

Numerical Recipes in C++

The Art of Scientific Computing
Second Edition

William H. Press

Los Alamos National Laboratory

Saul A. Teukolsky

Department of Physics, Cornell University

William T. Vetterling

Polaroid Corporation

Brian P. Flannery

EXXON Research and Engineering Company



PUBLISHED BY THE PRESS SYNDICATE OF THE UNIVERSITY OF CAMBRIDGE
The Pitt Building, Trumpington Street, Cambridge, United Kingdom

CAMBRIDGE UNIVERSITY PRESS
The Edinburgh Building, Cambridge CB2 2RU, UK
40 West 20th Street, New York, NY 10011-4211, USA
477 Williamstown Road, Port Melbourne, VIC, 3207, Australia
Ruiz de Alarcón 13, 28014 Madrid, Spain
Dock House, The Waterfront, Cape Town 8001, South Africa
<http://www.cambridge.org>

© Cambridge University Press 1988, 1992, 2002
except for §13.10 and Appendix B, which are placed into the public domain,
and except for all other computer programs and procedures, which are
© Numerical Recipes Software 1987, 1988, 1992, 1997, 2002
All Rights Reserved.

This book is copyright. Subject to statutory exception and to the provisions of relevant
collective licensing agreements, no reproduction of any part may take place without
the written permission of Cambridge University Press.

Some sections of this book were originally published, in different form, in *Computers
in Physics* magazine, © American Institute of Physics, 1988–1992.

First Edition originally published 1988; Second Edition originally published 1992;
C++ edition originally published 2002.

This printing is corrected to software version 2.10

Printed in the United States of America
Typeface Times 10/12 pt. System \TeX [AU]

Affiliations shown on title page are for purposes of identification only. No implication
that the works contained herein were created in the course of employment is intended,
nor is any knowledge of or endorsement of these works by the listed institutions to be inferred.

Without an additional license to use the contained software, this book is intended as a text
and reference book, for reading purposes only. A free license for limited use of the software
by the individual owner of a copy of this book who personally types one or more routines
into a single computer is granted under terms described on p. xviii. See the section “License
Information” (pp. xvii–xx) for information on obtaining more general licenses at low cost.

Machine-readable media containing the software in this book, with included licenses for
use on a single screen, are available from Cambridge University Press. See the order form at
the back of the book for further information.

The software may also be downloaded, with immediate purchase of a license also possible,
from the Numerical Recipes Software Web site (<http://www.nr.com>). Unlicensed transfer
of Numerical Recipes programs to any other format, or to any computer except one that is
specifically licensed, is strictly prohibited. Technical questions, corrections, and requests for
information should be addressed to Numerical Recipes Software, P.O. Box 380243, Cambridge,
MA 02238-0243 (USA), email “info@nr.com,” or fax 781 863-1739.

A catalog record for this book is available from the British Library.

Library of Congress Cataloging in Publication Data

Numerical recipes in C++ : the art of scientific computing / William H. Press

... [et al.]. – 2nd ed.

p. cm.

Includes bibliographical references and index.

ISBN 0-521-75033-4

1. C++ (Computer program language) 2. Numerical analysis. I. Press, William H.

QA76.73.C153 N85 2002

519.4'0285'5133–dc21

2001052699

ISBN 0 521 75033 4 Hardback

ISBN 0 521 75034 2 Example book in C++

ISBN 0 521 75037 7 C++/C CD-ROM (Windows/Macintosh)

ISBN 0 521 75035 0 Complete CD-ROM (Windows/Macintosh)

ISBN 0 521 75036 9 Complete CD-ROM (UNIX/Linux)

Contents

| | |
|---|--------------------|
| <i>Preface to the C++ Edition</i> | <i>xi</i> |
| <i>Preface to the Second Edition</i> | <i>xii</i> |
| <i>Preface to the First Edition</i> | <i>xv</i> |
| <i>License Information</i> | <i>xvii</i> |
| <i>Computer Programs by Chapter and Section</i> | <i>xxi</i> |
| 1 Preliminaries | 1 |
| 1.0 Introduction | 1 |
| 1.1 Program Organization and Control Structures | 5 |
| 1.2 Some C++ Conventions for Scientific Computing | 16 |
| 1.3 Implementation of the Vector and Matrix Classes | 25 |
| 1.4 Error, Accuracy, and Stability | 31 |
| 2 Solution of Linear Algebraic Equations | 35 |
| 2.0 Introduction | 35 |
| 2.1 Gauss-Jordan Elimination | 39 |
| 2.2 Gaussian Elimination with Backsubstitution | 44 |
| 2.3 LU Decomposition and Its Applications | 46 |
| 2.4 Tridiagonal and Band Diagonal Systems of Equations | 53 |
| 2.5 Iterative Improvement of a Solution to Linear Equations | 58 |
| 2.6 Singular Value Decomposition | 62 |
| 2.7 Sparse Linear Systems | 74 |
| 2.8 Vandermonde Matrices and Toeplitz Matrices | 93 |
| 2.9 Cholesky Decomposition | 99 |
| 2.10 QR Decomposition | 101 |
| 2.11 Is Matrix Inversion an N^3 Process? | 105 |
| 3 Interpolation and Extrapolation | 108 |
| 3.0 Introduction | 108 |
| 3.1 Polynomial Interpolation and Extrapolation | 111 |
| 3.2 Rational Function Interpolation and Extrapolation | 114 |
| 3.3 Cubic Spline Interpolation | 116 |
| 3.4 How to Search an Ordered Table | 120 |
| 3.5 Coefficients of the Interpolating Polynomial | 123 |
| 3.6 Interpolation in Two or More Dimensions | 126 |

| | | |
|----------|--|------------|
| 4 | <i>Integration of Functions</i> | 133 |
| 4.0 | Introduction | 133 |
| 4.1 | Classical Formulas for Equally Spaced Abscissas | 134 |
| 4.2 | Elementary Algorithms | 141 |
| 4.3 | Romberg Integration | 144 |
| 4.4 | Improper Integrals | 146 |
| 4.5 | Gaussian Quadratures and Orthogonal Polynomials | 152 |
| 4.6 | Multidimensional Integrals | 166 |
| 5 | <i>Evaluation of Functions</i> | 171 |
| 5.0 | Introduction | 171 |
| 5.1 | Series and Their Convergence | 171 |
| 5.2 | Evaluation of Continued Fractions | 175 |
| 5.3 | Polynomials and Rational Functions | 179 |
| 5.4 | Complex Arithmetic | 182 |
| 5.5 | Recurrence Relations and Clenshaw's Recurrence Formula | 184 |
| 5.6 | Quadratic and Cubic Equations | 189 |
| 5.7 | Numerical Derivatives | 192 |
| 5.8 | Chebyshev Approximation | 196 |
| 5.9 | Derivatives or Integrals of a Chebyshev-approximated Function | 201 |
| 5.10 | Polynomial Approximation from Chebyshev Coefficients | 203 |
| 5.11 | Economization of Power Series | 204 |
| 5.12 | Padé Approximants | 206 |
| 5.13 | Rational Chebyshev Approximation | 209 |
| 5.14 | Evaluation of Functions by Path Integration | 213 |
| 6 | <i>Special Functions</i> | 217 |
| 6.0 | Introduction | 217 |
| 6.1 | Gamma Function, Beta Function, Factorials, Binomial Coefficients | 218 |
| 6.2 | Incomplete Gamma Function, Error Function, Chi-Square Probability Function, Cumulative Poisson Function | 221 |
| 6.3 | Exponential Integrals | 227 |
| 6.4 | Incomplete Beta Function, Student's Distribution, F-Distribution, Cumulative Binomial Distribution | 231 |
| 6.5 | Bessel Functions of Integer Order | 235 |
| 6.6 | Modified Bessel Functions of Integer Order | 241 |
| 6.7 | Bessel Functions of Fractional Order, Airy Functions, Spherical Bessel Functions | 245 |
| 6.8 | Spherical Harmonics | 257 |
| 6.9 | Fresnel Integrals, Cosine and Sine Integrals | 259 |
| 6.10 | Dawson's Integral | 264 |
| 6.11 | Elliptic Integrals and Jacobian Elliptic Functions | 265 |
| 6.12 | Hypergeometric Functions | 275 |
| 7 | <i>Random Numbers</i> | 278 |
| 7.0 | Introduction | 278 |
| 7.1 | Uniform Deviates | 279 |

| | |
|--|------------|
| 7.2 Transformation Method: Exponential and Normal Deviates | 291 |
| 7.3 Rejection Method: Gamma, Poisson, Binomial Deviates | 294 |
| 7.4 Generation of Random Bits | 300 |
| 7.5 Random Sequences Based on Data Encryption | 304 |
| 7.6 Simple Monte Carlo Integration | 308 |
| 7.7 Quasi- (that is, Sub-) Random Sequences | 313 |
| 7.8 Adaptive and Recursive Monte Carlo Methods | 320 |
| 8 <i>Sorting</i> | 332 |
| 8.0 Introduction | 332 |
| 8.1 Straight Insertion and Shell's Method | 333 |
| 8.2 Quicksort | 336 |
| 8.3 Heapsort | 339 |
| 8.4 Indexing and Ranking | 341 |
| 8.5 Selecting the M th Largest | 344 |
| 8.6 Determination of Equivalence Classes | 348 |
| 9 <i>Root Finding and Nonlinear Sets of Equations</i> | 351 |
| 9.0 Introduction | 351 |
| 9.1 Bracketing and Bisection | 354 |
| 9.2 Secant Method, False Position Method, and Ridder's Method | 358 |
| 9.3 Van Wijngaarden–Dekker–Brent Method | 363 |
| 9.4 Newton-Raphson Method Using Derivative | 366 |
| 9.5 Roots of Polynomials | 373 |
| 9.6 Newton-Raphson Method for Nonlinear Systems of Equations | 383 |
| 9.7 Globally Convergent Methods for Nonlinear Systems of Equations | 387 |
| 10 <i>Minimization or Maximization of Functions</i> | 398 |
| 10.0 Introduction | 398 |
| 10.1 Golden Section Search in One Dimension | 401 |
| 10.2 Parabolic Interpolation and Brent's Method in One Dimension | 406 |
| 10.3 One-Dimensional Search with First Derivatives | 410 |
| 10.4 Downhill Simplex Method in Multidimensions | 413 |
| 10.5 Direction Set (Powell's) Methods in Multidimensions | 417 |
| 10.6 Conjugate Gradient Methods in Multidimensions | 424 |
| 10.7 Variable Metric Methods in Multidimensions | 430 |
| 10.8 Linear Programming and the Simplex Method | 434 |
| 10.9 Simulated Annealing Methods | 448 |
| 11 <i>Eigensystems</i> | 461 |
| 11.0 Introduction | 461 |
| 11.1 Jacobi Transformations of a Symmetric Matrix | 468 |
| 11.2 Reduction of a Symmetric Matrix to Tridiagonal Form: Givens and Householder Reductions | 474 |
| 11.3 Eigenvalues and Eigenvectors of a Tridiagonal Matrix | 481 |
| 11.4 Hermitian Matrices | 486 |
| 11.5 Reduction of a General Matrix to Hessenberg Form | 487 |

| | |
|--|------------|
| 11.6 The QR Algorithm for Real Hessenberg Matrices | 491 |
| 11.7 Improving Eigenvalues and/or Finding Eigenvectors by Inverse Iteration | 498 |
| 12 Fast Fourier Transform | 501 |
| 12.0 Introduction | 501 |
| 12.1 Fourier Transform of Discretely Sampled Data | 505 |
| 12.2 Fast Fourier Transform (FFT) | 509 |
| 12.3 FFT of Real Functions, Sine and Cosine Transforms | 515 |
| 12.4 FFT in Two or More Dimensions | 526 |
| 12.5 Fourier Transforms of Real Data in Two and Three Dimensions | 530 |
| 12.6 External Storage or Memory-Local FFTs | 536 |
| 13 Fourier and Spectral Applications | 542 |
| 13.0 Introduction | 542 |
| 13.1 Convolution and Deconvolution Using the FFT | 543 |
| 13.2 Correlation and Autocorrelation Using the FFT | 550 |
| 13.3 Optimal (Wiener) Filtering with the FFT | 552 |
| 13.4 Power Spectrum Estimation Using the FFT | 555 |
| 13.5 Digital Filtering in the Time Domain | 563 |
| 13.6 Linear Prediction and Linear Predictive Coding | 569 |
| 13.7 Power Spectrum Estimation by the Maximum Entropy (All Poles) Method | 577 |
| 13.8 Spectral Analysis of Unevenly Sampled Data | 580 |
| 13.9 Computing Fourier Integrals Using the FFT | 589 |
| 13.10 Wavelet Transforms | 596 |
| 13.11 Numerical Use of the Sampling Theorem | 611 |
| 14 Statistical Description of Data | 614 |
| 14.0 Introduction | 614 |
| 14.1 Moments of a Distribution: Mean, Variance, Skewness, and So Forth | 615 |
| 14.2 Do Two Distributions Have the Same Means or Variances? | 620 |
| 14.3 Are Two Distributions Different? | 625 |
| 14.4 Contingency Table Analysis of Two Distributions | 633 |
| 14.5 Linear Correlation | 641 |
| 14.6 Nonparametric or Rank Correlation | 644 |
| 14.7 Do Two-Dimensional Distributions Differ? | 650 |
| 14.8 Savitzky-Golay Smoothing Filters | 655 |
| 15 Modeling of Data | 661 |
| 15.0 Introduction | 661 |
| 15.1 Least Squares as a Maximum Likelihood Estimator | 662 |
| 15.2 Fitting Data to a Straight Line | 666 |
| 15.3 Straight-Line Data with Errors in Both Coordinates | 671 |
| 15.4 General Linear Least Squares | 676 |
| 15.5 Nonlinear Models | 686 |

| | |
|---|------------|
| 15.6 Confidence Limits on Estimated Model Parameters | 694 |
| 15.7 Robust Estimation | 704 |
| 16 Integration of Ordinary Differential Equations | 712 |
| 16.0 Introduction | 712 |
| 16.1 Runge-Kutta Method | 715 |
| 16.2 Adaptive Stepsize Control for Runge-Kutta | 719 |
| 16.3 Modified Midpoint Method | 727 |
| 16.4 Richardson Extrapolation and the Bulirsch-Stoer Method | 729 |
| 16.5 Second-Order Conservative Equations | 737 |
| 16.6 Stiff Sets of Equations | 739 |
| 16.7 Multistep, Multivalued, and Predictor-Corrector Methods | 751 |
| 17 Two Point Boundary Value Problems | 756 |
| 17.0 Introduction | 756 |
| 17.1 The Shooting Method | 760 |
| 17.2 Shooting to a Fitting Point | 762 |
| 17.3 Relaxation Methods | 765 |
| 17.4 A Worked Example: Spheroidal Harmonics | 775 |
| 17.5 Automated Allocation of Mesh Points | 785 |
| 17.6 Handling Internal Boundary Conditions or Singular Points | 787 |
| 18 Integral Equations and Inverse Theory | 790 |
| 18.0 Introduction | 790 |
| 18.1 Fredholm Equations of the Second Kind | 793 |
| 18.2 Volterra Equations | 796 |
| 18.3 Integral Equations with Singular Kernels | 799 |
| 18.4 Inverse Problems and the Use of A Priori Information | 806 |
| 18.5 Linear Regularization Methods | 811 |
| 18.6 Backus-Gilbert Method | 818 |
| 18.7 Maximum Entropy Image Restoration | 821 |
| 19 Partial Differential Equations | 829 |
| 19.0 Introduction | 829 |
| 19.1 Flux-Conservative Initial Value Problems | 836 |
| 19.2 Diffusive Initial Value Problems | 849 |
| 19.3 Initial Value Problems in Multidimensions | 855 |
| 19.4 Fourier and Cyclic Reduction Methods for Boundary Value Problems | 859 |
| 19.5 Relaxation Methods for Boundary Value Problems | 865 |
| 19.6 Multigrid Methods for Boundary Value Problems | 873 |
| 20 Less-Numerical Algorithms | 891 |
| 20.0 Introduction | 891 |
| 20.1 Diagnosing Machine Parameters | 891 |
| 20.2 Gray Codes | 896 |

| | |
|---|------------|
| 20.3 Cyclic Redundancy and Other Checksums | 898 |
| 20.4 Huffman Coding and Compression of Data | 906 |
| 20.5 Arithmetic Coding | 912 |
| 20.6 Arithmetic at Arbitrary Precision | 916 |
| References | 927 |
| Appendix A: Table of Function Declarations | 931 |
| Appendix B: Utility Routines and Classes | 939 |
| Appendix C: Converting to Single Precision | 957 |
| Index of Programs and Dependencies | 959 |
| General Index | 972 |

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

This is the revised and expanded second edition of the hugely popular Numerical Recipes: the Art of Scientific Computing. The product of a unique collaboration among four leading scientists in academic research and industry, Numerical Recipes is a complete text and reference book on scientific computing. About the Authors. N/A. Reviews and Rating: Amazon. Related Book Categories: Numerical Analysis and Scientific Computing. NUMERICAL RECIPES. The Art of Scientific Computing. Third Edition. William H. Press. Raymer Chair in Computer Sciences and Integrative Biology The University of Texas at Austin. Saul A. Teukolsky. Hans A. Bethe Professor of Physics and Astrophysics Cornell University. 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.