AN INTRODUCTION TO NUMERICAL METHODS AND ANALYSIS

Second Edition

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AN INTRODUCTION TO NUMERICAL METHODS AND ANALYSIS

To Mom (1920–1986) and Ed (1917–2012)
a story of love, faith, and grace

PREFACE

Preface to the Second Edition

This third version of the text is officially the Second Edition, because the second version was officially dubbed the Revised Edition. Now that the confusing explanation is out of the way, we can ask the important question: What is new?

- I continue to chase down typographical errors, a process that reminds me of herding cats. I'd like to thank everyone who has sent me information on this, especially Prof. Mark Mills of Central College in Pella, Iowa. I have become resigned to the notion that a typo-free book is the result of a (*slowly* converging) limiting process, and therefore is unlikely to be actually achieved. But I do keep trying.

- The text now assumes that the student is using MATLAB for computations, and many MATLAB routines are discussed and used in examples. I want to emphasize that this book is still a *mathematics* text, not a primer on how to use MATLAB.

- Several biographies were updated as more complete information has become widely available on the Internet, and a few have been added.

- Two sections, one on adaptive quadrature (§5.8.3) and one on adaptive methods for ODEs (§6.9) have been re-written to reflect the decision to rely more on MATLAB.

- Chapter 9 (A Survey of Numerical Methods for Partial Differential Equations) has been extensively re-written, with more examples and graphics.

- New material has been added:
  - Two sections on roots of polynomials. The first (§3.10) introduces the Durand–Kerner algorithm; the second (§8.5) discusses using the companion matrix to find polynomial roots as matrix eigenvalues.
  - A section (§3.12) on very high-order root-finding methods.
  - A section (§4.10) on splines under tension, also known as "taut splines;"
  - Sections on the finite element method for ODEs (§6.10.3) and some PDEs (§9.2);
  - An entire chapter (Chapter 10) on spectral methods[1].
- Several sections have been modified somewhat to reflect advances in computing technology.
- Later in this preface I devote some time to outlining possible chapter and section selections for different kinds of courses using this text.

It might be appropriate for me to describe how I see the material in the book. Basically, I think it breaks down into three categories:

- The fundamentals: All of Chapters 1 and 2, most of Chapters 3 (3.1, 3.2, 3.3, 3.5, 3.8, 3.9), 4 (4.1, 4.2, 4.3, 4.6, 4.7, 4.8, 4.11), and 5 (5.1, 5.2, 5.3, 5.4, 5.7); this is the basic material in numerical methods and analysis and should be accessible to any well-prepared students who have completed a standard calculus sequence.
- Second level: Most of Chapters 6, 7, and 8, plus much of the remaining sections from Chapters 3 (3.4, 3.6, 3.7, 3.10), 4 (4.4, 4.5), and 5 (5.5, 5.6), and some of 6 (6.8) and 7 (7.7); this is the more advanced material and much of it (from Chap. 6) requires a course in ordinary differential equations or (Chaps. 7 and 8) a course in linear algebra. It is still part of the core of numerical methods and analysis, but it requires more background.
- Advanced: Chapters 9 and 10, plus the few remaining sections from Chapters 3, 4, 5, 6, 7, and 8.
- It should go without saying that precisely *what* is considered "second level" or "advanced" is largely a matter of taste.

As always, I would like to thank my employer, *Mathematical Reviews*, and especially the Executive Editor, Graeme Fairweather, for the study leave that gave me the time to prepare (for the most part) this new edition; my editor at John Wiley & Sons, Susanne Steitz-Filler, who does a good job of putting up with me; an anonymous copy-editor at Wiley who saved me from a large number of self-inflicted wounds; and—most of all—my family of spouse Georgia, daughter Elinor, son James, and Border Collie mutts Samantha

[1]The material on spectral methods may well not meet with the approval of experts on the subject, as I presented the material in what appears to be a very non-standard way, and I left out a lot of important issues that make spectral methods, especially for time dependent problems, practical. I did it this way because I wanted to write an introduction to the material that would be accessible to students taking a first course in numerical analysis/methods, and also in order to avoid cluttering up the exposition with what I considered to be "side issues." I appreciate that these side issues have to be properly treated to make spectral methods practical, but since this tries to be an elementary text, I wanted to keep the exposition as clean as possible.

and Dylan. James was not yet born when I first began writing this text in 1997, and now he has finished his freshman year of high school; Elinor was in first grade at the beginning and graduated from college during the final editing process for this edition. I'm very proud of them both! And I can never repay the many debts that I owe to my dear spouse.

Online Material

There will almost surely be some online material to supplement this text. At a minimum, there will be

- MATLAB files for computing and/or reading Gaussian quadrature (§5.6) weights and abscissas for $N = 2^m$, $m = 0, 1, 2, \ldots, 10$.
- Similar material for computing and/or reading Clenshaw-Curtis (§10.3) weights and abscissas.
- Color versions of some plots from Chapter 9.
- It is possible that there will be an entire additional section for Chapter 3.

To access the online material, go to

`www.wiley.com/go/epperson2edition`

The webpage should be self-explanatory.

A Note About the Dedication

The previous editions were dedicated to six teachers who had a major influence on the author's mathematics education: Frank Crosby and Ed Croteau of New London High School, New London, CT; Prof. Fred Gehring and Prof. Peter Duren of the University of Michigan Department of Mathematics; and Prof. Richard MacCamy and Prof. George J. Fix of the Department of Mathematics, Carnegie-Mellon University, Pittsburgh, PA. (Prof. Fix served as the author's doctoral advisor.) I still feel an unpayable debt of gratitude to these men, who were outstanding teachers, but I felt it appropriate to express my feelings about my parents for this edition, hence the new dedication to the memory of my mother and step-father.

Course Outlines

One can define several courses from this book, based on the level of preparation of the students and the number of terms the course runs, as well as the level of theoretical detail the instructor wishes to address. Here are some example outlines that might be used.

- A single semester course that does not assume any background in linear algebra or differential equations, and which does not emphasize theoretical analysis of methods:

- Chapter 1 (all sections[2]);
- Chapter 2 (all sections[3]);
- Chapter 3 (Sections 3.1–3.3, 3.8–3.10);
- Chapter 4 (Sections 4.1–4.8);
- Chapter 5 (Sections 5.1–5.7).

- A two-semester course which assumes linear algebra and differential equations for the second semester:
  - Chapter 1 (all sections);
  - Chapter 2 (all sections);
  - Chapter 3 (Sections 3.1–3.3, 3.8–3.10);
  - Chapter 4 (Sections 4.1–4.8);
  - Chapter 5 (Sections 5.1–5.7).
  - Semester break should probably come here.
  - Chapter 6 (6.1–6.6; 6.10 if time/preparation permits)
  - Chapter 7 (7.1–7.6)
  - Chapter 8 (8.1–8.4)
  - Additional material at the instructor's discretion.
- A two-semester course for well-prepared students:
  - Chapter 1 (all sections);
  - Chapter 2 (all sections);
  - Chapter 3 (Sections 3.1–3.10; 3.11 at the discretion of the instructor);
  - Chapter 4 (Sections 4.1–4.11, 4.12.1, 4.12.3; 4.12.2 at the discretion of the instructor);
  - Chapter 5 (Sections 5.1–5.7, 5.8.1; other sections at the discretion of the instructor).
  - Semester break should probably come here.
  - Chapter 6 (6.1–6.8; 6.10 if time/preparation permits; other sections at the discretion of the instructor)
  - Chapter 7 (7.1–7.8; other sections at the discretion of the instructor)
  - Chapter 8 (8.1–8.4)
  - Additional material at the instructor's taste and discretion.

Some sections appear to be left out of all these outlines. Most textbooks are written to include extra material, to facilitate those instructors who would like to expose their students to different material, or as background for independent projects, etc.

I want to encourage anyone—teachers, students, random readers—to contact me with questions, comments, suggestions, or remaining typos. My professional email is still `jfe@ams.org`

[2]§§1.5 and 1.6 are included in order to expose students to the issue of approximation; if an instructor feels that the students in his or her class do not need this exposure, these sections can be skipped in favor of other material from later chapters.

[3]The material on ODEs and tridiagonal systems can be taught to students who have not had a normal ODE or linear algebra course.

Computer Access

Because the author no longer has a traditional academic position, his access to modern software is limited. Most of the examples were done using a very old and limited version of MATLAB from 1994. (Some were done on a Sun workstation, using FORTRAN code, in the late 1990s.) The more involved and newer examples were done using public access computers at the University of Michigan's Duderstadt Center, and the author would like to express his appreciation to this great institution for this.

A Note to the Student

(This is slightly updated from the version in the First Edition.) This book was written to be read. I am under no illusions that this book will compete with the latest popular novel for interest or thrilling narrative. But I have tried very hard to write a book on mathematics that can be read by students. So do not simply buy the book, work the exercises, and sell the book back to the bookstore at the end of the term. Read the text, think about what you have read, and ask your instructor questions about the things that you do not understand.

Numerical methods and analysis is a very different area of mathematics, certainly different from what you have seen in your previous courses. It is not harder, but the differentness of the material makes it seem harder. We worry about different issues than those in other mathematics classes. In a calculus course you are typically asked to compute the derivative or antiderivative of a given function, or to solve some equation for a particular unknown. The task is clearly defined, with a very concrete notion of "the right answer." Here, we are concerned with computing approximations, and this involves a slightly different kind of thinking. We have to understand what we are approximating well enough to construct a reasonable approximation, and we have to be able to think clearly and logically enough to analyze the accuracy and performance of that approximation. One former student has characterized this course material as "rigorously imprecise" or "approximately precise." Both are appropriate descriptions. Rote memorization of procedures is not of use here; it is vital in this course that the student learn the underlying concepts. Numerical mathematics is also *experimental* in nature. A lot can be learned simply by trying something out and seeing how the computation goes.

Preface to the Revised Edition

First, I would like to thank John Wiley for letting me do a Revised Edition of *An Introduction to Numerical Methods and Analysis*, and in particular I would like to thank Susanne Steitz and Laurie Rosatone for making it all possible.

So, what's new about this edition? A number of things. For various reasons, a large number of typographical and similar errors managed to creep into the original edition. These have been aggressively weeded out and fixed in this version. I'd like to thank everyone who emailed me with news of this or that error. In particular, I'd like to acknowledge Marzia Rivi, who translated the first edition into Italian and who emailed me with many typos, Prof. Nicholas Higham of Manchester University, Great Britain, and Mark Mills of Central College in Pella, Iowa. I'm sure there's a place or two where I did something silly like reversing the order of subtraction. If anyone finds any error of any sort, please email me at `jfe@ams.org`.

I considered adding sections on a couple of new topics, but in the end decided to leave the bulk of the text alone. I spent some time improving the exposition and presentation, but most of the text is the same as the first edition, except for fixing the typos.

I would be remiss if I did not acknowledge the support of my employer, the American Mathematical Society, who granted me a study leave so I could finish this project. Executive Director John Ewing and the Executive Editor of Mathematical Reviews, Kevin Clancey, deserve special mention in this regard. Amy Hendrikson of TeXnology helped with some LaTeX issues, as did my colleague at Mathematical Reviews, Patrick Ion. Another colleague, Maryse Brouwers, an extraordinary grammarian, helped greatly with the final copyediting process.

The original preface has the URL for the text website wrong; just go to `www.wiley.com` and use their links to find the book. The original preface also has my old professional email. The updated email is `jfe@ams.org`; anyone with comments on the text is welcome to contact me.

But, as is always the case, it is the author's immediate family who deserve the most credit for support during the writing of a book. So, here goes a big thank you to my wife, Georgia, and my children, Elinor and Jay. Look at it this way, kids: The end result will pay for a few birthdays.

Preface (To the First Edition)

This book is intended for introductory and advanced courses in numerical methods and numerical analysis, for students majoring in mathematics, sciences, and engineering. The book is appropriate for both single-term survey courses or year-long sequences, where students have a basic understanding of at least single-variable calculus and a programming language. (The usual first courses in linear algebra and differential equations are required for the last four chapters.)

To provide maximum teaching flexibility, each chapter and each section begins with the basic, elementary material and gradually builds up to the more advanced material. This same approach is followed with the underlying theory of the methods. Accordingly, one can use the text for a "methods" course that eschews mathematical analysis, simply by not covering the sections that focus on the theoretical material. Or, one can use the text for a survey course by only covering the basic sections, or the extra topics can be covered if you have the luxury of a full year course.

The objective of the text is for students to learn where approximation methods come from, why they work, why they sometimes don't work, and when to use which of many techniques that are available, and to do all this in a style that emphasizes readability and usefulness to the beginning student. While these goals are shared by other texts, it is the development and delivery of the ideas in this text that I think makes it different.

A course in numerical computation—whether it emphasizes the theory or the methods—requires that students think quite differently than in other mathematics courses, yet students are often not experienced in the kind of problem-solving skills and mathematical judgment that a numerical course requires. Many students react to mathematics problems by pigeonholing them by category, with little thought given to the meaning of the answer. Numerical mathematics demands much more judgment and evaluation in light of the underlying theory, and in the first several weeks of the course it is crucial for students to adapt their way of thinking about and working with these ideas, in order to succeed in the course.

To enable students to attain the appropriate level of mathematical sophistication, this text begins with a review of the important calculus results, and why and where these ideas play an important role in this course. Some of the concepts required for the study of computational mathematics are introduced, and simple approximations using Taylor's theorem are treated in some depth, in order to acquaint students with one of the most common and basic tools in the science of approximation. Computer arithmetic is treated in perhaps more detail than some might think necessary, but it is instructive for many students to see the actual basis for rounding error demonstrated in detail, at least once.

One important element of this text that I have not seen in other texts is the emphasis that is placed on "cause and effect" in numerical mathematics. For example, if we apply the trapezoid rule to (approximately) integrate a function, then the error should go down by a factor of 4 as the mesh decreases by a factor of 2; if this is not what happens, then almost surely there is either an error in the code or the integrand is not sufficiently smooth. While this is obvious to experienced practitioners in the field, it is not obvious to beginning students who are not confident of their mathematical abilities. Many of the exercises and examples are designed to explore this kind of issue.

Two common starting points to the course are root-finding or linear systems, but diving in to the treatment of these ideas often leaves the students confused and wondering what the point of the course is. Instead, this text provides a second chapter designed as a "toolbox" of elementary ideas from across several problem areas; it is one of the important innovations of the text. The goal of the toolbox is to acclimate the students to the culture of numerical methods and analysis, and to show them a variety of simple ideas before proceeding to cover any single topic in depth. It develops some elementary approximations and methods that the students can easily appreciate and understand, and introduces the students, in the context of very simple methods and problems, to the essence of the analytical and coding issues that dominate the course. At the same time, the early development of these tools allows them to be used later in the text in order to derive and explain some algorithms in more detail than is usually the case.

The style of exposition is intended to be more lively and "student friendly" than the average mathematics text. This does not mean that there are no theorems stated and proved correctly, but it does mean that the text is not slavish about it. There is a reason for this: The book is meant to be read by the students. The instructor can render more formal anything in the text that he or she wishes, but if the students do not read the text because they are turned off by an overly dry regimen of definition, theorem, proof, corollary, then all of our effort is for naught. In places, the exposition may seem a bit wordier than necessary, and there is a significant amount of repetition. Both are deliberate. While brevity is indeed better mathematical style, it is not necessarily better pedagogy. Mathematical textbook exposition often suffers from an excess of brevity, with the result that the students cannot follow the arguments as presented in the text. Similarly, repetition aids learning, by reinforcement.

Nonetheless I have tried to make the text mathematically complete. Those who wish to teach a lower-level survey course can skip proofs of many of the more technical results in order to concentrate on the approximations themselves. An effort has been made—not always successfully—to avoid making basic material in one section depend on advanced material from an earlier section.

The topics selected for inclusion are fairly standard, but not encyclopedic. Emerging areas of numerical analysis, such as wavelets, are not (in the author's opinion) appropriate for a first course in the subject. The same reasoning dictated the exclusion of other, more mature areas, such as the finite element method, although that might change in future editions should there be sufficient demand for it. A more detailed treatment of approximation theory, one of the author's favorite topics, was also felt to be poorly suited to a beginning text. It was felt that a better text would be had by doing a good job covering some of the basic ideas, rather than trying to cover everything in the subject.

The text is not specific to any one computing language. Most illustrations of code are made in an informal pseudo-code, while more involved algorithms are shown in a "macro-outline" form, and programming hints and suggestions are scattered throughout the text. The exercises assume that the students have easy access to and working knowledge of software for producing basic Cartesian graphs.

A diskette of programs is *not* provided with the text, a practice that sets this book at odds with many others, but which reflects the author's opinion that students must learn how to write and debug programs that implement the algorithms in order to learn the underlying mathematics. However, since some faculty and some departments structure their courses differently, a collection of program segments in a variety of languages is available on the text web site so that instructors can easily download and then distribute the code to their students. Instructors and students should be aware that these are program *segments*; none of them are intended to be ready-to-run complete programs. Other features of the text web site are discussed below. (*Note:* This material may be removed from the Revised Edition website.)

Exercises run the gamut from simple hand computations that might be characterized as "starter exercises" to challenging derivations and minor proofs to programming exercises designed to test whether or not the students have assimilated the important ideas of each chapter and section. Some of the exercises are taken from application situations, some are more traditionally focused on the mathematical issues for their own sake. Each chapter concludes with a brief section discussing existing software and other references for the topic at hand, and a discussion of material not covered in this text.

Historical notes are scattered throughout the text, with most named mathematicians being accorded at least a paragraph or two of biography when they are first mentioned. This not only indulges my interest in the history of mathematics, but it also serves to engage the interest of the students.

The web site for the text (http://www.wiley.com/epperson) will contain, in addition to the set of code segments mentioned above, a collection of additional exercises for the text, some application modules demonstrating some more involved and more realistic applications of some of the material in the text, and, of course, information about any updates that are going to be made in future editions. Colleagues who wish to submit exercises or make comments about the text are invited to do so by contacting the author at `epperson@math.uah.edu`.

Notation

Most notation is defined as it appears in the text, but here we include some commonplace items.

$\mathbb{R}$ — The real number line; $\mathbb{R} = (-\infty, \infty)$.

$\mathbb{R}^n$ — The vector space of real vectors of n components.

$\mathbb{R}^{n\times n}$ — The vector space of real $n \times n$ matrices.

$C([a, b])$ — The set of functions f which are defined on the interval $[a, b]$, continuous on all of (a, b), and continuous from the interior of $[a, b]$ at the endpoints.

$C^k([a, b])$ — The set of functions f such that f and its first k derivatives are all in $C([a, b])$.

$C^{p,q}(Q)$ — The set of all functions u that are defined on the two-dimensional domain $Q = \{(x, t) \mid a \leq x \leq b, 0 < t \leq T\}$, and that are p times continuously differentiable in x for all t, and q times continuously differentiable in t for all x.

$\approx$ — Approximately equal. When we say that $A \approx B$, we mean that A and B are approximations to each other. See §1.2.2.

$\equiv$ — Equivalent. When we say that $f(x) = g(x)$, we mean that the two functions agree at the single point x. When we say that $f(x) \equiv g(x)$, we mean that they agree at all points x. The same thing is said by using just the function names, i.e., $f = g$.

$\mathcal{O}$ — On the order of ("big O of"). We say that $A = B + \mathcal{O}(D(h))$ whenever $|A - B| \leq CD(h)$ for some constant C and for all h sufficiently small. See §1.2.3.

$\mathbf{u}$ — Machine epsilon. The largest number such that, in computer arithmetic, $1 + \mathbf{u} = 1$. Architecture dependent, of course. See §1.3.

sgn — Sign function. The value of $\text{sgn}(x)$ is 1, -1, or 0, depending on whether or not x is positive, negative, or zero, respectively.