

Numerical Methods

Numerical methods play an important role in solving complex engineering and science problems. This textbook provides essential information on a wide range of numerical techniques, and it is suitable for undergraduate and postgraduate/research students from various engineering and science streams. It covers numerical methods and their analysis to solve nonlinear equations, linear and nonlinear systems of equations, eigenvalue problems, interpolation and curve-fitting problems, splines, numerical differentiation and integration, ordinary and partial differential equations with initial and boundary conditions. C-programs for various numerical methods are presented to enrich problem-solving capabilities. The concepts of error and divergence of numerical methods are described by using unique examples. The introductions to all chapters carry graphical representations of the problems so that readers can visualize and interpret the numerical approximations.

C-Programs are available at www.cambridge.org/9781108716000

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Numerical Methods

Fundamentals and Applications

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To My Parents

Sh. Murari Lal and Smt. Santosh Devi

To My Teacher

Professor Karanjeet Singh

To My Wife and Children

Dr Usha Rani Gupta and Aaradhya and Reyansh

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Preface

There is no branch of mathematics, however abstract, which may not some day be applied to phenomena of the real world.

Nikolai Ivanovich Lobachevsky

(December 1, 1792–February 24, 1856)

His work is mainly on hyperbolic geometry, also known as Lobachevskian geometry.

The rapid growth of science and technology during the last few decades has made a tremendous change to the nature of various mathematical problems. It is not easy to solve these new problems for analytical solutions by conventional methods. In fact, the study of these mathematical problems for analytical solutions is not only regarded as a difficult endeavor, rather it is almost impossible to get analytical solutions in many cases. The tools for analysis and for obtaining the analytical solutions of complex and nonlinear mathematical systems are limited to very few special categories. Due to this reason, when confronted with such complex problems we usually simplify them by invoking certain restrictions on the problem and then solve it. But these solutions, however, fail to render much needed information about the system. These shortcomings of analytical solutions lead us to seek alternates, and various numerical techniques developed for different types of mathematical problems seem to be excellent options. During the last century, the numerical techniques have witnessed a veritable explosion in research, both in their application to complex mathematical systems and in the very development of these techniques. At many places in this book, we will compare numerical techniques with analytical techniques, and point out various problems which can not be solved through analytical techniques, and to which numerical techniques provide quite good approximate solutions.

Many researchers are using numerical techniques to investigate research problems. Numerical techniques are now widely used in a lot of engineering and science fields. Almost all universities now offer courses on introductory and advanced computer-oriented numerical methods to their engineering and science students, keeping in mind the utilization merits of these techniques. In addition, computer-oriented problems are part of various other courses of engineering/technology.

It gives me immense pleasure in presenting the book to our esteemed readers. This book is written keeping several goals in mind. It provides essential information on various numerical techniques to the students from various engineering and science streams. The aim of the book is to make the subject easy to understand, and to provide in-depth knowledge about various numerical tools in a simple and concise manner.

Students learn best when the course is problem-solution oriented, especially when studying mathematics and computing. This book contains many examples for almost all numerical techniques designed from a problem-solving perspective. In fact, theoretical and practical introductions to numerical techniques and worked examples make this book student-friendly.

While the main emphasis is on problem-solving, sufficient theory and examples are also included in this book to help students understand the basic concepts. The book includes theories related to errors and convergence, limitations of various methods, comparison of various methods for solving a specific type of problem and scope for further improvements, etc.

The practical knowledge of any subject is thought to be an essential part of the curriculum for an engineering student. Numerical methods require tedious and repetitive arithmetic operations, wherein for large-scale problems it is almost impossible to do such cumbersome arithmetic operations manually. Fortunately most numerical techniques are algorithmic in nature, so it is easy to implement them with the aid of a computer. To enrich problem-solving capabilities, we have presented the basic C-programs for a wide range of methods to solve algebraic and transcendental equations, linear and nonlinear systems of equations, eigenvalue problems, interpolation problems, curve fitting and splines, numerical integration, initial and boundary value problems, etc.

The section below provides an overview of the contents of the book. Each chapter contains a brief introduction and it also emphasizes the need for numerical techniques for solving specific problems. We have provided exercises in all chapters with the aim of helping students check their capabilities and understanding, and also illustrate how various numerical methods are the better problem solvers.

Chapter-by-chapter Introduction to the Book

The book comprises sixteen chapters.

Chapter 1: Number Systems explains integral and fractional numbers in the binary, octal, decimal and hexadecimal number systems. It also includes the conversion from one number system to another number system.

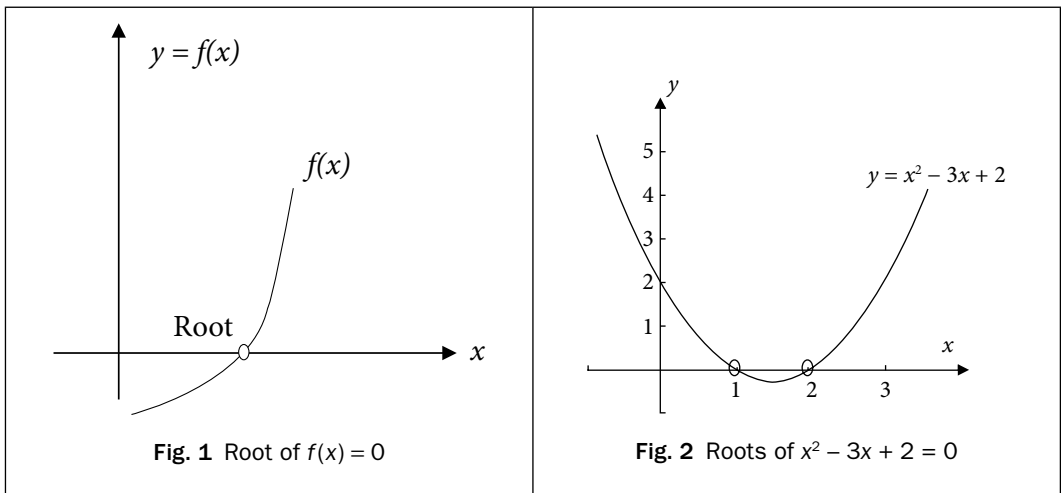
Chapter 2: Error Analysis primarily presents various types of errors, and some standard remedies to trace and reduce these errors.

Except Chapters 1 and 2, all other chapters of this book have been devoted to numerical techniques which are used to solve some specific type of problems. In each chapter, various numerical methods will be introduced to solve these problems.

Chapter 3: Nonlinear Equations consists of various techniques to solve nonlinear equations in single variable. Primary aim is to determine the value of variable or parameter x , called root of the equation that satisfies the equation

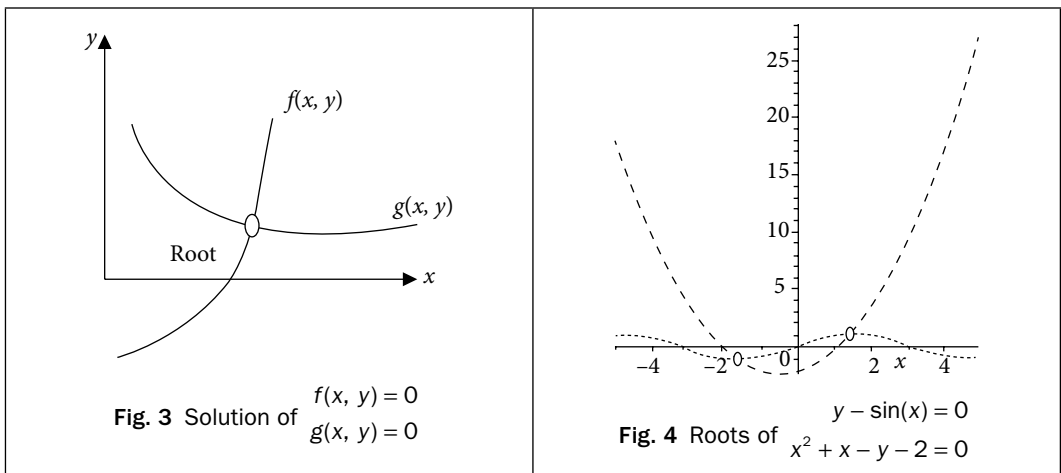
$$f(x) = 0$$

Roots of simple equations like quadratic equation $x^2 - 3x + 2 = 0$ can be obtained easily. But in the case of higher order polynomial equations like $3x^5 + x^4 + 3x^3 - 2x^2 - 3x + 9 = 0$ and transcendental equations viz. $2e^x \cos x - x = 0$, we do not have any general method to compute the roots of these equations. Numerical techniques will be helpful for computing roots of such equations.



These problems are especially valuable in engineering design contexts where due to the complexity of the design equations it is often impossible to solve these equations with analytical methods.

Chapter 4: *Nonlinear Systems and Polynomial Equations* deals with the numerical techniques to solve the systems of nonlinear equations, say, the system of two equations
$$\begin{cases} f(x, y) = 0 \\ g(x, y) = 0 \end{cases}$$



The aim is to find coordinate (x, y) , which satisfies these two equations simultaneously. Since there is no general analytical method for the solution of such systems of nonlinear equations, therefore we will apply numerical methods to solve such kind of problems. This chapter also includes some numerical methods for the roots of polynomial equations.

Chapter 5: *Systems of Linear Equations* is devoted to obtain solution of the system of linear algebraic equations

$$\begin{array}{l}
 a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1 \\
 a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2 \\
 \vdots \\
 \vdots \\
 a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nn}x_n = b_n
 \end{array}
 \quad \text{e.g.,} \quad
 \begin{array}{l}
 x_1 - 2x_2 + 3x_3 = 15 \\
 2x_1 - x_2 + 3x_3 = 15 \quad \text{with } n = 3. \\
 x_1 + x_2 - 3x_3 = -9
 \end{array}$$

In case of system of two algebraic equations, we have two lines, and their point of intersection is the solution.

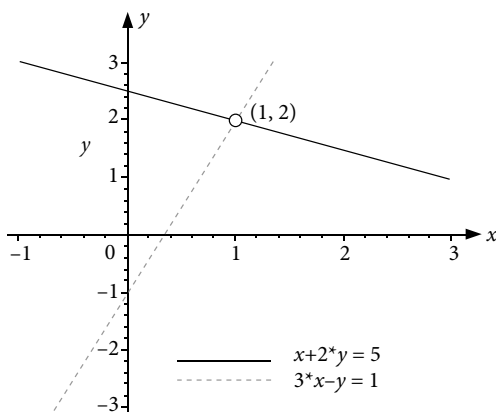


Fig. 5 Linear system in two variables (x, y)

Such equations have many important applications in science and engineering, specifically in the mathematical modeling of large systems of interconnected elements such as electrical circuits, structures, lattice and fluid networks, etc. In this chapter, we will discuss various direct and iterative methods to solve these systems of linear equations. Also, we will discuss problems that arise in applying these methods on the computer and some remedies for these problems.

Chapter 6: *Eigenvalues and Eigenvectors* is to deduce eigenvalues and eigenvectors for a square matrix A . A column vector X is an eigenvector corresponding to eigenvalue λ of a square matrix A , if

$$AX = \lambda X. \quad (\text{or}) \quad (A - \lambda I)X = 0$$

The nontrivial solutions of this homogeneous system exist, only if

$$p(\lambda) = \det(A - \lambda I) = 0$$

$p(\lambda)$ is the polynomial of degree n for a square matrix of order n . There are only n eigenvalues of matrix A , including repetitions (eigenvalues may be complex). The polynomial $p(\lambda)$ is known as characteristic polynomial, and the equation $p(\lambda) = 0$ is called characteristic equation.

For example, the characteristic equation for the matrix $A = \begin{bmatrix} 1 & 2 \\ 3 & 2 \end{bmatrix}$ is given by

$$p(\lambda) = |A - \lambda I| = \begin{vmatrix} 1 - \lambda & 2 \\ 3 & 2 - \lambda \end{vmatrix} = (\lambda - 4)(\lambda + 1) = 0$$

The roots of the characteristic equation give eigenvalues -1 and 4 .

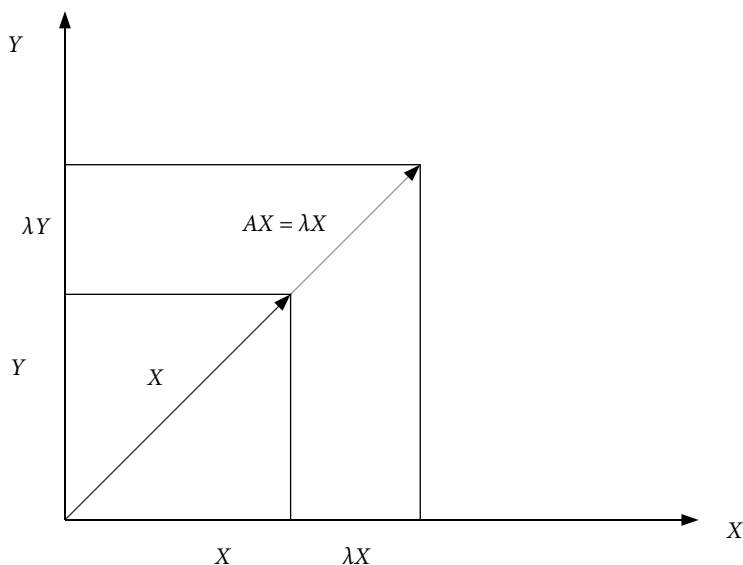


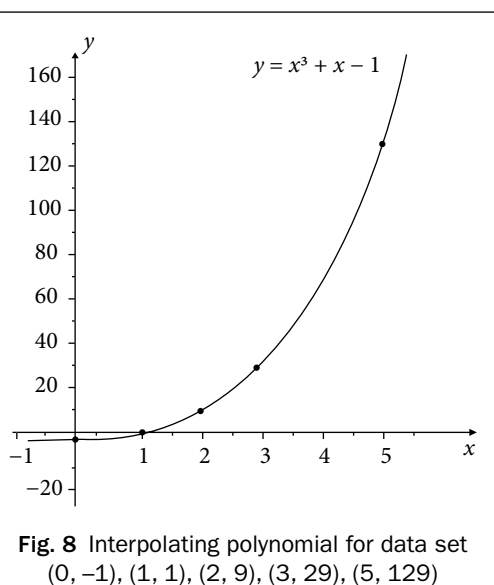
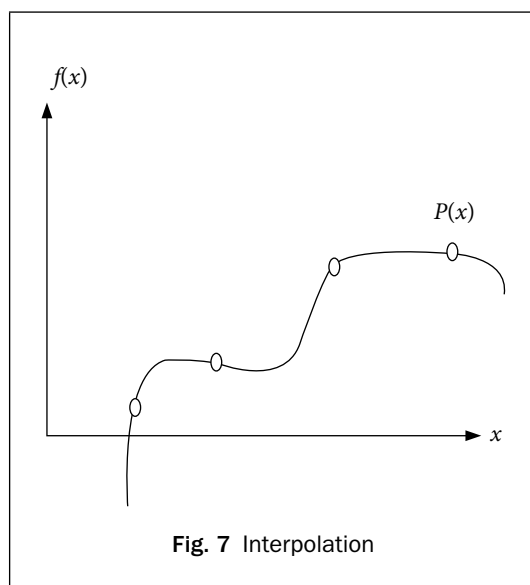
Fig. 6 Eigenvalue λ and eigenvector X of matrix A

These types of problems arise in different streams of science and engineering especially in the case of oscillatory systems like elasticity, vibrations, etc.

Chapter 7: Eigenvalues and Eigenvectors of Real Symmetric Matrices deals with the eigenvalues and eigenvectors of real symmetric matrices. Some methods are applicable only to real symmetric matrices. Since these methods are easy to implement and provide all the eigenvalues and eigenvectors at a time, hence need more exploration.

Chapter 8: Interpolation is most important part of numerical methods, as it deals with the approximation of the data sets with the polynomials. This chapter deals with the task of constructing a polynomial function $P(x)$ of minimum degree, which passes through a given set of discrete data points (x_i, y_i) , $i = 0, 1, \dots, n$. This polynomial is known as interpolating polynomial. It estimates the value of the dependent variable y for any intermediate value of the independent variable, x .

For example: consider the data set $(0, -1), (1, 1), (2, 9), (3, 29), (5, 129)$. The aim is to construct a polynomial of minimum degree which passes through all these points. We will discuss methods to construct such polynomial. The polynomial $P(x) = x^3 + x - 1$ is the required polynomial and it passes through all these points.



A data set is either the table of values of well-defined functions or the table of data points from observations during an experiment. These types of problems are most common in various experiments where only inputs and corresponding outputs are known. In most of the experimental cases, we have data points, i.e., inputs (x) and correspondingly outputs (y). Also, many practical problems involve data points instead of the mathematical model for the problem. For example, Indian government carries out national census after a gap of 10 years to speculate about the development in population of country. Hence, we have populations in these years as follows:

Years	Population (in crores)
1961	43.9235
1971	54.8160
1981	68.3329
1991	84.6421
2001	102.8737
2011	121.0193

This population data is exact up to four decimal digits. But, in intermediate years such as 1977, 2010, etc., we do not have exact population. The numerical techniques can be used to compute approximate populations in these years.

Except for data points, sometimes, we also require approximating different functions with polynomials due to the simple structure of the polynomials. The polynomials are also easy for analysis like differentiation and integration etc.

This chapter is devoted to various techniques for the polynomial approximations of functions and data points. The chapter also includes the piecewise interpolation.

Chapter 9: Finite Operators introduces various finite operators including finite difference operators (forward, backward and central difference operators) and other operators like average or mean operator, shift operator, and differential operator. The chapter contains the relations between these operators. This chapter also presents construction of finite difference tables and the error propagation in these tables.

These finite difference operators are helpful in constructing solutions of difference equations and also used to construct interpolating polynomials for equally spaced points, as discussed in Chapter 10.

Chapter 10: Interpolation for Equal Intervals and Bivariate Interpolation contains some interpolation methods for equally spaced points. The methods discussed in Chapter 8 are applicable for both unequally as well as equally spaced points. Rather, the interpolating polynomial obtained from any formula is unique, but for equally spaced points, the calculations for interpolation become simpler and hence need more exploration.

We will also discuss the extension of interpolation from one independent variable to two independent variables known as bivariate interpolation.

Chapter 11: Splines, Curve Fitting, and Other Approximating Curves discusses approximations of data set other than interpolation. In interpolation, we fit a polynomial of the degree $\leq n$ to $(n + 1)$ data points. But if the data set is large, say 50 data points, then it is impractical to fit a polynomial of degree 49 to the data set. In this case, other approximation techniques like least squares curve fitting, spline fitting, etc., can be used. In this chapter, we will discuss different approximation techniques which have certain advantages over interpolation in some real time problems.

Curve fitting is to construct an approximate function $f(x)$ (like exponential, polynomial, logistic curve, etc.) for a table of data points.

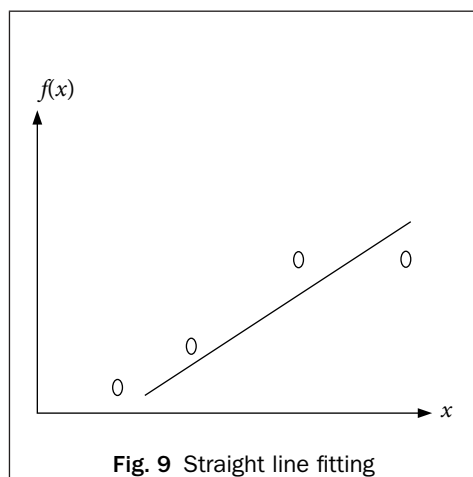


Fig. 9 Straight line fitting

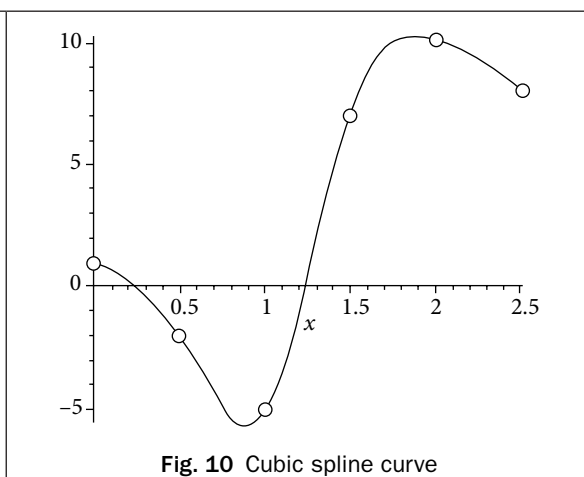


Fig. 10 Cubic spline curve

Interpolating polynomials have global effect, i.e., if we change a point in the data set, then complete polynomial will change. Also if we change the order of data points, the interpolating polynomial remain same, which is not recommended for certain applications like computer graphics and designing, etc. In these cases, we can apply Bézier and B-Spline curves.

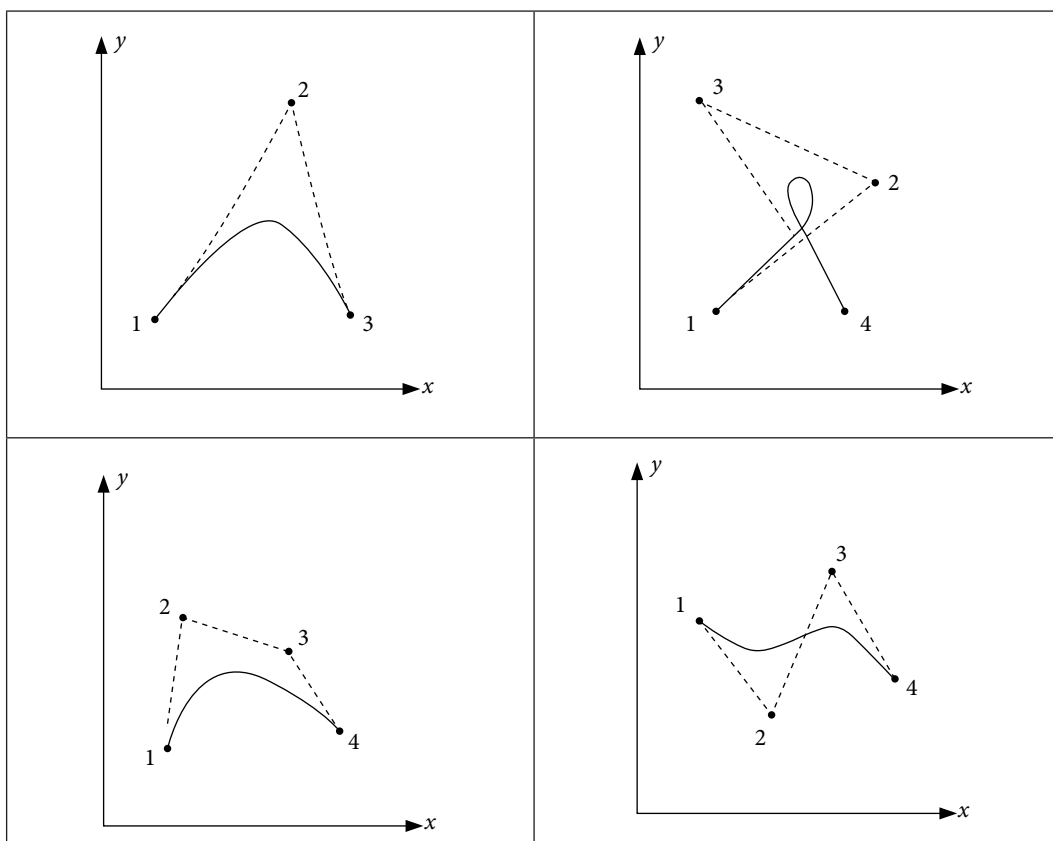


Fig. 11 Bézier curves

In approximations of any polynomial by lower order polynomial, the maximum absolute error can be minimized by Chebyshev polynomials. We can deduce best lower order approximation to a given polynomial by using Chebyshev polynomials.

The polynomial approximations are best approximations for smooth functions and experiments (data set). But if function/experiment behaves in chaos or singular manner (i.e. tends to infinity at some points), then we have to approximate with some other function. One of the functions is a rational function of polynomials, and the approximation is known as Padé approximation.

Chapter 12: Numerical Differentiation is devoted to obtaining numerical differentiation from discrete data points. This chapter elaborates some numerical differentiation techniques based on interpolation.

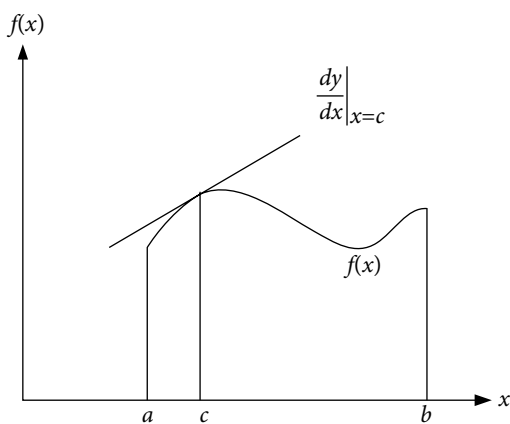


Fig. 12 Differentiation

Chapter 13: Numerical Integration deals with approximating the finite integral of the functions, which are complicated enough to integrate analytically. For example, we don't have exact closed form solutions of integrations like $\int_0^{\pi} \sqrt{1 + \cos^2 x} dx$, $\int_1^2 \frac{\sin x}{x} dx$, $\int_0^2 e^{-x^2} dx$ etc. In these cases, we can simply apply numerical methods for the approximate solutions. Sometimes we have to find the integration from a set of discrete data points $\{(x_i, y_i), i = 0, 1, \dots, n\}$. It is not possible to integrate data points analytically, so it is imperative to approximate these integrations by numerical methods. For example, the value of integral $\int_0^5 y(x) dx$ for the given data set $(0, -1), (1, 1), (2, 9), (3, 29), (5, 129)$ can be obtained only through numerical methods.

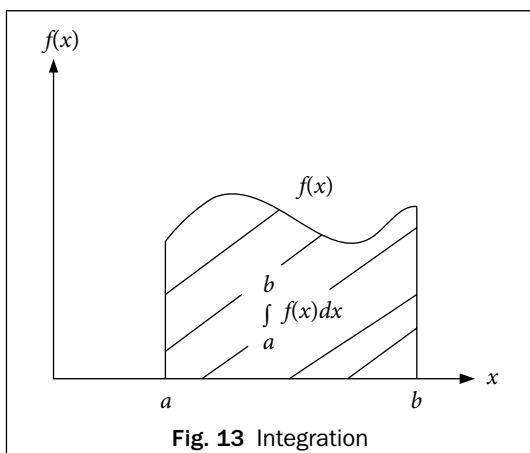


Fig. 13 Integration

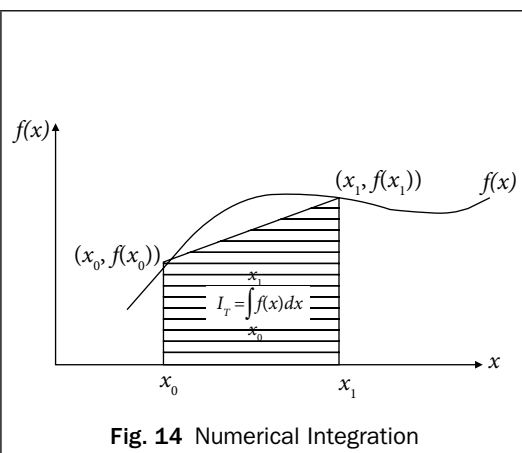


Fig. 14 Numerical Integration

Chapter 14: First Order Ordinary Differential Equations: Initial Value Problems provides a detailed description of standard numerical techniques for the solution of first order ordinary differential equation (ODE) with the initial condition

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0$$

The ODE with initial conditions is known as initial value problem (IVP). Most of the physical laws have a rate of change of quantity rather than the magnitude of the quantity itself; e.g., velocity of any fluid (rate of change of distance), radioactive decay (rate of change of radioactive material), etc. Differential equations govern all these physical phenomena. This chapter contains some basic definitions on differential equations.

The main aim of this chapter is to study numerical methods for the solutions of first order IVP. Differential equations, especially nonlinear, are not easy to solve analytically, as very few analytical methods exist in the literature for a limited class of differential equations. Hence, numerical methods play an important role in the theories of the differential equations.

Consider the following examples

i) $\frac{dy}{dx} = x + y^2, \quad y(1) = 2$

ii) $\frac{d^2 y}{dx^2} = x \frac{dy}{dx} + \sin y; \quad y(0) = 1, \quad y'(0) = 1, \text{ etc.}$

These examples are difficult to solve analytically, but we can use numerical techniques for approximate solutions of such ODEs.

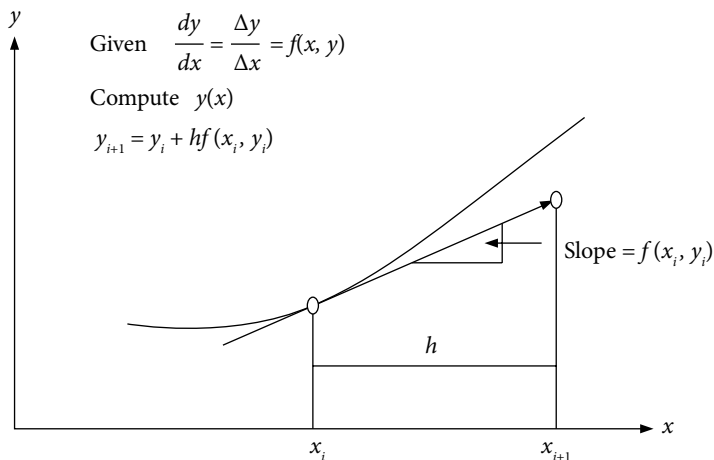


Fig. 15 First order ODE

Chapter 15: Systems of First Order ODEs and Higher Order ODEs: Initial and Boundary Value Problems elucidates the steps involved for finding numerical solutions of a system of first order ODEs and higher order ODEs with initial and boundary conditions, for examples

Preface

Systems of First Order ODEs:

$$\begin{array}{ll} \frac{dy}{dx} = x + y - z^2 & \frac{dy}{dx} = w + \sin(x)y - z^2 \\ \text{i) } \frac{dz}{dx} = z - \sin(xy) & \text{ii) } \frac{dz}{dx} = z^2 - \sin(xy) \\ y(0) = 1, z(0) = -1 & \frac{dw}{dx} = x + w - 2y \\ & y(1) = 1, z(1) = -1, w(1) = 1.3 \end{array}$$

Second and Higher Order Initial Value Problems

$$\begin{array}{ll} \text{i) } \frac{d^2y}{dx^2} + x \frac{dy}{dx} + y = 3; & y(0) = 1, y'(0) = 2 \\ \text{ii) } \frac{d^3y}{dx^3} + \sin x \frac{d^2y}{dx^2} + xy = \cos x; & y(0) = 1, y'(0) = 2, y''(0) = 2 \end{array}$$

Second and Higher Order Boundary Value Problems

$$\begin{array}{ll} \text{i) } x^2 \frac{d^2y}{dx^2} + (x-1) \frac{dy}{dx} + y = 3; & y(0) + 2y'(0) = 1, y(1) = 3 \\ \text{ii) } \frac{d^3y}{dx^3} + \sin x \frac{d^2y}{dx^2} + xy = \cos x; & y(0) = 1, y'(1) = 2, y(3) + y''(3) = -4 \end{array}$$

In last chapter, we have described various numerical methods for the solutions of the first order ODE $\frac{dy}{dx} = f(x, y)$; $y(x_0) = y_0$. In this chapter, we will generalize these methods to find the numerical solutions of system of first order ODEs.

The chapter deals with the conversion of higher order ODEs to the systems of first order ODEs. This chapter also includes the finite difference approximations of derivatives and further solutions of boundary value problems using these finite differences.

Chapter 16: Partial Differential Equations: Finite Difference Methods presents various finite difference methods for the solutions of some standard linear partial differential equations (PDEs). The finite difference method is a simple and most commonly used method to solve PDEs. In this method, we select some node points in the domain of the PDE. Various derivative terms in the PDE and the derivate boundary conditions are replaced by their finite difference approximations at these node points. The PDE is converted to a set of linear algebraic equations at node points. This system of linear algebraic equations can be solved by any direct/iterative procedure discussed in Chapter 5. The solution of this system of linear equations leads to the solution of PDE at node points. An important advantage of this method is that the procedure is algorithmic, and the calculations can be carried out on the computer. So, the solutions can be obtained in a systematic and easy way.

PDEs are of great significance in describing the systems in which the behavior of any physical quantity depends on two or more independent variables. Laplace and Poisson equations (steady-state flow, fluid mechanics, electromagnetic theory and torsion problems), heat conduction equation (temperature distribution) and wave equation (vibrations, fluid dynamics, etc.) are some important examples of second order linear PDEs. Numerical techniques for the solution

of PDEs include finite difference methods (FDMs), finite volume methods (FVMs) and finite element methods (FEMs). This chapter contains only a few finite difference techniques for the solutions of following PDEs governing some important physical phenomena.

Parabolic Equation (Heat Conduction or Diffusion Equation)

$$\frac{\partial u}{\partial t} = c \frac{\partial^2 u}{\partial x^2} \quad (1\text{-Dimensional heat conduction equation})$$

$$\frac{\partial u}{\partial t} = c \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = c \nabla^2 u \quad (2\text{-Dimensional heat conduction equation})$$

Elliptic Equation (Laplace and Poisson Equations)

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad (\text{Laplace equation in 2-dimensions})$$

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \quad (\text{Poisson equation in 2-dimensions})$$

Hyperbolic Equation (Wave Equation)

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \quad (1\text{-Dimensional wave equation})$$

The primary focus is on the preliminary material and the basic concepts of the finite difference techniques used in the book along with their application procedures to derive the numerical solutions of the PDEs.

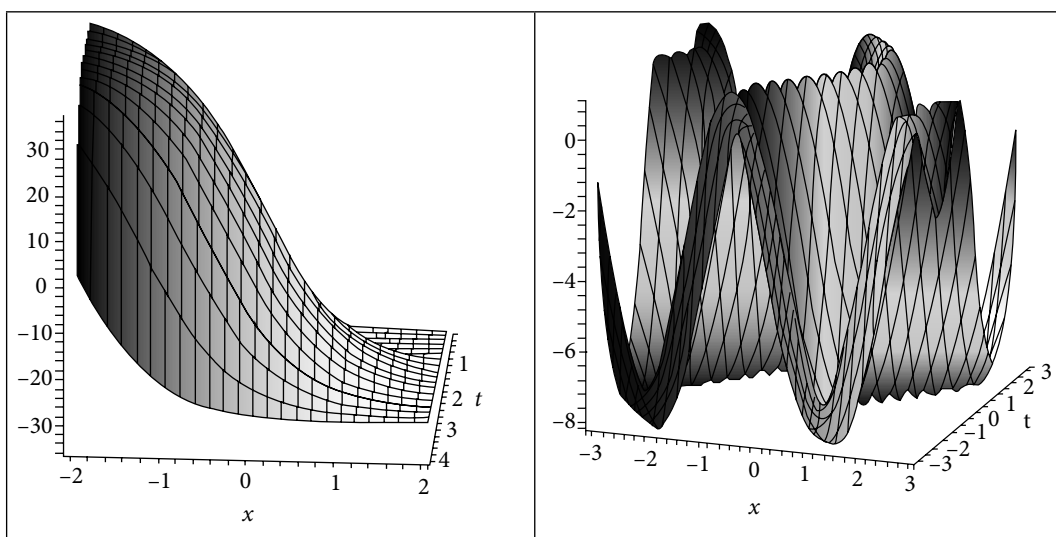


Fig. 16 Partial differential equations

Any Information concerning corrections/errors in this book will be gratefully received.

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