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Sujit Kumar Bose

Numerical Methods of Mathematics Implemented in Fortran

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Sujit Kumar Bose
S. N. Bose National Centre for Basic
Sciences
Kolkata, West Bengal, India

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|| Mangalācaranam ||

Om sahanāvavatu sahanaubhunaktu
sahavíryyaṁkarvāvahai |
Tejasvināvadhítamastu mā vidvíśāvahai ||

|| *Om* Ś*ānti*ḥ Ś*ānti*ḥ Ś*ānti*ḥ ||

{O the Universal Consciousness protect and nourish us (both teacher and student) to work with great vigour to enlighten our intellect, without creation of any jealousy or rancour whatsoever (in that endeavour). Let peace, peace, peace be everywhere.}

Preface

Numerical computation of mathematically formulated problems is universal in sciences and engineering. The mathematical models appearing in the two disciplines essentially boil down to formalisms of analysis and linear algebra, and for obtaining useful results from them, numerical methods were devised from time to time. The numerical methods were laid on a firm mathematical foundation later on, during the course of development of the subject. The invention of computing machines, such as the present-day digital computer, has greatly increased the power of numerically solving difficult scientific problems.

The gamut of scientific computation consists of the development of methods of treating different mathematical models, their mathematical analysis and writing computer codes for obtaining desired results. A course on numerical methods of mathematics is an integral part of the undergraduate science and engineering studies. This study sometimes forms a part of the postgraduate courses as well. The emphasis on methods, analysis and coding for computer implementation varies in different course types. A typical course may consist of the principal methods, and some programming, with little intricacies of analysis. However, a theoretical course may emphasise the methods together with their analyses and possibly some algorithms of the methods developed. This book is designed in such a manner that a course instructor can draw requisite material for any of the courses leaving the remaining parts for reference purposes. For laying emphasis on the methods that form the bulk of the courses, simple examples and exercises are given for hand calculation with the aid of a calculator. For courses emphasising the underlying mathematical theory, the topics are presented in separate sections. At the other end where the reader would like to have complete computer codes, concise computer programs are provided that follow the diverse methods developed in a general manner. In some cases, programming tricks become necessary for obtaining correct and accurately computed results from computer programs. Such tricks are rarely employed in this book. The succinct programs presented as subroutine procedures in the text are applicable under very general settings, so as to be useful even in research investigations. Special packages often popular with students sometimes give disappointingly incorrect results and are hard to debug on account of their opacity. Open source codes, however, are often long-drawn statements, not clearly reflecting the corresponding algorithm followed. The subroutines presented in the book are free from these difficulties on account of their transparency.

For writing the computer codes, I have chosen to use the Fortran programming language. Fortran is a powerful, easy-to-learn and traditional language for scientific computation in which there are a number of inbuilt intrinsic functions. The present version Fortran 2003 is fully backwards-compatible with its earlier popular versions FORTRAN 77 and Fortran 90/95. The language has been upgraded to Fortran 2010, and a future version Fortran 2018 is proposed to be launched during this year. The latest versions are the only ones usable in supercomputers and in modern multiprocessor desktops. There is, therefore, some merit in retaining Fortran for the purpose of scientific computation, especially because of the fact that a large number of source codes mentioned in Chap. 1 are written in that language. At present, to my knowledge, the output in Fortran is alphanumeric in nature. Conversion of output to desirable graphic displays, however, is easily accomplished by using some graphic software.

The book is divided into ten chapters. Chapter 1 gives a brief description of computer software and types of errors encountered in computing due to truncation of mathematical formulae and digitisation of decimal numbers. Elements of Fortran statements used in the book are also described in this chapter. Elementary illustrative examples are given in the chapter for initiation in Fortran programming to beginners. Chapters 2 and 3 treat the fundamental problem of solving a single equation or a system of several equations possessing real and complex roots, respectively. A major part of Chap. 3 deals with the most important topic of solving a system of linear equations. Chapter 4 provides the study of the classic problem of approximation of a function by interpolation over the given data points, deferring the treatment of the more theoretical topics of approximation to Chap. 8. Chapter 4 provides the methods which lead to the topics of numerical differentiation and integration and to the solution of ordinary and partial differential equations numerically. These topics are respectively covered in Chaps. 5–7. Chapters 9 and 10 treat the computationally fascinating, but mathematically difficult subjects of the matrix—eigenvalues and the fast Fourier transform for computing Fourier integrals. Short biographical sketches of the principal discoverers of the weighty material have been given to enliven the reader as one proceeds to uncover the masterly techniques. Tomes have been written by mathematicians and programmers on topics of each of the ten chapters. In a moderately sized book like the present one, the selection of the material arranged in some logical manner, therefore, became a necessity. I have kept the benchmark of choice to understand the basics, keeping in view the utility of application of the routines to the extent of research-level problems. A suite of 38 ready-to-use subroutines is given that directly follow the different methods developed in the book.

The book is an outcome of teaching the subject to undergraduate and postgraduate students of engineering in which the students provided a huge contribution as feedback. No less has been the effect on my own travails in computing for my research problems that have spanned for at least the past five decades. The compilation of this book is a reflection of these experiences. As writing progressed, I had to sift through several books including one of my own that strayed away from the benchmark laid down by myself. The ones that I found useful to varying degrees are thankfully acknowledged at the end of the book. Thanks are also due to S. N. Bose National Centre for Basic Sciences, Kolkata, for providing me the library facility to look at new texts that have appeared in recent years.

Kolkata, India Sujit Kumar Bose

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About the Author

Sujit Kumar Bose is a distinguished computer educationist and author of several useful books on computational and numerical mathematics. He was a Research Consultant at the Department of Civil Engineering, Indian Institute of Technology Kharagpur, from 2002 to 2014. He was also member of the Guest Faculty at the Department of Computer Science, Jadavpur University, Kolkata, from 1998 to 2006; a Senior Professor of Mathematics at the S. N. Bose National Centre for Basic Sciences, Kolkata, India, from 1993 to 1998; Professor and Head of the Department of Mathematics at the National Institute of Technology, Durgapur, India, from 1975 to 1993; an Assistant Professor at the West Bengal Educational Service, from 1965 to 1975; and a Lecturer at the West Bengal Junior Educational Service, from 1960 to 1965. In addition, he was a postdoctoral fellow at the University of California, Los Angeles, from 1972 to 1974.

Professor Bose is associated with several respected research institutes: Fellow of the Indian Academy of Sciences, India; member of the Indian Society of Theoretical and Applied Mechanics at the Department of Mathematics, Indian Institute of Technology Kharagpur; member of the Calcutta Mathematical Society; and member of the Indian Statistical Institute, Kolkata. He is awarded the Prof. B. Sen Memorial Gold Medal for the Best Research in Elasticity, in 1978, and the Sardar Vallabhbhai Patel Award for the Excellence in Researches in Mathematical Sciences, in 2012. He obtained B.Sc. (Math Hons, 1957) and M.Sc. (Applied Mathematics, 1959) as well as D.Sc. (Applied Mathematics, 1971), all from the University of Calcutta, winning several gold medals. He was a Visiting Scholar at the Computational Mechanics Center, Georgia Institute of Technology, USA, and the Department of Applied Mathematics at the University of Twente, The Netherlands in 1989. Professor Bose has research interests in applied mathematics, solid mechanics, fluid mechanics and sediment transport.