Fundamental Numerical Methods and Data Analysis

by

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Preface

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The origins of this book can be found years ago when I was a doctoral candidate working on my thesis and finding that I needed numerical tools that I should have been taught years before. In the intervening decades, little has changed except for the worse. All fields of science have undergone an information explosion while the computer revolution has steadily and irrevocability been changing our lives. Although the crystal ball of the future is at best "seen through a glass darkly", most would declare that the advent of the digital electronic computer will change civilization to an extent not seen since the coming of the steam engine. Computers with the power that could be offered only by large institutions a decade ago now sit on the desks of individuals. Methods of analysis that were only dreamed of three decades ago are now used by students to do homework exercises. Entirely new methods of analysis have appeared that take advantage of computers to perform logical and arithmetic operations at great speed. Perhaps students of the future may regard the multiplication of two two-digit numbers without the aid of a calculator in the same vein that we regard the formal extraction of a square root. The whole approach to scientific analysis may change with the advent of machines that communicate orally. However, I hope the day never arrives when the investigator no longer understands the nature of the analysis done by the machine.

Unfortunately instruction in the uses and applicability of new methods of analysis rarely appears in the curriculum. This is no surprise as such courses in any discipline always are the last to be developed. In rapidly changing disciplines this means that active students must fend for themselves. With numerical analysis this has meant that many simply take the tools developed by others and apply them to problems with little knowledge as to the applicability or accuracy of the methods. Numerical algorithms appear as neatly packaged computer programs that are regarded by the user as "black boxes" into which they feed their data and from which come the publishable results. The complexity of many of the problems dealt with in this manner makes determining the validity of the results nearly impossible. This book is an attempt to correct some of these problems.

Some may regard this effort as a survey and to that I would plead guilty. But I do not regard the word survey as pejorative for to survey, condense, and collate, the knowledge of man is one of the responsibilities of the scholar. There is an implication inherent in this responsibility that the information be made more comprehensible so that it may more readily be assimilated. The extent to which I have succeeded in this goal I will leave to the reader. The discussion of so many topics may be regarded by some to be an impossible task. However, the subjects I have selected have all been required of me during my professional career and I suspect most research scientists would make a similar claim. Unfortunately few of these subjects were ever covered in even the introductory level of treatment given here during my formal education and certainly they were never placed within a coherent context of numerical analysis.

The basic format of the first chapter is a very wide ranging view of some concepts of mathematics based loosely on axiomatic set theory and linear algebra. The intent here is not so much to provide the specific mathematical foundation for what follows, which is done as needed throughout the text, but rather to establish, what I call for lack of a better term, "mathematical sophistication". There is a general acquaintance with mathematics that a student should have before embarking on the study of numerical methods. The student should realize that there is a subject called mathematics which is artificially broken into sub-disciplines such a linear algebra, arithmetic, calculus, topology, set theory, etc. All of these disciplines are related and the sooner the student realizes that and becomes aware of the relations, the sooner mathematics will become a convenient and useful language of scientific expression. The ability to use mathematics in such a fashion is largely what I mean by "mathematical sophistication". However, this book is primarily intended for scientists and engineers so while there is a certain familiarity with mathematics that is assumed, the rigor that one expects with a formal mathematical presentation is lacking. Very little is proved in the traditional mathematical sense of the word. Indeed, derivations are resorted to mainly to emphasize the assumptions that underlie the results. However, when derivations are called for, I will often write several forms of the same expression on the same line. This is done simply to guide the reader in the direction of a mathematical development. I will often give "rules of thumb" for which there is no formal proof. However, experience has shown that these "rules of thumb" almost always apply. This is done in the spirit of providing the researcher with practical ways to evaluate the validity of his or her results.

The basic premise of this book is that it can serve as the basis for a wide range of courses that discuss numerical methods used in science. It is meant to support a series of lectures, not replace them. To reflect this, the subject matter is wide ranging and perhaps too broad for a single course. It is expected that the instructor will neglect some sections and expand on others. For example, the social scientist may choose to emphasize the chapters on interpolation, curve-fitting and statistics, while the physical scientist would stress those chapters dealing with numerical quadrature and the solution of differential and integral equations. Others might choose to spend a large amount of time on the principle of least squares and its ramifications. All these approaches are valid and I hope all will be served by this book. While it is customary to direct a book of this sort at a specific pedagogic audience, I find that task somewhat difficult. Certainly advanced undergraduate science and engineering students will have no difficulty dealing with the concepts and level of this book. However, it is not at all obvious that second year students couldn't cope with the material. Some might suggest that they have not yet had a formal course in differential equations at that point in their career and are therefore not adequately prepared. However, it is far from obvious to me that a student’s first encounter with differential equations should be in a formal mathematics course. Indeed, since most equations they are liable to encounter will require a numerical solution, I feel the case can be made that it is more practical for them to be introduced to the subject from a graphical and numerical point of view. Thus, if the instructor exercises some care in the presentation of material, I see no real barrier to using this text at the second year level in some areas. In any case I hope that the student will at least be exposed to the wide range of the material in the book lest he feel that numerical analysis is limited only to those topics of immediate interest to his particular specialty.

Nowhere is this philosophy better illustrated that in the first chapter where I deal with a wide range of mathematical subjects. The primary objective of this chapter is to show that mathematics is "all of a piece". Here the instructor may choose to ignore much of the material and jump directly to the solution of linear equations and the second chapter. However, I hope that some consideration would be given to discussing the material on matrices presented in the first chapter before embarking on their numerical manipulation. Many will feel the material on tensors is irrelevant and will skip it. Certainly it is not necessary to understand covariance and contravariance or the notion of tensor and vector densities in order to numerically interpolate in a table of numbers. But those in the physical sciences will generally recognize that they encountered tensors for the first time too late in their educational experience and that they form the fundamental basis for understanding vector algebra and calculus. While the notions of set and group theory are not directly required for the understanding of cubic splines, they do form a unifying basis for much of mathematics. Thus, while I expect most instructors will heavily select the material from the first chapter, I hope they will encourage the students to at least read through the material so as to reduce their surprise when the see it again.

The next four chapters deal with fundamental subjects in basic numerical analysis. Here, and throughout the book, I have avoided giving specific programs that carry out the algorithms that are discussed. There are many useful and broadly based programs available from diverse sources. To pick specific packages or even specific computer languages would be to unduly limit the student's range and selection. Excellent packages are contain in the IMSL library and one should not overlook the excellent collection provided along with the book by Press et al. (see reference 4 at the end of Chapter 2). In general collections compiled by users should be preferred for they have at least been screened initially for efficacy.

Chapter 6 is a lengthy treatment of the principle of least squares and associated topics. I have found that algorithms based on least squares are among the most widely used and poorest understood of all algorithms in the literature. Virtually all students have encountered the concept, but very few see and understand its relationship to the rest of numerical analysis and statistics. Least squares also provides a logical bridge to the last chapters of the book. Here the huge field of statistics is surveyed with the hope of providing a basic understanding of the nature of statistical inference and how to begin to use statistical analysis correctly and with confidence. The foundation laid in Chapter 7 and the tests presented in Chapter 8 are not meant to be a substitute for a proper course of study in the subject. However, it is hoped that the student unable to fit such a course in an already crowded curriculum will at least be able to avoid the pitfalls that trap so many who use statistical analysis without the appropriate care.

Throughout the book I have tried to provide examples integrated into the text of the more difficult algorithms. In testing an earlier version of the book, I found myself spending most of my time with students giving examples of the various techniques and algorithms. Hopefully this initial shortcoming has been overcome. It is almost always appropriate to carry out a short numerical example of a new method so as to test the logic being used for the more general case. The problems at the end of each chapter are meant to be generic in nature so that the student is not left with the impression that this algorithm or that is only used in astronomy or biology. It is a fairly simple matter for an instructor to find examples in diverse disciplines that utilize the techniques discussed in each chapter. Indeed, the student should be encouraged to undertake problems in disciplines other than his/her own if for no other reason than to find out about the types of problems that concern those disciplines.

Here and there throughout the book, I have endeavored to convey something of the philosophy of numerical analysis along with a little of the philosophy of science. While this is certainly not the central theme of the book, I feel that some acquaintance with the concepts is essential to anyone aspiring to a career in science. Thus I hope those ideas will not be ignored by the student on his/her way to find some tool to solve an immediate problem. The philosophy of any subject is the basis of that subject and to ignore it while utilizing the products of that subject is to invite disaster.

There are many people who knowingly and unknowingly had a hand in generating this book. Those at the Numerical Analysis Department of the University of Wisconsin who took a young astronomy student and showed him the beauty of this subject while remaining patient with his bumbling understanding have my perpetual gratitude. My colleagues at The Ohio State University who years ago also saw the need for the presentation of this material and provided the environment for the development of a formal course in the subject. Special thanks are due Professor Philip C. Keenan who encouraged me to include the sections on statistical methods in spite of my shortcomings in this area. Peter Stoychoeff has earned my gratitude by turning my crude sketches into clear and instructive drawings. Certainly the students who suffered through this book as an experimental text have my admiration and well as my thanks.

George W. Collins, II
September 11, 1990

A Note Added for the Internet Edition

A significant amount of time has passed since I first put this effort together. Much has changed in Numerical Analysis. Researchers now seem often content to rely on packages prepared by others even more than they did a decade ago. Perhaps this is the price to be paid by tackling increasingly ambitious problems. Also the advent of very fast and cheap computers has enabled investigators to use inefficient methods and still obtain answers in a timely fashion. However, with the avalanche of data about to descend on more and more fields, it does not seem unreasonable to suppose that numerical tasks will overtake computing power and there will again be a need for efficient and accurate algorithms to solve problems. I suspect that many of the techniques described herein will be rediscovered before the new century concludes. Perhaps efforts such as this will still find favor with those who wish to know if numerical results can be believed.

George W. Collins, II
January 30, 2001

A Further Note for the Internet Edition

Since I put up a version of this book two years ago, I have found numerous errors which largely resulted from the generations of word processors through which the text evolved. During the last effort, not all the fonts used by the text were available in the word processor and PDF translator. This led to errors that were more wide spread that I realized. Thus, the main force of this effort is to bring some uniformity to the various software codes required to generate the version that will be available on the internet. Having spent some time converting *Fundamentals of Stellar Astrophysics* and *The Virial Theorem in Stellar Astrophysics* to Internet compatibility, I have learned to better understand the problems of taking old manuscripts and setting then in the contemporary format. Thus I hope this version of my Numerical Analysis book will be more error free and therefore useable. Will I have found all the errors? That is most unlikely, but I can assure the reader that the number of those errors is significantly reduced from the earlier version. In addition, I have attempted to improve the presentation of the equations and other aspects of the book so as to make it more attractive to the reader. All of the software coding for the index was lost during the travels through various word processors. Therefore, the current version was prepared by means of a page comparison between an earlier correct version and the current presentation. Such a table has an intrinsic error of at least ± 1 page and the index should be used with that in mind. However, it should be good enough to guide the reader to general area of the desired subject.

Having re-read the earlier preface and note I wrote, I find I still share the sentiments expressed therein. Indeed, I find the flight of the student to “black-box” computer programs to obtain solutions to problems has proceeded even faster than I thought it would. Many of these programs such as MATHCAD are excellent and provide quick and generally accurate ‘first looks’ at problems. However, the researcher would be well advised to understand the methods used by the “black-boxes” to solve their problems. This effort still provides the basis for many of the operations contained in those commercial packages and it is hoped will provide the researcher with the knowledge of their applicability to his/her particular problem. However, it has occurred to me that there is an additional view provided by this book. Perhaps, in the future, a historian may wonder what sort of numerical skills were expected of a researcher in the mid twentieth century. In my opinion, the contents of this book represent what I feel scientists and engineers of the mid twentieth century should have known and many did. I am confident that the knowledge-base of the mid twenty first century scientist will be quite different. One can hope that the difference will represent an improvement.

Finally, I would like to thank John Martin and Charles Knox who helped me adapt this version for the Internet and the Astronomy Department at the Case Western Reserve University for making the server-space available for the PDF files. As is the case with other books I have put on the Internet, I encourage anyone who is interested to down load the PDF files as they may be of use to them. I would only request that they observe the courtesy of proper attribution should they find my efforts to be of use.

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April, 2003
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