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978-0-521-88068-8 - Numerical Recipes: The Art of Scientific Computing, Third Edition

William H. Press, Saul A. Teukolsky, William T. Vetterling and Brian P. Flannery

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NUMERICAL RECIPES

The Art of Scientific Computing

Third Edition

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The Art of Scientific Computing

Third Edition

William H. Press

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Preface to the Third Edition (2007)

“I was just going to say, when I was interrupted...” begins Oliver Wendell Holmes in the second series of his famous essays, *The Autocrat of the Breakfast Table*. The interruption referred to was a gap of 25 years. In our case, as the autocrats of *Numerical Recipes*, the gap between our second and third editions has been “only” 15 years. Scientific computing has changed enormously in that time.

The first edition of *Numerical Recipes* was roughly coincident with the first commercial success of the personal computer. The second edition came at about the time that the Internet, as we know it today, was created. Now, as we launch the third edition, the practice of science and engineering, and thus scientific computing, has been profoundly altered by the mature Internet and Web. It is no longer difficult to find *somebody’s* algorithm, and usually free code, for almost any conceivable scientific application. The critical questions have instead become, “How does it work?” and “Is it any good?” Correspondingly, the second edition of *Numerical Recipes* has come to be valued more and more for its text explanations, concise mathematical derivations, critical judgments, and advice, and less for its code implementations per se.

Recognizing the change, we have expanded and improved the text in many places in this edition and added many completely new sections. We seriously considered leaving the code out entirely, or making it available only on the Web. However, in the end, we decided that without code, it wouldn’t be *Numerical Recipes*. That is, without code you, the reader, could never know whether our advice was in fact honest, implementable, and practical. Many discussions of algorithms in the literature and on the Web omit crucial details that can only be uncovered by actually coding (our job) or reading compilable code (your job). Also, we needed actual code to teach and illustrate the large number of lessons about object-oriented programming that are implicit and explicit in this edition.

Our wholehearted embrace of a style of object-oriented computing for scientific applications should be evident throughout this book. We say “*a* style,” because, contrary to the claims of various self-appointed experts, there can be no one rigid style of programming that serves all purposes, not even all scientific purposes. Our style is ecumenical. If a simple, global, C-style function will fill the need, then we use it. On the other hand, you will find us building some fairly complicated structures for something as complicated as, e.g., integrating ordinary differential equations. For more on the approach taken in this book, see §1.3 – §1.5.

In bringing the text up to date, we have luckily not had to bridge a full 15-year gap. Significant modernizations were incorporated into the second edition versions in Fortran 90 (1996)* and C++ (2002), in which, notably, the last vestiges of unit-based arrays were expunged in favor of C-style zero-based indexing. Only with this third edition, however, have we incorporated a substantial amount (several hundred pages!) of completely new material. Highlights include:

- a new chapter on classification and inference, including such topics as Gaussian mixture models, hidden Markov modeling, hierarchical clustering (phylogenetic trees), and support vector machines

*“Alas, poor Fortran 90! We knew him, Horatio: a programming language of infinite jest, of most excellent fancy: he hath borne us on his back a thousand times.”

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- a new chapter on computational geometry, including topics like KD trees, quad- and octrees, Delaunay triangulation and applications, and many useful algorithms for lines, polygons, triangles, spheres, etc.
- many new statistical distributions, with pdfs, cdfs, and inverse cdfs
- an expanded treatment of ODEs, emphasizing recent advances, and with completely new routines
- much expanded sections on uniform random deviates and on deviates from many other statistical distributions
- an introduction to spectral and pseudospectral methods for PDEs
- interior point methods for linear programming
- more on sparse matrices
- interpolation on scattered data in multidimensions
- curve interpolation in multidimensions
- quadrature by variable transformation and adaptive quadrature
- more on Gaussian quadratures and orthogonal polynomials
- more on accelerating the convergence of series
- improved incomplete gamma and beta functions and new inverse functions
- improved spherical harmonics and fast spherical harmonic transforms
- generalized Fermi-Dirac integrals
- multivariate Gaussian deviates
- algorithms and implementations for hash memory functions
- incremental quantile estimation
- chi-square with small numbers of counts
- dynamic programming
- hard and soft error correction and Viterbi decoding
- eigensystem routines for real, nonsymmetric matrices
- multitaper methods for power spectral estimation
- wavelets on the interval
- information-theoretic properties of distributions
- Markov chain Monte Carlo
- Gaussian process regression and kriging
- stochastic simulation of chemical reaction networks
- code for plotting simple graphs from within programs

The *Numerical Recipes* Web site, www.nr.com, is one of the oldest active sites on the Internet, as evidenced by its two-letter domain name. We will continue to make the Web site useful to readers of this edition. Go there to find the latest bug reports, to purchase the machine-readable source code, or to participate in our readers' forum. With this third edition, we also plan to offer, by subscription, a completely electronic version of *Numerical Recipes* — accessible via the Web, downloadable, printable, and, unlike any paper version, always up to date with the latest corrections. Since the electronic version does not share the page limits of the print version, it will grow over time by the addition of completely new sections, available only electronically. This, we think, is the future of *Numerical Recipes* and perhaps of technical reference books generally. If it sounds interesting to you, look at <http://www.nr.com/electronic>.

This edition also incorporates some “user-friendly” typographical and stylistic improvements: Color is used for headings and to highlight executable code. For code, a label in the margin gives the name of the source file in the machine-readable distribution. Instead of printing repetitive `#include` statements, we provide a con-

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venient Web tool at <http://www.nr.com/dependencies> that will generate exactly the statements you need for any combination of routines. Subsections are now numbered and referred to by number. References to journal articles now include, in most cases, the article title, as an aid to easy Web searching. Many references have been updated; but we have kept references to the grand old literature of classical numerical analysis when we think that books and articles deserve to be remembered.

Acknowledgments

Regrettably, over 15 years, we were not able to maintain a systematic record of the many dozens of colleagues and readers who have made important suggestions, pointed us to new material, corrected errors, and otherwise improved the *Numerical Recipes* enterprise. It is a tired cliché to say that “you know who you are.” Actually, in most cases, *we* know who you are, and we are grateful. But a list of names would be incomplete, and therefore offensive to those whose contributions are no less important than those listed. We apologize to both groups, those we might have listed and those we might have missed.

We prepared this book for publication on Windows and Linux machines, generally with Intel Pentium processors, using LaTeX in the TeTeX and MiKTeX implementations. Packages used include amsmath, amfonts, txfonts, and graphicx, among others. Our principal development environments were Microsoft Visual Studio / Microsoft Visual C++ and GNU C++. We used the SourceJammer cross-platform source control system. Many tasks were automated with Perl scripts. We could not live without GNU Emacs. To all the developers: “You know who you are,” and we thank you.

Research by the authors on computational methods was supported in part by the U.S. National Science Foundation and the U.S. Department of Energy.

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Preface to the Second Edition (1992)

Our aim in writing the original edition of *Numerical Recipes* was to provide a book that combined general discussion, analytical mathematics, algorithmics, and actual working programs. The success of the first edition puts us now in a difficult, though hardly unenviable, position. We wanted, then and now, to write a book that is informal, fearlessly editorial, unesoteric, and above all useful. There is a danger that, if we are not careful, we might produce a second edition that is weighty, balanced, scholarly, and boring.

It is a mixed blessing that we know more now than we did six years ago. Then, we were making educated guesses, based on existing literature and our own research, about which numerical techniques were the most important and robust. Now, we have the benefit of direct feedback from a large reader community. Letters to our alter-ego enterprise, Numerical Recipes Software, are in the thousands per year. (Please, *don't telephone* us.) Our post office box has become a magnet for letters pointing out that we have omitted some particular technique, well known to be important in a particular field of science or engineering. We value such letters and digest them carefully, especially when they point us to specific references in the literature.

The inevitable result of this input is that this second edition of *Numerical Recipes* is substantially larger than its predecessor, in fact about 50% larger in both words and number of included programs (the latter now numbering well over 300). “Don’t let the book grow in size,” is the advice that we received from several wise colleagues. We have tried to follow the intended spirit of that advice, even as we violate the letter of it. We have not lengthened, or increased in difficulty, the book’s principal discussions of mainstream topics. Many new topics are presented at this same accessible level. Some topics, both from the earlier edition and new to this one, are now set in smaller type that labels them as being “advanced.” The reader who ignores such advanced sections completely will not, we think, find any lack of continuity in the shorter volume that results.

Here are some highlights of the new material in this second edition:

- a new chapter on integral equations and inverse methods
- a detailed treatment of multigrid methods for solving elliptic partial differential equations
- routines for band-diagonal linear systems
- improved routines for linear algebra on sparse matrices
- Cholesky and QR decomposition
- orthogonal polynomials and Gaussian quadratures for arbitrary weight functions
- methods for calculating numerical derivatives
- Padé approximants and rational Chebyshev approximation
- Bessel functions, and modified Bessel functions, of fractional order and several other new special functions
- improved random number routines
- quasi-random sequences
- routines for adaptive and recursive Monte Carlo integration in high-dimensional spaces
- globally convergent methods for sets of nonlinear equations
- simulated annealing minimization for continuous control spaces

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- fast Fourier transform (FFT) for real data in two and three dimensions
- fast Fourier transform using external storage
- improved fast cosine transform routines
- wavelet transforms
- Fourier integrals with upper and lower limits
- spectral analysis on unevenly sampled data
- Savitzky-Golay smoothing filters
- fitting straight line data with errors in both coordinates
- a two-dimensional Kolmogorov-Smirnoff test
- the statistical bootstrap method
- embedded Runge-Kutta-Fehlberg methods for differential equations
- high-order methods for stiff differential equations
- a new chapter on “less-numerical” algorithms, including Huffman and arithmetic coding, arbitrary precision arithmetic, and several other topics

Consult the Preface to the first edition, following, or the Contents, for a list of the more “basic” subjects treated.

Acknowledgments

It is not possible for us to list by name here all the readers who have made useful suggestions; we are grateful for these. In the text, we attempt to give specific attribution for ideas that appear to be original and are not known in the literature. We apologize in advance for any omissions.

Some readers and colleagues have been particularly generous in providing us with ideas, comments, suggestions, and programs for this second edition. We especially want to thank George Rybicki, Philip Pinto, Peter Lepage, Robert Lupton, Douglas Eardley, Ramesh Narayan, David Spergel, Alan Oppenheim, Sallie Baliunas, Scott Tremaine, Glennys Farrar, Steven Block, John Peacock, Thomas Loredo, Matthew Choptuik, Gregory Cook, L. Samuel Finn, P. Deuffhard, Harold Lewis, Peter Weinberger, David Syer, Richard Ferch, Steven Ebstein, Bradley Keister, and William Gould. We have been helped by Nancy Lee Snyder’s mastery of a complicated \TeX manuscript. We express appreciation to our editors Lauren Cowles and Alan Harvey at Cambridge University Press, and to our production editor Russell Hahn. We remain, of course, grateful to the individuals acknowledged in the Preface to the first edition.

Special acknowledgment is due to programming consultant Seth Finkelstein, who wrote, rewrote, or influenced many of the routines in this book, as well as in its Fortran-language twin and the companion Example books. Our project has benefited enormously from Seth’s talent for detecting, and following the trail of, even very slight anomalies (often compiler bugs, but occasionally our errors), and from his good programming sense. To the extent that this edition of *Numerical Recipes in C* has a more graceful and “C-like” programming style than its predecessor, most of the credit goes to Seth. (Of course, we accept the blame for the Fortranish lapses that still remain.)

We prepared this book for publication on DEC and Sun workstations running the UNIX operating system and on a 486/33 PC compatible running MS-DOS 5.0 / Windows 3.0. We enthusiastically recommend the principal software used: GNU Emacs, \TeX , Perl, Adobe Illustrator, and PostScript. Also used were a variety of C

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compilers — too numerous (and sometimes too buggy) for individual acknowledgment. It is a sobering fact that our standard test suite (exercising all the routines in this book) has uncovered compiler bugs in many of the compilers tried. When possible, we work with developers to see that such bugs get fixed; we encourage interested compiler developers to contact us about such arrangements.

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Preface to the First Edition (1985)

We call this book *Numerical Recipes* for several reasons. In one sense, this book is indeed a “cookbook” on numerical computation. However, there is an important distinction between a cookbook and a restaurant menu. The latter presents choices among complete dishes in each of which the individual flavors are blended and disguised. The former — and this book — reveals the individual ingredients and explains how they are prepared and combined.

Another purpose of the title is to connote an eclectic mixture of presentational techniques. This book is unique, we think, in offering, for each topic considered, a certain amount of general discussion, a certain amount of analytical mathematics, a certain amount of discussion of algorithmics, and (most important) actual implementations of these ideas in the form of working computer routines. Our task has been to find the right balance among these ingredients for each topic. You will find that for some topics we have tilted quite far to the analytic side; this where we have felt there to be gaps in the “standard” mathematical training. For other topics, where the mathematical prerequisites are universally held, we have tilted toward more in-depth discussion of the nature of the computational algorithms, or toward practical questions of implementation.

We admit, therefore, to some unevenness in the “level” of this book. About half of it is suitable for an advanced undergraduate course on numerical computation for science or engineering majors. The other half ranges from the level of a graduate course to that of a professional reference. Most cookbooks have, after all, recipes at varying levels of complexity. An attractive feature of this approach, we think, is that the reader can use the book at increasing levels of sophistication as his/her experience grows. Even inexperienced readers should be able to use our most advanced routines as black boxes. Having done so, we hope that these readers will subsequently go back and learn what secrets are inside.

If there is a single dominant theme in this book, it is that practical methods of numerical computation can be simultaneously efficient, clever, and — important — clear. The alternative viewpoint, that efficient computational methods must necessarily be so arcane and complex as to be useful only in “black box” form, we firmly reject.

Our purpose in this book is thus to open up a large number of computational black boxes to your scrutiny. We want to teach you to take apart these black boxes and to put them back together again, modifying them to suit your specific needs. We assume that you are mathematically literate, i.e., that you have the normal mathematical preparation associated with an undergraduate degree in a physical science, or engineering, or economics, or a quantitative social science. We assume that you know how to program a computer. We do not assume that you have any prior formal knowledge of numerical analysis or numerical methods.

The scope of *Numerical Recipes* is supposed to be “everything up to, but not including, partial differential equations.” We honor this in the breach: First, we *do* have one introductory chapter on methods for partial differential equations. Second, we obviously cannot include *everything* else. All the so-called “standard” topics of a numerical analysis course have been included in this book: linear equations, interpolation and extrapolation, integration, nonlinear root finding, eigensystems, and ordinary differential equations. Most of these topics have been taken beyond their

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standard treatments into some advanced material that we have felt to be particularly important or useful.

Some other subjects that we cover in detail are not usually found in the standard numerical analysis texts. These include the evaluation of functions and of particular special functions of higher mathematics; random numbers and Monte Carlo methods; sorting; optimization, including multidimensional methods; Fourier transform methods, including FFT methods and other spectral methods; two chapters on the statistical description and modeling of data; and two-point boundary value problems, both shooting and relaxation methods.

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Many colleagues have been generous in giving us the benefit of their numerical and computational experience, in providing us with programs, in commenting on the manuscript, or with general encouragement. We particularly wish to thank George Rybicki, Douglas Eardley, Philip Marcus, Stuart Shapiro, Paul Horowitz, Bruce Musicus, Irwin Shapiro, Stephen Wolfram, Henry Abarbanel, Larry Smarr, Richard Muller, John Bahcall, and A.G.W. Cameron.

We also wish to acknowledge two individuals whom we have never met: Forman Acton, whose 1970 textbook *Numerical Methods That Work* (New York: Harper and Row) has surely left its stylistic mark on us; and Donald Knuth, both for his series of books on *The Art of Computer Programming* (Reading, MA: Addison-Wesley), and for \TeX , the computer typesetting language that immensely aided production of this book.

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Routines by Chapter and Section

Previous editions included a table of all the routines in the book, along with a short description, arranged by chapter and section. This information is now available as an interactive Web page at <http://www.nr.com/routines>. The following illustration gives the idea.

Each line corresponds to a printed piece of code in the book. These pieces have unique internal names (not visible in the book, though related to the struct or function names), as well as chapter, section, and page numbers. Multiple pieces are combined into source code #include files. The following table shows the correspondences.

sort by name	sort by section			sort by file
Internal Name	Chapter	Section	Page	File
flmoon	1	1.0	2	calendar.h
julday	1	1.0	6	calendar.h
caldat	1	1.0	6	calendar.h
gaussj	2	2.1	43	gaussj.h
ludcmp	2	2.3	51	ludcmp.h
ludcmp_ludcmp	2	2.3	51	ludcmp.h
ludcmp_solve	2	2.3	52	ludcmp.h
ludcmp_inverse	2	2.3	53	ludcmp.h
ludcmp_dat	2	2.3	54	ludcmp.h