHOD
C   H- THE INITIAL SIMPLEX SIZE
C   N- THE NUMBER OF UNKNOWNNS
C   X(I)- THE UNKNOWNNS
C
C*****
C
1   IMPLICIT REAL*8(A-H,O-Z)
2   COMMON/TWO/NFUN
3   DIMENSION X(10)
C
C   SET THE INITIAL SIMPLEX SIZE AND SELECT PRINT OPTION
C
4   H=.1
5   IPRINT=0
C
C   INPUT INITIAL GUESSES
C
6   X(1)=10.0
7   X(2)=10.0
C
C   CALL NELDER-MEAD OPTIMIZER
C
8   CALL NMEAD(X,2,H,IPRINT)
9   WRITE (6,22)NFUN

```

```

10 22 FORMAT(10X, ' NUMBER OF FUNCTION EVALUATIONS=', I4)
11 STOP
12 END

C
C
C***** ABSTRACT *****
C
C THIS SUBROUTINE CALCULATES THE VALUE OF F GIVEN THE VALUES OF X(I)
C
C*****
C
1 SUBROUTINE NSOLV(X,F)
2 IMPLICIT REAL*8(A-H,O-Z)
3 COMMON/TWO/NFUN
4 DIMENSION X(10)
5 F=10.*(X(2)-X(1)*X(1))**2+(1.-X(1))**2
6 NFUN=NFUN+1
7 RETURN
8 END

```

THE FINAL VALUES AT THE OPTIMUM ARE:

X(1)= .1000000D+01

X(2)= .9999999D+00

THE FINAL VALUE OF THE OBJECTIVE FUNCTION = .39056D-13

NUMBER OF FUNCTION EVALUATIONS = 219

## Example 6.11 Conjugate Gradient Method

### Problem Statement

Apply the library program CONGRAD to the Rosenbrock function (Example 6.10)

### Solution

A subroutine that calculates the gradient (subroutine DER) must be provided as well as a subroutine to calculate the function value (subroutine FUN). The program listing and results follow.

## PROGRAM LISTING FOR EXAMPLE 6.11

```

C
C***** ABSTRACT *****
C
C THIS PROGRAM USES THE LIBRARY ROUTINE CONGRAD TO OPTIMIZE A FORM OF
C THE ROSENBOCK FUNCTION. CONGRAD USES BOTH THE FUNCTION VALUES AND
C THE GRADIENT TO FIND THE OPTIMUM.
C
C***** NOMENCLATURE *****
C
C IPRINT- THE PRINT OPTION FOR CONGRAD

```

```

C  N- THE NUMBER OF UNKNOWNNS
C  X(I)- THE UNKNOWNNS
C
C*****
C
1      IMPLICIT REAL*8(A-H,O-Z)
2      DIMENSION X(10),GRAD(10)
3      EXTERNAL FUN,DER
C
C  SET INPUT DATA
C
4      N=2
5      IPRINT=0
C
C  INPUT INITIAL GUESSES
C
6      X(1)=10.0
7      X(2)=10.0
C
C  CALL CONGRAD
C
8      CALL CONGRAD(FUN,DER,N,X,GRAD,NFUN,NDEV,IPRINT,FY)
C
C  PRINT OUT RESULTS
C
9      WRITE(6,2080)NFUN,NDEV
10 2080 FORMAT( 10X,' NFUN=',I4,5X,' NDER=',I4)
11      WRITE(6,2222)FY,(X(I),I=1,N)
12 2222 FORMAT( 5X,' OPTIMUM FUNCTION VALUE=',D12.5,5X,' X=',10D12.5)
13      STOP
14      END

C
C***** ABSTRACT *****
C
C  THIS SUBROUTINE CALCULATES THE VALUE OF F GIVEN THE VALUES OF X(I)
C
C*****
C
1      SUBROUTINE FUN(N,X,F,NFUN)
2      IMPLICIT REAL*8(A-H,O-Z)
3      DIMENSION X(10)
4      F=10.*(X(2)-X(1)*X(1))**2+(1.-X(1))**2
5      NFUN=NFUN+1
6      RETURN
7      END

C
C***** ABSTRACT *****
C
C  THIS SUBROUTINE CALCULATES THE GRADIENT OF F GIVEN THE VALUES OF X(I)
C
C*****
C
1      SUBROUTINE DER(N,X,GRAD,NDER)

```

```

2      IMPLICIT REAL*8(A-H,O-Z)
3      DIMENSION X(10),GRAD(10)
4      GRAD(1)=-40.*X(1)*(X(2)-X(1)**2)-2.*(1.-X(1))
5      GRAD(2)=20.*(X(2)-X(1)**2)
6      NDER=NDER+1
7      RETURN
8      END

```

```

      NFUN= 159      NDER= 16
OPTIMUM FUNCTION VALUE= .14329D-17      X= .10000D+00 .10000D+00

```

### 6.2.3 Linear Programming

Many economically important engineering problems can be characterized by a linear objective function subject to a set of linear constraints. This type of problem is a linear programming (LP) problem. LP methods are used to solve resource allocation problems in which some commodity or product can be distributed in a variety of ways. LP methods allow the determination of the most efficient (usually economic) distribution pattern.

An example of a small LP problem is as follows:

Maximize

$$y = 2x_1 + 3x_2$$

subject to

$$x_2 - x_1 \leq 5$$

$$x_1 + x_2 \leq 10$$

In addition, with LP problems the independent variables are always assumed to be nonnegative; i.e.,

$$x_1 \geq 0$$

$$x_2 \geq 0$$

This problem is shown graphically in **Figure 6.15**. Note that the constraints form the boundaries of the valid region of the problem. Also, the family of lines for different values of  $y$  is indicated on this figure. It can be seen that the intersection of the two constraints is the location of the largest value of the objective function. For all LP problems, the solution occurs at an intersection of constraints; therefore, only the intersections of constraints (vertices) have to be examined in order to solve a LP problem. But for large-scale problems, there are an excessive number of vertices.

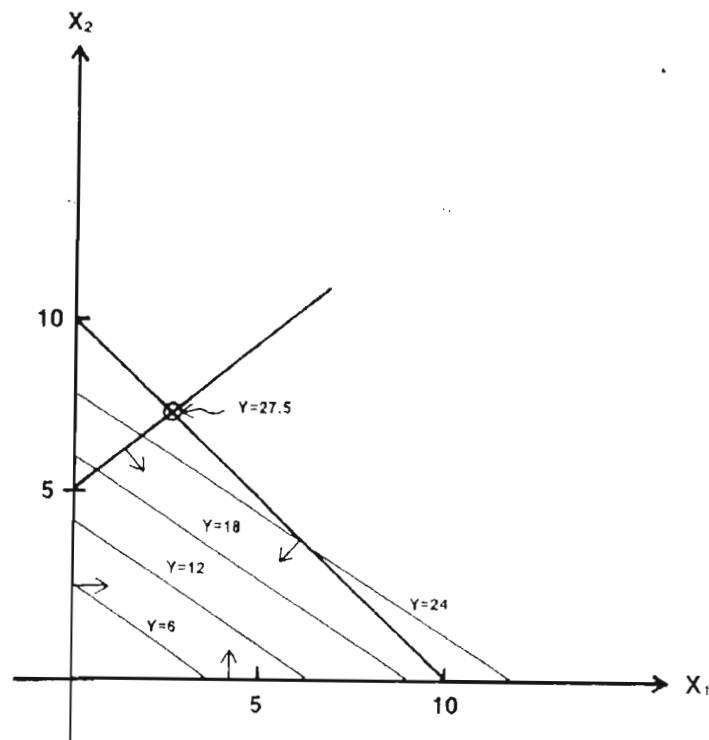


Figure 6.15 LP problem.

Let us consider how to systematically search the vertices to find the optimum using the simplex method. The first step is to find a starting point, that is, a vertex that satisfies all the constraints. Since

$$x_1 = x_2 = 0$$

satisfies all the constraints and is the intersection of the implied constraints on the independent variables, it will be used as the starting point (also called the basic solution).

Next, we must add slack variables to the constraints to convert them from inequality constraints to equality constraints.

$$x_2 - x_1 + x_3 = 5$$

$$x_1 + x_2 + x_4 = 10$$

Then this problem can be rearranged into the following form:

$$y = 2x_1 + 3x_2$$

$$x_3 = 5 + x_1 - x_2$$

$$x_4 = 10 - x_1 - x_2$$

where  $x_i \geq 0$  ( $i=1, 2, 3, 4$ ). Since at the basic solution,

$$x_1 = 0$$

$$x_2 = 0$$

the values of  $y$ ,  $x_3$ , and  $x_4$  can be read directly from the equations as their respective constant terms.

At this point the value of the objective function is zero. We want to move from this vertex in such a way that the greatest improvement in the objective function results. By analysis of the objective function, one can see that for the same change in  $x_1$  or  $x_2$ , the change in  $x_2$  provides a greater increase in the objective function. As a result, we should increase  $x_2$  until a constraint is encountered. Another way to identify which variable should be increased is to choose the variable with the largest positive coefficient when searching for a maximum.

Since  $x_1$  is to remain at zero, the first constraint indicates that the maximum value that  $x_2$  can attain is 5. Note that this occurs when  $x_3 = 0$ . The second constraint places a maximum value of  $x_2$  at 10 when  $x_4 = 0$ . Therefore, the first constraint is encountered first, as can be seen from **Figure 6.15**. This vertex is formed by the intersection of the first constraint and the implied constraint on  $x_1$ . At this point,

$$x_1 = 0$$

$$x_3 = 0$$

Now we should write the objective function and the constraints in terms of  $x_1$  and  $x_3$  since they are the current zeroed variables. So solving the second constraint in terms of  $x_2$  results in

$$x_2 = 5 + x_1 - x_3$$

This equation can be used to eliminate  $x_2$  from the objective function and the second constraint, yielding

$$y = 15 + 5x_1 - 3x_3$$

$$x_2 = 5 + x_1 - x_3$$

$$x_4 = 5 - 2x_1 + x_3$$

Therefore, at this vertex

$$y = 15$$

$$x_2 = 5$$

$$x_4 = 5$$

Note that since  $x_3 = 0$ , this indicates that this vertex lies on the first constraint (**Figure 6.15**).

Once again, we want to move away from the vertex in such a way that we obtain the greatest increase in the objective function. In this case, we want to increase the value of  $x_1$  since  $x_1$  has the only positive coefficient.

The first constraint places no limit on the value of  $x_1$ , while the second constraint limits  $x_1$  to less than or equal to 2.5; therefore, the second constraint is encountered first. At this vertex  $x_3 = x_4 = 0$ . Solving for  $x_1$  using the second constraint yields

$$x_1 = 2.5 + 0.5x_3 - 0.5x_4$$

Then writing the objective function and constraints in terms of  $x_3$  and  $x_4$  results in

$$y = 27.5 - 0.5x_3 - 2.5x_4$$

$$x_1 = 2.5 + 0.5x_3 - 0.5x_4$$

$$x_2 = 7.5 - 0.5x_3 - 0.5x_4$$

Note that now any increase in  $x_3$  or  $x_4$  results in a decrease in the value of the objective function; therefore, this vertex is the solution to this LP problem. At this vertex,  $x_1 = 2.5$  and  $x_2 = 7.5$ . Also, the coefficients of  $x_3$  and  $x_4$  in the objective function represent the sensitivity of the optimum value of  $y$  to relatively small changes in the two original constraints. For example, relaxing the second constraint (i.e., moving the constraint upward) provides a greater increase in the objective function than relaxing the first constraint. This results because  $x_4$  has a larger negative coefficient. A sensitivity analysis can be useful in analyzing the influence of sales and pricing structure on overall profits for LP problems. A more thorough presentation of a sensitivity analysis using the simplex method is presented by Beightler, Phillips, and Wilde [7].

The simplex method can also be applied to LP problems in which the goal is to minimize the objective function. The only changes are (1) that the variable to be increased in the objective function has the largest negative coefficient, and (2) that the solution is obtained when all coefficients of the variables in the objective function are positive.

The overall simplex algorithm can be summarized as follows:

1. Add the slack variables.
2. Find the basic solution.
3. Write the objective function and constraints in terms of zeroed variables.
4. Identify which zeroed variable should be increased.
5. Determine which constraint will be encountered first (this will locate the next vertex).
6. Write the objective function and constraints in terms of zeroed variables.
7. If the vertex is not an optimum, return to number 4.

In the implementation of a LP method to an industrial problem (i.e., as many as 1000 independent variables), several problems can result. The most challenging problem is usually finding the basic solution in order to begin the solution procedure. In addition, multiple solutions can result or the constraints can be mutually exclusive.



### Example 6.12 Minimization of a LP

#### Problem Statement

Find the minimum of the following LP problem:

$$y = 10 - 3x_1 - 2x_2$$

where

$$x_2 - x_1 \leq 5$$

$$x_1 + x_2 \leq 10$$

$$x_1 - x_2 \leq 5$$

#### Solution

Since  $x_1$  and  $x_2$  equal to zero satisfies all the constraints, it can be used as the basic solution. Now add in the slack variables and rearrange.

$$y = 10 - 3x_1 - 2x_2$$

$$x_3 = 5 + x_1 - x_2$$

$$x_4 = 10 - x_1 - x_2$$

$$x_5 = 5 - x_1 + x_2$$

Since  $x_1$  has the largest negative coefficient,  $x_1$  will be increased. The third constraint is encountered first. At this vertex,  $x_2$  and  $x_5$  are equal to zero. Using the third constraint to eliminate  $x_1$  from the rest of the problem results in

$$y = -5 - 5x_2 + 3x_5$$

$$x_3 = 10 - x_5$$

$$x_4 = 5 - 2x_2 + x_5$$

$$x_1 = 5 + x_2 - x_5$$

Note that values of  $y$ ,  $x_3$ ,  $x_4$ , and  $x_1$  can be read directly since  $x_2$  and  $x_5$  are equal to zero. Now increase  $x_2$  since  $x_2$  has the largest negative coefficient. Note that the first and third constraints place no upper limit on  $x_2$  but the second constraint does. Solving for  $x_2$  and substituting results in

$$y = -17.5 + 2.5x_4 + 0.5x_5$$

$$x_3 = 10 - x_5$$

$$x_2 = 2.5 - 0.5x_4 + 0.5x_5$$

$$x_1 = 7.5 - 0.5x_4 - 0.5x_5$$

which is the solution, since there are only positive coefficients remaining. Note that the optimum value of  $y$  is  $-17.5$ , which occurs at  $x_2 = 2.5$  and  $x_1 = 7.5$ .



**Table 6.4** Crude Yield and Availability

Crude		1	2	3	4
Fractional Yield	Gasoline	.10	.6	.35	.25
	Heating Oil	.30	.2	.25	.29
	Jet Fuel	.20	.1	.28	.20
	Lube Oil	.25	0	0	.15
	Loss	.15	.1	.12	.11
Availability 1000 Barrels/Day		25	20	30	35

**Table 6.5** Product Costs and Demand

Product	Total Cost of Processing \$/Barrel	Wholesale Price \$/Barrel	Maximum Demand 1000 Barrels/Day
Gasoline	50	55	35
Heating Oil	47	50	20
Jet Fuel	54	60	25
Lube Oil	57	65	4

**Example 6.13 Refinery LP****Problem Statement**

Consider a refinery that has the choice of processing four different crudes in any proportion it chooses. The yield and availability of each crude is shown in **Table 6.4**. For example, there are 35,000 barrels of crude 4 available for processing each day and for every 100 barrels processed, 25 barrels of gasoline, 29 barrels of heating oil, 20 barrels of jet fuel, and 15 barrels of lube oil are produced.

**Table 6.5** lists the total processing costs, wholesale price, and maximum market demand for gasoline, heating oil, jet fuel, and lube oil. For example, jet fuel costs \$54 per barrel to process and sells for \$60 per barrel and there is a market demand for 25,000 barrels per day. Find the amount of each crude that should be processed per day for a maximum profit.

**Solution**

First we must convert this problem into a LP. Define  $x_i$  as the amount of each crude (1000 barrels/day) processed. But the profit is based upon the amount of each

product produced; therefore, the fractional yields (Table 6.4) must be used with the  $x_i$  to get the overall profit. For example, the profit from processing crude 1 is

$$x_1 [(55 - 50)0.1 + (50 - 47)0.3 + (60 - 54)0.2 + (65 - 57)0.25] 1000 = \$4600x_1/\text{day}$$

Likewise, the profit for each crude can be calculated in terms of their respective processing rates,  $x_i$ 's. Combining these yields, the total profit  $y$  (\$/day) is

$$y = 4600x_1 + 4200x_2 + 4180x_3 + 4520x_4$$

There are two kinds of constraints on this problem: crude availability and market demand. Crude availability yields the following constraints directly:

$$x_1 \leq 25$$

$$x_2 \leq 20$$

$$x_3 \leq 30$$

$$x_4 \leq 35$$

In order to construct the market demand constraints, the fractional yields must be used.

$$\text{Gasoline} \quad 0.1x_1 + 0.6x_2 + 0.35x_3 + 0.25x_4 \leq 35$$

$$\text{Heating Oil} \quad 0.3x_1 + 0.2x_2 + 0.25x_3 + 0.29x_4 \leq 20$$

$$\text{Jet Fuel} \quad 0.2x_1 + 0.1x_2 + 0.28x_3 + 0.20x_4 \leq 25$$

$$\text{Lube Oil} \quad 0.25x_1 + 0.15x_4 \leq 4$$

Now that this problem has been converted into the form of a LP, it can be solved using the IMSL subroutine ZX3LP. Note that ZX3LP was set up to find the maximum of a LP problem; therefore, if you want to find the minimum of a LP problem, simply multiply the objective function by  $-1$ , leaving the constraints unchanged.

### PROGRAM LISTING FOR EXAMPLE 6.13

```

C
C***** ABSTRACT *****
C
C   THIS PROGRAM SOLVES EXAMPLE 6.13 USING THE IMSL LIBRARY
C   ROUTINE ZX3LP, WHICH SOLVES LINEAR PROGRAMMING PROBLEMS,
C   USING THE REVISED SIMPLEX METHOD (EASY TO USE VERSION)
C
C***** NOMENCLATURE *****
C
C   A(I,J)- THE COEFFICIENT OF THE JTH VARIABLE IN THE ITH
C           CONSTRAINT
C   B(I)- THE CONSTANT FOR THE ITH CONSTRAINT
C   C(I)- THE COEFFICIENT OF THE ITH VARIABLE IN THE OBJECTIVE
C           FUNCTION
C   IA- EQUAL TO M1+M2+2
C   IW- WORK VECTOR
C   M1- NUMBER OF INEQUALITY CONSTRAINTS

```

```

C  M2- NUMBER OF EQUALITY CONSTRAINTS
C  N- NUMBER OF INDEPENDENT VARIABLES
C  PSOL(I)- THE VALUE OF THE ITH VARIABLE AT THE OPTIMUM VERTEX
C  RW- WORK VECTOR
C
C *****
C
1  DIMENSION A(10,4),B(10),C(4),RW(128),IW(28),PSOL(20)
2  DIMENSION DSOL(10)
C
C  INPUT DATA FOR LP PROBLEM
C
3  N=4
4  IA=10
5  M1=8
6  M2=0
C  ZERO A MATRIX
7  DO 1 I=1,N
8  DO 1 J=1,IA
9  1 A(J,I)=0.0
10 DO 2 I=1,N
11 2 A(I,I)=1.0
C  SPECIFY NON-ZERO VALUES OF A MATRIX
12 A(5,1)=.1
13 A(5,2)=.6
14 A(5,3)=.35
15 A(5,4)=.25
16 A(6,1)=.3
17 A(6,2)=.2
18 A(6,3)=.25
19 A(6,4)=.29
20 A(7,1)=.2
21 A(7,2)=.1
22 A(7,3)=.28
23 A(7,4)=.2
24 A(8,1)=.25
25 A(8,4)=.15
C  SPECIFY B VECTOR
26 B(1)=25.
27 B(2)=20.
28 B(3)=30.
29 B(4)=35.
30 B(5)=35.
31 B(6)=20.
32 B(7)=25.
33 B(8)=4.
C  SPECIFY C VECTOR
34 C(1)=4600.
35 C(2)=4200.
36 C(3)=4180.
37 C(4)=4520.
C
C  CALL IMSL SUBROUTINE ZX3LP
C
38 CALL ZX3LP(A, IA, B, C, N, M1, M2, S, PSOL, DSOL, RW, IW, IER)
C
C  PRINT OUT RESULTS

```

```

C
39      PRINT 11,S
40      11 FORMAT( 22H THE MAXIMUM PROFIT IS,F10.2,2X,15H
          *DOLLARS PER DAY)
41      PRINT 12
42      12 FORMAT( 36H THE OPTIMAL PROCESSING SCHEDULE IS)
43      13 FORMAT( 5X,9H CRUDE NO,I2,15H THE FLOW RATE=,E11.4,21H
          *1000 BARRELS PER DAY)
44      DO 20 I=1,N
45      20 PRINT 13,I,PSOL(I)
46      END

```

THE MAXIMUM PROFIT IS 329933.31 DOLLARS PER DAY

THE OPTIMAL PROCESSING SCHEDULE IS

CRUDE NO 1 THE FLOW RATE = 0.0000E+00 1000 BARRELS PER DAY  
 CRUDE NO 2 THE FLOW RATE = 0.2000E+02 1000 BARRELS PER DAY  
 CRUDE NO 3 THE FLOW RATE = 0.3000E+02 1000 BARRELS PER DAY  
 CRUDE NO 4 THE FLOW RATE = 0.2667E+02 1000 BARRELS PER DAY

### 6.2.4 Industrial Practice

An industrial scale nonlinear optimization problem will typically have in the range of 20 to 100 independent variables subject to as many as 500 constraints. A special class of optimization methods has evolved to handle this type of problem: successive linear programming (SLP), successive quadratic programming (SQP), and the generalized reduced gradient method (GRG). These methods have been applied to a wide range of large-scale nonlinear problems ranging from chemical process optimization to complex resource allocation problems. Lasdon [8] presents a detailed analysis of the general problem with specific discussion of the SLP, SQP, and GRG methods.

**Successive Linear Programming.** With this method, the objective function and constraints are linearized about a starting point, converting the nonlinear problem into a LP problem. The LP is solved using conventional techniques, generating an improved estimate of the solution. Once again, the objective function and constraints are linearized, yielding another LP. In this manner, the optimum of the nonlinear problem is approached by successively converting the nonlinear problem into a LP.

This method is relatively easy to implement and is the method that is usually used for larger problems (greater than 50 independent variables). It tends to work quite well when the optimum lies at the intersection of constraints (i.e., at a vertex), but converges slowly for a nonvertex optimum.

**Successive Quadratic Programming.** In a manner similar to SLP, SQP successively converts the nonlinear problem into a quadratic programming problem which is solved at each step. A quadratic programming problem has linear constraints and a quadratic objective function of the following form:

$$y = \sum_{i=1}^n \sum_{j=1}^n a_{i,j} x_i x_j$$

There are algorithms [9] that have been developed to solve optimization problems of this particular form.

SQP is usually harder to implement than SLP but usually requires fewer function evaluations than either the SLP or GRG methods. SQP has evolved as the leading method for large-scale problems.

**Generalized Reduced Gradient Method.** The GRG method successively converts the optimization problems with constraints into an unconstrained problem which is usually solved using a gradient method (Section 6.2.2). First, slack variables are added to convert all the inequality constraints into equality constraints. Then each constraint is used to eliminate one degree of freedom in the objective function. Then the problem is converted into an unconstrained search with a lower dimensionality. When the reduced problem is solved, it produces an improved estimate of the optimum of the overall problem.

The GRG method is probably the most reliable method but is the hardest to implement. It tends to work well for both vertex optimization and nonvertex optimization.

**Table 6.6** Summary of Industrial Optimizers

Method	Advantages	Disadvantages
SLP	Easy to implement Effective on large problems Rapid convergence for vertex optimum	Slow convergence for non-vertex optimum
SQP	Most efficient method Best overall method	Harder to implement than SLP
GRG	Most reliable method Effective for both vertex and nonvertex optimum	Hardest to implement

### Section Summary

In most cases, the application of analytical methods to the solution of multidimensional optimization is not practical, but these methods do provide insight into multidimensional optimization. There are different types of multidimensional optimization problems: unconstrained problems, problems with equality constraints, and problems with equality and inequality constraints.

For unconstrained problems, there are necessary and sufficiency conditions which can be used to determine the location and character of the stationary points. For equality constrained problems, the method of constrained variation or the Lagrangian multipliers method can be used. Using slack variables, inequality constraints can be converted into equality constraints. For inequality constrained problems, it is usually more efficient to use the Lagrangian multiplier method.



There are two classes of unconstrained multidimensional numerical optimization methods: nongradient and gradient methods. Nongradient methods use only function values in searching for the optimum. Gradient methods use the gradient of the function as well as the function values. The multidimensional optimization methods used by the text are the Nelder-Mead method, which is a pattern search method that both expands and contracts, and a conjugate gradient method.

A linear objective function subject to linear constraints constitutes a LP problem. The solution of a LP is located at the vertex formed by the constraints of the problem. The simplex method provides a systematic means of searching the vertices of a problem to locate the optimum.

The SLP, SQP, and GRG methods can be applied to solve industrial scale optimization problems (i.e., greater than 20 independent variables). SLP is the easiest to implement and is usually used on the larger problems. SQP is usually the most efficient method, while GRG is the most reliable but the hardest to implement. Table 6.6 presents a comparison of advantages and disadvantages of each of these methods.

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## 6.3 Problems

### Section 1

- 6.1 Find the global maximum and minimum for the following objective function:

$$y = x^3 - 6x^2 + 36x + 7$$

$$1 \leq x \leq 5$$

- 6.2 Find the global maximum and minimum for the following objective function:

$$y = 2x^3 + 3x^2 - 7x + 5$$

$$0.5 \leq x \leq 5$$

- 6.3. Find the global minimum of

$$y = x^2 + \exp(2/x^2)$$

where  $x > 0$ .

- 6.4 Find the global maximum and global minimum of

$$y = \frac{x^2 + 3x + 1}{x - 3}$$

- 6.5 Using  $x = 0$  as the starting point, bound the following function:

$$\min(y) = x^2 - 20x + 100$$

Using

- a. a constant step size  $\Delta x$  of 1.0
- b. a step size doubling procedure with an initial step size of 1.0

- 6.6 Using the results of the previous problem, part b, perform by hand 3 cycles of search using the modified Fibonacci method.
- 6.7 Perform by hand 3 cycles of search for the minimum using the modified Fibonacci method on **Problem 6.2**.
- 6.8 Solve **Problem 6.3** numerically. First bound the optimum by hand; then, using the computer program presented in **Example 6.9**, find the solution to an accuracy of 0.01.
- 6.9 Solve **Problem 6.2** using the computer program (**Example 6.9**).

## Section 2

6.10 Using the computer code for the Nelder-Mead method, find the minimum of

$$y = 3x_1^2 + 3x_2^2 + 5x_1x_2 - 6x_1 + 4x_2 + 8$$

6.11 Find the maximum of

$$y = x_1^2 + x_2^2$$

subject to

$$x_1 + x_2 < 5$$

$$x_1 > 0$$

$$x_2 > 0$$

$$3x_1 - x_2 < 7$$

using a penalty function approach to convert the problem into an unconstrained search.

6.12 Solve the following LP problem by hand:

Maximize

$$y = 2x_1 + 3x_2 + 5x_3$$

subject to

$$2x_1 + 2x_2 + 2x_3 \leq 3$$

$$5x_1 - x_2 + 2x_3 \leq 5$$

$$x_1 + 3x_2 - 2x_3 \leq 2$$

6.13 You are required to produce an alloy that has at least 30% Pb and at least 30% Zn by mixing a number of available Pb-Zn-Sn alloys. Find the cheapest blend.

Available Alloy	Analysis (%)			Cost (\$/lb)
	Pb	Zn	Sn	
1	20	20	60	6.0
2	10	40	50	6.3
3	40	50	10	7.5
4	50	30	20	8.0