6 Analytical Multidimensional (Multivariable) Unconstrained Optimization

Learning Objectives

After studying this chapter, you should be able to:

1. Describe the method of solving problems of multivariable unconstrained optimization.
2. Classify the multivariable optimization problems.
3. Explain the necessary and sufficient conditions for solving multivariable unconstrained optimization problems.
4. Solve unconstrained multivariable functions.

In Chapter 5, we formulated the single variable optimization problems without constraints. Now let us extend those concepts to solve multivariable optimization problems without constraints. The optimization of such problems is routed in more than one direction. For instance, if there are two variables in the objective function, we call such problems *two-dimensional* as we have to search from two directions. Similarly, a three-variable problem can be called *three-dimensional*, and so on. However, the method of solving is similar in all such cases, and, therefore, all these problems can be named *multidimensional* or *multivariable unconstrained optimization* problems.

Recollect that we made use of complete differentiation to solve single variable unconstrained optimization problems. Here we use the concept of partial differentiation in solving multivariable unconstrained optimization problems using analytical methods.

6.1 Classification of Multivariable Optimization Problems

The multivariable optimization problems can be classified broadly into two categories: multivariable unconstrained optimization, i.e. without constraints, and multivariable constrained optimization, i.e. with constraints. Further, since we categorize the constraints into two types, such as equality and inequality type we can further classify the multivariable constrained optimization problems into two types. Summarily, the classification of multivariable optimization problems is shown in Figure 6.1.

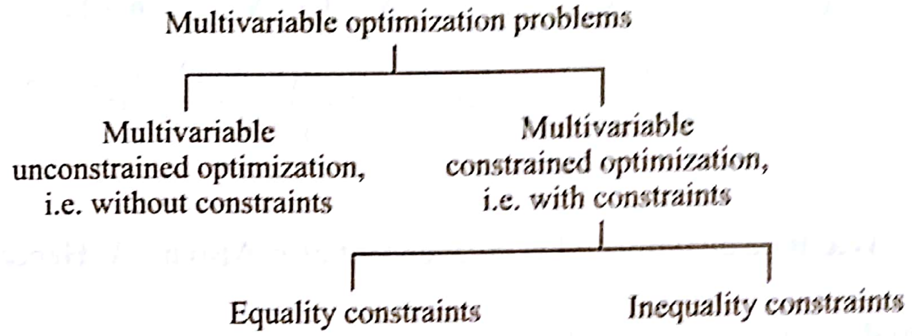

Figure 6.1 Classification of multivariable optimization problems.

In this chapter, we discuss the analytical solution methods for multivariable unconstrained optimization.

6.2 Optimization Techniques to Solve Unconstrained Multivariable Functions

Let us now discuss the necessary and sufficient conditions for optimization of an unconstrained (without constraints) multivariable function for which we make use of Taylor's series expansion of a multivariable function. Taylor's theorem/series expansion is given in Exhibit 6.1.

Exhibit 6.1
Taylor's Theorem/Series Expansion

Taylor's Series

In the Taylor's formula with remainder [Eqs. (i) and (ii)], if the remainder $R_n(x) \to 0$ as $n \to \infty$, then we obtain

$$f(x) = f(a) + \frac{(x-a)}{1!} f'(a) + \frac{(x-a)^2}{1!} f''(a) + \cdots + \frac{(x-a)^n}{n!} f^{(n)}(a) + \cdots \quad \text{(i)}$$

which is called the *Taylor's series*. When $a = 0$, we obtain the *Maclaurin's series*

$$f(x) = f(0) + \frac{x}{1!} f'(0) + \frac{x^2}{2!} f''(0) + \cdots + \frac{x^n}{n!} f^{(n)}(0) + \cdots \quad \text{(ii)}$$

Since it is assumed that $f(x)$ has continuous derivatives up to $(n+1)$th order, $f^{(n+1)}(x)$ is bounded in the interval (a, x). Hence, to establish that $\lim_{n\to\infty} |R_n(x)| = 0$, it is sufficient to show that $\lim_{n\to\infty} \frac{|x-a|^{n+1}}{(n+1)!} = 0$ for any fixed numbers x and a. Now, for any fixed numbers x and a,

6.3 Necessary Condition (Theorem 6.1)

If $f(x)$ has an extreme point (maximum or minimum) at $x = x^*$ and if the first derivative of $f(x)$ exists at x^*, then

$$\frac{\partial f(x^*)}{\partial x_1} = \frac{\partial f(x^*)}{\partial x_2} = \cdots = \frac{\partial f(x^*)}{\partial x_n} = 0$$

6.4 Sufficient Condition (Theorem 6.2)

A sufficient condition for a stationary point x^* to be an extreme point is that the matrix of second partial derivatives (Hessian matrix) of $f(x)$ evaluated at x^* is:

(i) Positive definite when x^* is a relative minimum point.
(ii) Negative definite when x^* is a relative maximum point.

6.5 Working Rule (Algorithm) for Unconstrained Multivariable Optimization

From Theorems 6.1 and 6.2, we can obtain the following procedure to solve the problems of multivariable functions without constraints.

Step 1: Check the function to ensure that it belongs to the category of multivariable unconstrained optimization problems, i.e. it should contain more than one variable, say, $x_1, x_2, \ldots, x_n$ and no constraints.

Step 2: Find the first partial derivatives of the function w.r.t. $x_1, x_2, \ldots, x_n$.

Step 3: Equate all the first partial derivatives (obtained from Step 2) to zero to find the values of $x_1^*, x_2^*, \ldots, x_n^*$.

Step 4: Find all the second partial derivatives of the function.

Step 5: Prepare the Hessian matrix. For example, if we have two variables x_1, x_2, in $f(x)$, then the Hessian matrix is

$$J_{(x_1^*, x_2^*)} = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1 \partial x_2} \\ \dfrac{\partial^2 f}{\partial x_1 \partial x_2} & \dfrac{\partial^2 f}{\partial x_2^2} \end{bmatrix}$$

Step 6: Find the values of determinants of square sub-matrices

$$J_1, J_2, \ldots, J_n$$

In our example,
$$J_1 = \left| \frac{\partial^2 f}{\partial x_1^2} \right|$$

and
$$J_2 = \begin{vmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1 \partial x_2} \\ \dfrac{\partial^2 f}{\partial x_1 \partial x_2} & \dfrac{\partial^2 f}{\partial x_2^2} \end{vmatrix}$$

Step 7: Evaluate whether x_1^*, x_2^* are relative maxima or minima depending on the positive or negative nature of J_1, J_2 and so on.

Thus, the sign of J_1 decides whether J is positive or negative while the sign of J_2 decides definite or indefiniteness of J (Table 6.1). More clearly,

If (i) $J_1 > 0, J_2 > 0$, then J is positive definite and x^* is a relative minimum.
(ii) $J_1 > 0, J_2 < 0$, then J is indefinite and x^* is a saddle point.
(iii) $J_1 < 0, J_2 > 0$, then J is negative definite and x^* is a relative maximum.
(iv) $J_1 < 0, J_2 < 0$, then J is indefinite and x^* is a saddle point.

Table 6.1 presents the sign notation of J.

Table 6.1 Sign Notation of J

J_1 / J_2	**J_1 positive or $J_1 > 0$ (J is positive)**	**J_1 negative or $J_1 < 0$ (J is negative)**
J_2 positive or $J_2 > 0$ (J is definite)	J is positive definite and x^* is a relative minimum	J is negative definite and x^* is a relative maximum
J_2 negative or $J_2 < 0$ (J is indefinite)	J is indefinite and x^* is a saddle point	J is indefinite and x^* is a saddle point

Note: If in a function of two variables $f(x_1, x_2)$ the Hessian matrix is neither positive nor negative definite, then the point (x_1^*, x_2^*) at which $\partial f/\partial x_1^* = \partial f/\partial x_2^*$ is called the *saddle point*, which means it may be a maximum or minimum with one variable when the other is fixed.

Illustration 6.2 Determine the extreme points as well as evaluate the following function $f(x)$:

$$f(x) = x_1^3 + x_2^3 + 2x_1^2 + 4x_2^2 + 6$$

Solution The necessary conditions for the existence of an extreme point are

$$\frac{\partial f}{\partial x_1} = 0 \quad \text{and} \quad \frac{\partial f}{\partial x_2} = 0$$

$$\frac{\partial f}{\partial x_1} = 3x_1^2 + 4x_1 = x_1(3x_1 + 4) = 0 \qquad \text{(i)}$$

$$\frac{\partial f}{\partial x_2} = 3x_2^2 + 8x_2 = x_2(3x_2 + 8) = 0 \qquad \text{(ii)}$$

From Eq. (i), we get $x_1 = 0$ or $-\dfrac{4}{3}$

And from Eq. (ii), we get $x_2 = 0$ or $-\dfrac{8}{3}$

Hence, the above equations are satisfied by the following points:

$$(0, 0), (0, -8/3), (-4/3, 0) \text{ and } (-4/3, -8/3)$$

Now, let us find the nature of these extreme points for which we use the sufficiency conditions, i.e. by the second order partial differentiation of f.

$$\frac{\partial^2 f}{\partial x_1^2} = 6x_1 + 4$$

$$\frac{\partial^2 f}{\partial x_2^2} = 6x_2 + 8$$

$$\frac{\partial^2 f}{\partial x_1 \partial x_2} = 0$$

The Hessian matrix of f is given by

$$J = \begin{bmatrix} 6x_1 + 4 & 0 \\ 0 & 6x_2 + 8 \end{bmatrix}$$

Hence,

$$J_1 = |6x_1 + 4|$$

and

$$J_2 = \begin{vmatrix} 6x_1 + 4 & 0 \\ 0 & 6x_2 + 8 \end{vmatrix}$$

The values of J_1 and J_2 and the nature of the extreme points are given in Table 6.2.

Table 6.2 Sign Notation of J in Illustration 6.2

Point x	Value of J_1	Value of J_2	Nature of J	Nature of x	$f(x)$
(0, 0)	+ 4	+ 32	Positive definite	Relative minimum	6
(0, –8/3)	+ 4	–32	Indefinite	Saddle point since $\partial f/\partial x_1 = \partial f/\partial x_2$	418/27
(–4/3, 0)	–4	–32	Indefinite	Saddle point	194/27
(–4/3, –8/3)	–4	+ 32	Negative definite	Relative maximum	50/3

Illustration 6.3 Find the extreme values of the function $f(x_1, x_2) = x_1^2 - x_2^2$.

Solution Applying the necessary conditions $\partial f/\partial x_1 = 0$ and $\partial f/\partial x_2 = 0$, we have

$$\frac{\partial f}{\partial x_1} = 2x_1 = 0 \Rightarrow x_1 = 0$$

$$\frac{\partial f}{\partial x_2} = -2x_2 = 0 \Rightarrow x_2 = 0$$

Now, applying the sufficient conditions

$$\frac{\partial^2 f}{\partial x_1^2} = 2, \quad \frac{\partial^2 f}{\partial x_2^2} = -2 \quad \text{and} \quad \frac{\partial^2 f}{\partial x_1 \partial x_2} = 0$$

Therefore, the Hessian matrix $J = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}$

Thus at $x_1 = 0, x_2 = 0$.

We have $J_1 = |2| = 2$ and $J_2 = \begin{vmatrix} 2 & 0 \\ 0 & -2 \end{vmatrix} = -4$

Since J_1 is positive (+2) and J_2 is negative (–4), the nature of J is indefinite and the point at $x_1 = 0, x_2 = 0$ is a saddle point, and also the value the function at this saddle point is $f(0,0) = 0$.

Note: At the saddle point if one of the values of x_1 or x_2 is fixed, the other may show extremity.

Illustration 6.5 Two frictionless rigid bodies R_1 and R_2 are connected by three linear elastic springs of constants k_1, k_2 and k_3 as shown in Figure 6.3. The springs are at their natural positions when the applied force P is zero. Find the displacements x_1 and x_2 under the force of 26 units by using the principle of minimum potential energy assuming the spring constants k_1, k_2 and k_3 as 2, 3 and 4 respectively. Examine whether the displacements correspond to the minimum potential energy.

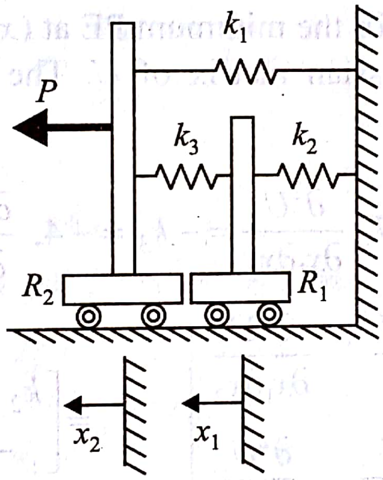

Figure 6.3 Illustration 6.5.

Solution We know that the potential energy U is given by

Potential energy, U = strain energy of springs – work done by external forces.

$$= [(1/2)k_2x_1^2 + (1/2)k_3(x_2 - x_1)^2 + (1/2)k_1x_2^2] - Px_2$$

where k_1, k_2 and k_3 are the spring constants.

Now taking k_1, k_2 and k_3 as 2, 3 and 4 respectively, we get the potential energy, U as

$$U = \left[\frac{1}{2}k_2x_1^2 + \frac{1}{2}k_3(x_2 - x_1)^2 + \frac{1}{2}k_1x_2^2\right] - Px_2$$

$$= \left[\frac{1}{2}\times 3x_1^2 + \frac{1}{2}\times 4(x_2 - x_1)^2 + \frac{1}{2}\times 2x_2^2\right] - Px_2$$

$$= \frac{3}{2}x_1^2 + 2(x_2 - x_1)^2 + x_2^2 - Px_2$$

Applying the necessary condition for the minimum of U, and substituting the value of spring constants, we get

$$\frac{\partial U}{\partial x_1} = k_2x_1 - k_3(x_2 - x_1) = 0 \quad \text{(i)}$$

$$= 3x_1 - 4(x_2 - x_1) = 0$$

and

$$\frac{\partial U}{\partial x_2} = k_3(x_2 - x_1) + k_1x_2 - P = 0 \quad \text{(ii)}$$

$$= 4(x_2 - x_1) + 2x_2 - P = 0$$

The values of x_1 and x_2 corresponding to the equilibrium state obtained by the above equations are

$$x_1^* = \frac{Pk_3}{k_1k_2 + k_2k_3 + k_3k_1} = \frac{4P}{(2\times 3)+(3\times 4)+(4\times 2)} = \frac{4P}{26}$$

$$x_2^* = \frac{P(k_2 + k_3)}{k_1k_2 + k_2k_3 + k_3k_1} = \frac{4P}{(2\times 3)+(3\times 4)+(4\times 2)} = \frac{7P}{26}$$

At P = 26 units, x_1^* = 4 units and x_2^* = 7 units.

Now, the sufficiency condition for the minimum PE at (x_1^*, x_2^*) can also be verified by testing the positive definiteness of the Hessian matrix of U. The Hessian matrix of U evaluated at (x_1^*, x_2^*) is

$$\frac{\partial^2 U}{\partial x_1^2} = k_2 + k_3 = 7, \quad \frac{\partial^2 U}{\partial x_1 \partial x_2} = -k_3 = -4, \quad \frac{\partial^2 U}{\partial x_2^2} = k_1 + k_3 = 6$$

$$J_{(x_1^*, x_2^*)} = \begin{bmatrix} \dfrac{\partial^2 U}{\partial x_1^2} & \dfrac{\partial^2 U}{\partial x_1 \partial x_2} \\ \dfrac{\partial^2 U}{\partial x_1 \partial x_2} & \dfrac{\partial^2 U}{\partial x_2^2} \end{bmatrix}_{(x_1^*, x_2^*)} = \begin{bmatrix} k_2 + k_3 & -k_3 \\ -k_3 & k_1 + k_3 \end{bmatrix}$$

$$= \begin{bmatrix} 7 & -4 \\ -4 & 6 \end{bmatrix}$$

The determinants of sub-matrices of J are

$$J_1 = |k_2 + k_3| = k_2 + k_3 = 7 > 0$$

and
$$J_2 = \begin{vmatrix} k_2 + k_3 & -k_3 \\ -k_3 & k_1 + k_3 \end{vmatrix} = \begin{vmatrix} 7 & -4 \\ -4 & 6 \end{vmatrix} = 42 + 16 = 58 > 0$$

Since the values of J are positive, the matrix J is positive definite and hence the values x_1^* and x_2^* correspond to the minimum potential energy.

$\therefore$ $x_1^* = 4$ and $x_2^* = 7$.

Illustration 6.6 The profit on a contract of road laying is estimated as $26x_1 + 20x_2 + 4x_1x_2 - 3x_1^2 - 4x_2^2$, where x_1 and x_2 denote the labour cost and the material cost respectively. Find the values of labour cost and material cost that can maximize the profit on the contract.

Solution Given, profit $Z(x_1, x_2) = 26x_1 + 20x_2 + 4x_1x_2 - 3x_1^2 - 4x_2^2$

Applying the necessary conditions, i.e.

$$\frac{\partial Z}{\partial x_1} = \frac{\partial Z}{\partial x_2} = 0$$

$$\frac{\partial Z}{\partial x_1} = 26 + 4x_2 - 6x_1 = 0 \qquad \text{(i)}$$

and
$$\frac{\partial Z}{\partial x_2} = 20 + 4x_1 - 8x_2 = 0 \qquad \text{(ii)}$$

On solving Eqs. (i) and (ii), we get $x_1^* = 9$, $x_2^* = 7$.

Now, let us apply the sufficiency condition to maximize the profit (Z) at (x_1^*, x_2^*). This is verified by testing the negative definiteness of the Hessian matrix. The Hessian matrix of Z at (x_1^*, x_2^*) is calculated as

$$\frac{\partial Z}{\partial x_1^2} = -6, \quad \frac{\partial Z}{\partial x_2^2} = -8 \text{ and } \frac{\partial^2 Z}{\partial x_1 \partial x_2} = 4$$

$\therefore$ Hessian matrix $J_{(x_1^*, x_2^*)} = \begin{bmatrix} -6 & 4 \\ 4 & -8 \end{bmatrix}$

The determinants of the square sub-matrices of J are

$$J_1 = |-6| = -6 < 0$$

$$J_2 = \begin{vmatrix} -6 & 4 \\ 4 & -8 \end{vmatrix} = 48 - 16 = 32 > 0$$

Since J_1 is negative (i.e. -6) and J_2 is positive (i.e. $+32$) which is definite, the nature of J is negative definite. Hence, the values of x_1 and x_2 show a relative maximum for Z at x_1^* and x_2^* respectively.

$\therefore$
$$x_1^* = 9, \; x_2^* = 7$$

Hence max profit,
$$Z_{max} = 26(9) + 20(7) + 4(9)(7) - 3(9)^2 - 4(7)^2$$
$$= 234 + 140 + 252 - 243 - 196 = 187 \text{ units}$$

Summary

Multivariable optimization problems without constraints are explained in this chapter. The optimization problems of multivariable functions without constraints make use of Taylor's series expansion of multivariable functions and partial differentiations. The basic idea behind the solution methods of these problems is trying to convert them nearest to the single variable problems, i.e. the partial differentiation which is the differentiation of one variable at a time keeping the other variables fixed. However, the mathematical concepts of matrices, calculus and other simple algebraic principles are prerequisites to these problems. We will take up the multivariable constrained problems in the next chapter.

Key Concepts

Multidimensional optimization: The optimization problems routed in more than one direction, i.e. having more than one variable.

Saddle point: If there is a function of two variables $f(x_1, x_2)$ whose Hessian matrix is neither positive definite nor negative definite, then the point (x_1^*, x_2^*) at which $\partial f/\partial x_1^* = \partial f/\partial x_2^*$ is called the saddle point.

Hessian matrix: $J_{x = x^*} = [\partial^2 f/\partial x_i \partial x_j|_{x=x^*}]$ is the matrix of the second partial derivative.

Positive definite: If $J_1 > 0$, $J_2 > 0$, then J is positive definite and x^* is a relative minimum.

Positive indefinite: If $J_1 > 0$, $J_2 < 0$, then J is indefinite and x^* is a saddle point.

Negative definite: If $J_1 < 0$, $J_2 > 0$, then J is negative definite and x^* is a relative maximum.

Negative indefinite: If $J_1 < 0$, $J_2 < 0$, then J is indefinite and x^* is a saddle point.