

NUMERICAL RECIPES in C++

The Art of Scientific Computing
Second Edition

William H. Press

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Preface to the C++ Edition

C++ has gradually become the dominant language for computer programming, displacing C and Fortran even in many scientific and engineering applications. This version of *Numerical Recipes* contains the entire text of the Second Edition with all the programs presented in C++.

C++ poses special problems for numerical work. In particular, it is difficult to treat vectors and matrices in a manner that is simultaneously efficient and yet allows programming with high-level constructs. The fact that there is still no universally accepted standard library for doing this makes the problem even more difficult for authors of a book like this one. In Chapter 1 and the Appendices we describe how we have solved this problem. The default option is for you, the reader, to use a very simple class library that we provide. You can be up and running in a few minutes. We also show you how you can alternatively use any other matrix/vector class library of your choosing. This may take you a few minutes to set up the first time, but thereafter will provide transparent access to the Recipes with essentially no loss in efficiency.

We have taken this opportunity to respond to a clear consensus from our C readers, and converted all arrays and matrices to be “zero-based.” We have also taken this opportunity to fix errors in the text and programs that have been reported to us by our readers. There are too many people to acknowledge individually, but to all who have written to us we are very grateful.

September 2001

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

Preface to the Second Edition

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 both in 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
- fast Fourier transform (FFT) for real data in two and three dimensions
- fast Fourier transform (FFT) 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 table of 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 Lored, Matthew Choptuik, Gregory Cook, L. Samuel Finn, P. Deuflhard, Harold Lewis, Peter Weinberger, David Syer, Richard Ferch, Steven Epstein, 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. (See §1.0 for a list of additional computers used in

program tests.) We enthusiastically recommend the principal software used: GNU Emacs, TeX, Perl, Adobe Illustrator, and PostScript. Also used were a variety of C 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.

WHP and SAT acknowledge the continued support of the U.S. National Science Foundation for their research on computational methods. D.A.R.P.A. support is acknowledged for §13.10 on wavelets.

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

Preface to the First Edition

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 towards more in-depth discussion of the nature of the computational algorithms, or towards 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 (Chapter 19). 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 (Chapter 2), interpolation and extrapolation (Chapter 3), integration (Chapter 4), nonlinear root-finding (Chapter 9), eigensystems (Chapter 11), and ordinary differential equations (Chapter 16). Most of these topics have been taken beyond their standard treatments into some advanced material which 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 (Chapters 5 and 6); random numbers and Monte Carlo methods (Chapter 7); sorting (Chapter 8); optimization, including multidimensional methods (Chapter 10); Fourier transform methods, including FFT methods and other spectral methods (Chapters 12 and 13); two chapters on the statistical description and modeling of data (Chapters 14 and 15); and two-point boundary value problems, both shooting and relaxation methods (Chapter 17).

The programs in this book are included in ANSI-standard C. Versions of the book in Fortran, Pascal, and BASIC are available separately. We have more to say about the C language, and the computational environment assumed by our routines, in §1.1 (Introduction).

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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 in 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 T_EX, the computer typesetting language which immensely aided production of this book.

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Computer Programs by Chapter and Section

1.0	flmoon	calculate phases of the moon by date
1.1	julday	Julian Day number from calendar date
1.1	badluk	Friday the 13th when the moon is full
1.1	caldat	calendar date from Julian day number
2.1	gaussj	Gauss-Jordan matrix inversion and linear equation solution
2.3	ludcmp	linear equation solution, <i>LU</i> decomposition
2.3	lubksb	linear equation solution, backsubstitution
2.4	tridag	solution of tridiagonal systems
2.4	banmul	multiply vector by band diagonal matrix
2.4	bandec	band diagonal systems, decomposition
2.4	banbks	band diagonal systems, backsubstitution
2.5	mprove	linear equation solution, iterative improvement
2.6	svbksb	singular value backsubstitution
2.6	svdcmp	singular value decomposition of a matrix
2.6	pythag	calculate $(a^2 + b^2)^{1/2}$ without overflow
2.7	cyclic	solution of cyclic tridiagonal systems
2.7	sprsin	convert matrix to sparse format
2.7	spr sax	product of sparse matrix and vector
2.7	sprstx	product of transpose sparse matrix and vector
2.7	sprstp	transpose of sparse matrix
2.7	sprspm	pattern multiply two sparse matrices
2.7	sprstm	threshold multiply two sparse matrices
2.7	linbcg	biconjugate gradient solution of sparse systems
2.7	snrm	used by linbcg for vector norm
2.7	atimes	used by linbcg for sparse multiplication
2.7	asolve	used by linbcg for preconditioner
2.8	vander	solve Vandermonde systems
2.8	toeplz	solve Toeplitz systems
2.9	choldc	Cholesky decomposition
2.9	cholsl	Cholesky backsubstitution
2.10	qrdcmp	QR decomposition
2.10	qrsolv	QR backsubstitution
2.10	rsolv	right triangular backsubstitution
2.10	qrupdt	update a QR decomposition
2.10	rotate	Jacobi rotation used by qrupdt
3.1	polint	polynomial interpolation
3.2	ratint	rational function interpolation
3.3	spline	construct a cubic spline
3.3	splint	cubic spline interpolation
3.4	locate	search an ordered table by bisection

3.4	hunt	search a table when calls are correlated
3.5	polcoe	polynomial coefficients from table of values
3.5	polcof	polynomial coefficients from table of values
3.6	polin2	two-dimensional polynomial interpolation
3.6	bcucof	construct two-dimensional bicubic
3.6	bcuint	two-dimensional bicubic interpolation
3.6	splie2	construct two-dimensional spline
3.6	splin2	two-dimensional spline interpolation
4.2	trapzd	trapezoidal rule
4.2	qtrap	integrate using trapezoidal rule
4.2	qsimp	integrate using Simpson's rule
4.3	qromb	integrate using Romberg adaptive method
4.4	midpnt	extended midpoint rule
4.4	qromo	integrate using open Romberg adaptive method
4.4	midinf	integrate a function on a semi-infinite interval
4.4	midsql	integrate a function with lower square-root singularity
4.4	midsqu	integrate a function with upper square-root singularity
4.4	midexp	integrate a function that decreases exponentially
4.5	qgaus	integrate a function by Gaussian quadratures
4.5	gauleg	Gauss-Legendre weights and abscissas
4.5	gaulag	Gauss-Laguerre weights and abscissas
4.5	gauher	Gauss-Hermite weights and abscissas
4.5	gaujac	Gauss-Jacobi weights and abscissas
4.5	gaucof	quadrature weights from orthogonal polynomials
4.5	orthog	construct nonclassical orthogonal polynomials
4.6	quad3d	integrate a function over a three-dimensional space
5.1	eulsum	sum a series by Euler-van Wijngaarden algorithm
5.3	ddpoly	evaluate a polynomial and its derivatives
5.3	poldiv	divide one polynomial by another
5.3	ratval	evaluate a rational function
5.7	dfridr	numerical derivative by Ridders' method
5.8	chebft	fit a Chebyshev polynomial to a function
5.8	chebev	Chebyshev polynomial evaluation
5.9	chder	derivative of a function already Chebyshev fitted
5.9	chint	integrate a function already Chebyshev fitted
5.10	chebpc	polynomial coefficients from a Chebyshev fit
5.10	pcshft	polynomial coefficients of a shifted polynomial
5.11	pccheb	inverse of chebpc; use to economize power series
5.12	pade	Padé approximant from power series coefficients
5.13	ratlsq	rational fit by least-squares method
6.1	gammln	logarithm of gamma function
6.1	factrl	factorial function
6.1	bico	binomial coefficients function
6.1	factln	logarithm of factorial function

6.1	beta	beta function
6.2	gamm	incomplete gamma function
6.2	gammq	complement of incomplete gamma function
6.2	gser	series used by gamm and gammq
6.2	gcf	continued fraction used by gamm and gammq
6.2	erff	error function
6.2	erffc	complementary error function
6.2	erfcc	complementary error function, concise routine
6.3	expint	exponential integral E_n
6.3	ei	exponential integral E_i
6.4	betai	incomplete beta function
6.4	betacf	continued fraction used by betai
6.5	bessj0	Bessel function J_0
6.5	bessy0	Bessel function Y_0
6.5	bessj1	Bessel function J_1
6.5	bessy1	Bessel function Y_1
6.5	bessy	Bessel function Y of general integer order
6.5	bessj	Bessel function J of general integer order
6.6	bessi0	modified Bessel function I_0
6.6	bessk0	modified Bessel function K_0
6.6	bessi1	modified Bessel function I_1
6.6	bessk1	modified Bessel function K_1
6.6	bessk	modified Bessel function K of integer order
6.6	bessi	modified Bessel function I of integer order
6.7	bessjy	Bessel functions of fractional order
6.7	beschb	Chebyshev expansion used by bessjy
6.7	bessik	modified Bessel functions of fractional order
6.7	airy	Airy functions
6.7	sphbes	spherical Bessel functions j_n and y_n
6.8	plgndr	Legendre polynomials, associated (spherical harmonics)
6.9	frenel	Fresnel integrals $S(x)$ and $C(x)$
6.9	cisi	cosine and sine integrals Ci and Si
6.10	dawson	Dawson's integral
6.11	rf	Carlson's elliptic integral of the first kind
6.11	rd	Carlson's elliptic integral of the second kind
6.11	rj	Carlson's elliptic integral of the third kind
6.11	rc	Carlson's degenerate elliptic integral
6.11	ellf	Legendre elliptic integral of the first kind
6.11	elle	Legendre elliptic integral of the second kind
6.11	ellpi	Legendre elliptic integral of the third kind
6.11	sncndn	Jacobian elliptic functions
6.12	hypgeo	complex hypergeometric function
6.12	hypser	complex hypergeometric function, series evaluation
6.12	hypdrv	complex hypergeometric function, derivative of
7.1	ran0	random deviate by Park and Miller minimal standard
7.1	ran1	random deviate, minimal standard plus shuffle

7.1	ran2	random deviate by L'Ecuyer long period plus shuffle
7.1	ran3	random deviate by Knuth subtractive method
7.2	expdev	exponential random deviates
7.2	gasdev	normally distributed random deviates
7.3	gamdev	gamma-law distribution random deviates
7.3	poidev	Poisson distributed random deviates
7.3	bnldev	binomial distributed random deviates
7.4	irbit1	random bit sequence
7.4	irbit2	random bit sequence
7.5	psdes	"pseudo-DES" hashing of 64 bits
7.5	ran4	random deviates from DES-like hashing
7.7	sobseq	Sobol's quasi-random sequence
7.8	vegas	adaptive multidimensional Monte Carlo integration
7.8	rebin	sample rebinning used by vegas
7.8	miser	recursive multidimensional Monte Carlo integration
7.8	ranpt	get random point, used by miser
8.1	piksort	sort an array by straight insertion
8.1	piksr2	sort two arrays by straight insertion
8.1	shell	sort an array by Shell's method
8.2	sort	sort an array by quicksort method
8.2	sort2	sort two arrays by quicksort method
8.3	hpsort	sort an array by heapsort method
8.4	indexx	construct an index for an array
8.4	sort3	sort, use an index to sort 3 or more arrays
8.4	rank	construct a rank table for an array
8.5	select	find the N th largest in an array
8.5	selip	find the N th largest, without altering an array
8.5	hpsel	find M largest values, without altering an array
8.6	eclclass	determine equivalence classes from list
8.6	eclazz	determine equivalence classes from procedure
9.0	scrsho	graph a function to search for roots
9.1	zbrac	outward search for brackets on roots
9.1	zbrak	inward search for brackets on roots
9.1	rtbis	find root of a function by bisection
9.2	rtflsp	find root of a function by false-position
9.2	rtsec	find root of a function by secant method
9.2	zriddr	find root of a function by Ridders' method
9.3	zbrent	find root of a function by Brent's method
9.4	rtnewt	find root of a function by Newton-Raphson
9.4	rtsafe	find root of a function by Newton-Raphson and bisection
9.5	laguer	find a root of a polynomial by Laguerre's method
9.5	zroots	roots of a polynomial by Laguerre's method with deflation
9.5	zrhqr	roots of a polynomial by eigenvalue methods
9.5	qroot	complex or double root of a polynomial, Bairstow