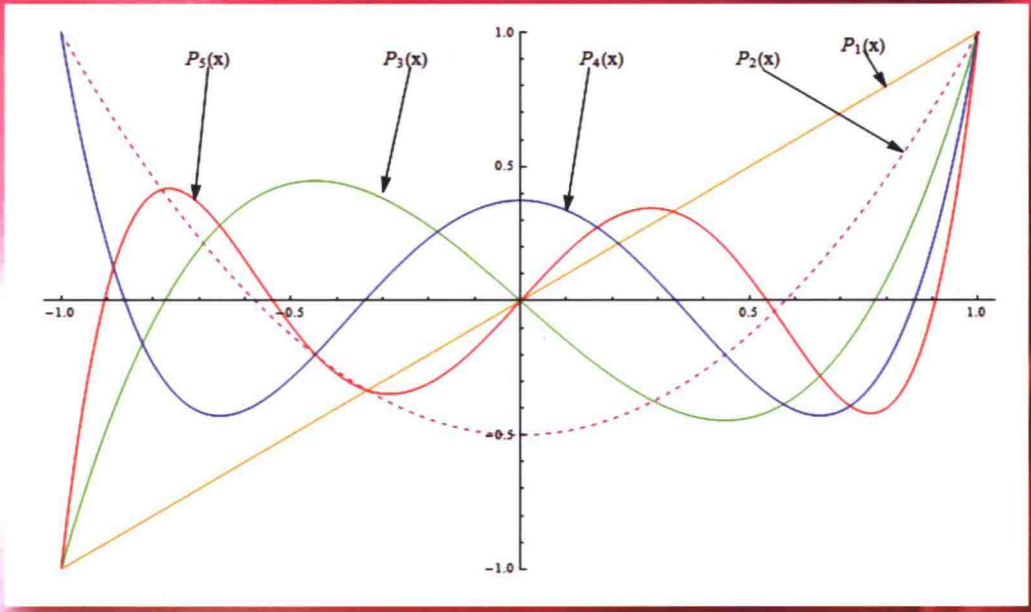
# NUMERICAL ANALYSIS WITH ALGORITHMS AND PROGRAMMING




Santanu Saha Ray

CRC Press
Taylor & Francis Group
A CHAPMAN & HALL BOOK

**Numerical Analysis with Algorithms and Programming** is the first comprehensive textbook to provide detailed coverage of numerical methods, their algorithms, and corresponding computer programs. It presents many techniques for the efficient numerical solution of problems in science and engineering.

Along with numerous worked-out examples, end-of-chapter exercises, and *Mathematica*® programs, the book includes the standard algorithms for numerical computation:

- Root finding for nonlinear equations
- Interpolation and approximation of functions by simpler computational building blocks, such as polynomials and splines
- The solution of systems of linear equations and triangularization
- Approximation of functions and least square approximation
- Numerical differentiation and divided differences
- Numerical quadrature and integration
- Numerical solutions of ordinary differential equations and boundary value problems
- Numerical solution of partial differential equations

This text develops readers' understanding of the construction of numerical algorithms and the applicability of the methods. By thoroughly studying the algorithms, readers will discover how various methods provide accuracy, efficiency, scalability, and stability for large-scale systems.

**Features**

- Emphasizes the multidisciplinary aspect of numerical analysis involving science, computer science, engineering, and mathematics
- Describes the computational implementation of algorithms, illustrating the major issues of accuracy, computational work effort, and stability
- Includes the *Mathematica* programming codes for each numerical method, enabling readers to gain practical experience applying the methods
- Gives a brief introduction to the finite element method

CRC Press
Taylor & Francis Group
an informa business
www.crcpress.com

6000 Broken Sound Parkway, NW
Suite 300, Boca Raton, FL 33487
711 Third Avenue
New York, NY 10017
2 Park Square, Milton Park
Abingdon, Oxon OX14 4RN, UK

K26760
ISBN: 978-1-4987-4174-3
90000
9 781498 741743
www.crcpress.com

Saha Ray

# NUMERICAL ANALYSIS WITH ALGORITHMS AND PROGRAMMING

CRC

# NUMERICAL ANALYSIS WITH ALGORITHMS AND PROGRAMMING

Santanu Saha Ray

CRC Press
Taylor & Francis Group
Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an **informa** business

A CHAPMAN & HALL BOOK

CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742



Printed on acid-free paper
Version Date: 20160401

International Standard Book Number-13: 978-1-4987-4174-3 (Hardback)



**Library of Congress Cataloging-in-Publication Data**

Names: Saha Ray, Santanu.
Title: Numerical analysis with algorithms and programming / Santanu Saha Ray.
Description: Boca Raton : Taylor & Francis, 2016. | "A CRC title."
Identifiers: LCCN 2016003230 | ISBN 9781498741743 (alk. paper)
Subjects: LCSH: Numerical analysis--Problems, exercises, etc. | Engineering mathematics--Problems, exercises, etc. | Numerical analysis--Data processing--Problems, exercises, etc. | Algorithms--Problems, exercises, etc.
Classification: LCC QA297 .S24 2016 | DDC 518--dc23
LC record available at http://lccn.loc.gov/2016003230

**Visit the Taylor & Francis Web site at**
**http://www.taylorandfrancis.com**

**and the CRC Press Web site at**
**http://www.crcpress.com**

# NUMERICAL ANALYSIS WITH ALGORITHMS AND PROGRAMMING

# Dedication

*This work is dedicated to my grandfather the late Sri Chandra Kumar Saha Ray, my parents, my beloved wife Lopamudra, and my son Sayantan.*

# Preface

The utmost aim of this book is to provide an extensive study of expedient procedures for obtaining useful acceptable solutions to the desired accuracy of mathematical problems occurring in disciplines of science and engineering and for acquiring useful information from available solutions. The main feature of this book is its multidisciplinary aspect involving science, computer science, engineering, and mathematics. It can be used as a text for various disciplines of science and engineering in which this subject is pertinent to a given curriculum. This book provides a comprehensive foundation of numerical analysis that includes substantial ground work in the algorithms of computation, approximation, numerical solutions of nonlinear equations, interpolation, numerical differentiation and integration, numerical solutions of linear algebraic equation systems, numerical solutions of ordinary differential equations, eigenvalue problems in matrix, approximations of functions, and numerical solutions of partial differential equations (PDEs). In addition, a brief introduction to the finite element method (FEM) is also provided. To gain practical knowledge for applications of the methods, MATHEMATICA® programs are provided at the end of almost each and every method. In very few cases, programs have been intentionally excluded and left for the exercises of the readers. It is a comprehensive textbook in which the subject matter is presented in a well-organized and systematic manner.

This book has 11 chapters. Each chapter presents a thorough analysis of the theory, principles, and methods, followed by many illustrative examples. There are a large number of problems given as exercises for the students to practice, in order to enhance their knowledge and skill involved while solving these problems. In addition, this book may be helpful for numerical computation with high-end digital computer. Nowadays, computational experience is very important and indispensable, and it manifests perception to enter into the deeper sense for most of the theoretical aspects. This experience has prompted the real impetus for preparation of this book.

It is a well-known fact that analytical solutions of many important physical problems are not readily available; hence, numerical approximate solutions are the only alternative. These solutions will contain errors, for which a discussion at the beginning of the book is a must.

Chapter 1 provides fundamental concepts of errors in numerical computations. Some basic ideas about numerical stability, condition number, and convergence are also discussed.

Chapter 2 presents detailed discussions of several methods for solving nonlinear algebraic and transcendental equations. The order of convergence and condition of convergence have also been described in detail. Numerical solutions of systems of nonlinear equations have also been discussed using different numerical methods.

In Chapter 3, different types of interpolation formulas are presented. All the forward, backward, and central interpolation formulas have been included explicitly. Cubic spline has been described exhaustively. A pretty clear idea may be perceived from the pictorial representation of the cubic spline graph. The error analysis of the cubic spline has been presented very elegantly.

Numerical differentiation and numerical integration have been discussed rigorously in Chapters 4 and 5, respectively. Different numerical integration formulas have been derived from Newton–Cotes quadrature formula as well as from the interpolation formula. The numerical integration procedures are also graphically presented. Richardson extrapolation along with Romberg integration and different types of Gauss quadrature formulas are extensively discussed. Different numerical methods for double integration have also been presented. At the end of Chapter 5, theories and properties of Bernoulli polynomials, Bernoulli numbers, and the Euler–Maclaurin formula have been discussed.

Chapter 6 is devoted to the presentation of various direct methods along with their algorithms and operational counts or time complexities. Several important iterative methods have been presented along with their algorithms and convergence analysis. Ill-conditioned systems are also discussed in detail. Moreover, for solving tridiagonal systems, the Thomas algorithm has also been included.

In Chapter 7, several numerical methods including single-step and multistep ones are discussed in detail for numerical solutions of differential equations. Various types of Runge–Kutta (R–K) methods are derived according to their order. Particular attention has been paid to the derivation of the fourth order R–K method. The Runge–Kutta–Fehlberg method is discussed rigorously. The multistep methods, especially the Adams–Bashforth and the Adams–Moulton predictor–corrector methods are also discussed. The numerical solutions of differential equation systems are also taken into consideration. Various methods, such as finite difference method, shooting method, collocation method, and the Galerkin method, have been implemented for solving boundary value problems. Algorithms are also presented with implementations of various numerical techniques for numerical solutions of differential equations. Stability analysis of single-step and multistep methods has also been presented extensively. The fundamental concepts of stiff differential equations, that is, A-stability and L-stability, are also well explored. To get rid of the lack of organized algorithms for the implementation of the methods discussed in this chapter, an emphasis is laid on details regarding the description of algorithms with its applications through computer programs, along with solved examples, which yields the lengthiest chapter in this book.

In Chapter 8, various methods have been included to determine the eigenvalues of a square matrix. The Householder's method and *QR* method are elegantly described with great intent. A meticulous effort has been paid for the comprehensive descriptions of the power method, inverse power method, and other relevant methods for finding eigenvalues of a square matrix, because the matrix is a very good tool for solving engineering problems.

Chapter 9 deals with the approximation of functions. First, Bernstein polynomials and their properties are introduced. Next, least square curve fitting techniques are presented. The Gram–Schmidt orthogonalization process is also discussed to find a set of orthogonal polynomials. Special emphasis is laid on the minimax polynomial approximation and its corresponding theorems with proofs. Function approximation by cubic B-spline has been also introduced. In the end, the Padé approximation has been discussed considerably.

Chapter 10 deals with indispensable salient methods for the numerical solutions of parabolic, hyperbolic, and elliptic PDEs. At the end of the descriptions of each technique, algorithms with MATHEMATICA® programs with some solved problems have been provided for the better perception and comprehension of these different numerical techniques applied to the PDEs. Moreover, for numerical solutions of two-dimensional parabolic PDEs, an alternating direction implicit method has also been described in detail with its algorithm, along with the corresponding computer program. In the end, the stability analysis of the numerical schemes has been explored.

Finally, in Chapter 11, a brief introduction to the FEM is also presented. The FEM constitutes a general tool for the numerical solution of PDEs appearing in applied science and engineering. The notable work of L. Rayleigh (1870) and W. Ritz (1909) on variational methods and the weighted-residual approach adopted by B. G. Galerkin (1915) and others form the theoretical groundwork for the FEM. For this purpose, the Rayleigh–Ritz method is explained intensively with its algorithm and the corresponding computer program. Furthermore, relevant literature has also been referred to for further details regarding the mathematical theory and implementation of the FEM.

This book contains sufficient materials to be adjudged as a text book with respect to the scenario that it covers the numerical analysis course thoroughly. In this book, every concept is illustrated by worked-out examples. In addition, it contains many exercises, covering various application areas. A number of computer programs have been developed by using MATHEMATICA®, with the aid of implementation of the corresponding algorithms related to numerical methods.

The bibliographic material to the relevant literature has been provided to serve as helpful sources for further study and research for interested readers.

**Santanu Saha Ray**

# Acknowledgments

I express my deepest sense of sincere gratitude to Dr. R. K. Bera, former professor and head, Department of Science, National Institute of Technical Teacher's Training and Research, Kolkata, India, and Dr. K. S. Chaudhuri, FNA (India), FIMA (United Kingdom), former professor and emeritus fellow, Department of Mathematics, Jadavpur University, Kolkata, India, for their encouragement in the preparation of this book. I acknowledge, with the deepest thanks, the valuable suggestions provided by Professor Lokenath Debnath, Department of Mathematics, The University of Texas–Pan American, Edinburg, Texas; Professor Abdul-Majid Wazwaz, Department of Mathematics and Computer Science, Saint Xavier University, Chicago, Illinois. I am also highly thankful to Professor Edward J. Allen, Texas Tech University, Lubbock, Texas; Professor Xiao-Jun Yang, China University of Mining and Technology, Xuzhou, Jiangsu, China; Professor Vasily E. Tarasov, Lomonosov Moscow State University, Moscow, Russia; Professor Mehdi Dehghan, Department of Applied Mathematics, Faculty of Mathematics and Computer Science, Amirkabir University of Technology, Tehran, Iran; Professor Santos Bravo Yuste, Departamento de Física, Facultad de Ciencias, Universidad de extremadura, Badajoz, Spain; Professor Dumitru Baleanu, Çankaya University, Ankara, Turkey; Professor Siddhartha Sen, Department of Electrical Engineering, Indian Institute of Technology, Kharagpur, India; Professor J. A. Tenreiro Machado, Institute of Engineering, Polytechnic of Porto, Portugal; and Professor Shantanu Das, senior scientist, Reactor Control Division, Bhabha Atomic Research Centre, Mumbai, India.

It is not out of place to acknowledge the sincere and meticulous efforts of my PhD scholar students who had worked hard to assist me in the preparation of this book.

I also express my sincere gratitude to the director of National Institute of Technology (NIT), Rourkela, India, for his kind cooperation and support. The moral support received from my colleagues at the NIT, Rourkela, India, is also acknowledged.

I express my sincere thanks to everyone involved in the preparation of this book. I take the opportunity to acknowledge the efforts of all those who were directly or indirectly involved in helping me throughout this difficult mission.

Moreover, I am especially grateful to the Taylor & Francis Group/CRC Press for their cooperation in all aspects for the production of this book.

Last, but not the least, special mention should be made of my parents and my beloved wife Lopamudra, for her patience, unequivocal support, and generous encouragement throughout the period of my work. In addition, I acknowledge the allowance of my only son Sayantan for not sparing my pleasant company in his childhood playtime and also in his valuable educational activities.

I look forward to receive comments and suggestions from students, teachers, and researchers.

**Santanu Saha Ray**

# Author

**Dr. Santanu Saha Ray** is an associate professor in the Department of Mathematics, National Institute of Technology, Rourkela, India. Dr. Saha Ray obtained his PhD in 2008 from Jadavpur University, Kolkata, India and MCA (Masters of Computer Applications) degree in 2001 from the Indian Institute of Engineering Science and Technology (IIEST; formerly the Bengal Engineering College) Sibpur, India. He completed a master's degree in applied mathematics at the Calcutta University, Kolkata, India, in 1998 and a bachelor's (honors) degree in mathematics at St. Xavier's College, Kolkata, India, in 1996.

Dr. Saha Ray has 15 years of teaching experience at the undergraduate and postgraduate levels. He has also about 14 years of research experience in various fields of applied mathematics. He has published many peer-reviewed research papers in numerous fields and various international SCI journals of repute, including *Applied Mathematics and Computation*, *Communication in Nonlinear Science and Numerical Simulation*, *Transaction ASME Journal of Applied Mechanics*, *Journal of Computational and Nonlinear Dynamics*, *Computers and Mathematics with Applications*, *Journal of Computational and Applied Mathematics*, *Mathematical Methods in the Applied Sciences*, *Computers & Fluids*, *Physica Scripta*, *Communications in Theoretical Physics*, *Nuclear Engineering and Design*, *International Journal of Nonlinear Science and Numerical Simulation*, *Annals of Nuclear Energy*, and *Journal of Mathematical Chemistry*. For a detail citation overview, the reader may refer to *Scopus*. To date, he has more than 100 research papers published in journals of international repute, including more than 80 SCI journal papers.

He is the author of *Graph Theory with Algorithms and Its Applications: in Applied Science and Technology* (Springer, 2013) and *Fractional Calculus with Applications for Nuclear Reactor Dynamics* (CRC Press, 2015). He is the editor-in-chief for the Springer journal entitled *International Journal of Applied and Computational Mathematics*.

He has contributed papers on several topics, such as fractional calculus, mathematical modeling, mathematical physics, stochastic modeling, integral equations, and wavelet methods. He is a member of the Society for Industrial and Applied Mathematics and the American Mathematical Society.

He was the principal investigator of a Board of Research in Nuclear Sciences project, with grants from the Bhabha Atomic Research Centre, Mumbai, India. He was also the principal investigator of a research project financed by the Department of Science and Technology, Government of India. He is the principal investigator of another two research projects financed by the Board of Research in Nuclear Sciences, Bhabha Atomic Research Centre, Mumbai, India and National Board for Higher Mathematics, Department of Atomic Energy, Government of India, respectively.

A research scholar was awarded with PhD from the National Institute of Technology, Rourkela, India under his supervision. In addition, he is supervising five research scholars, including three senior research fellowship scholars. He had also been the lead guest editor of the international SCI journals of the Hindawi Publishing Corporation, New York.

# Contents