TURING 图灵原版数学·统计学系列

数值计算领域圣经

矩阵计算

Matrix Computations

4th Edition

（英文版·第4版）

[美] Gene H. Golub
Charles F. Van Loan 著

人民邮电出版社
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内 容 提 要

本书是数值计算领域的名著，系统介绍了矩阵计算的基本理论和方法。内容包括：矩阵乘法、矩阵分析、线性方程组、正交化和最小二乘法、特征值问题、Lanczos 方法、矩阵函数及专题讨论等。书中的许多算法都有现成的软件包实现，每节后附有习题，并有注释和大量参考文献。新版增加约四分之一内容，反映了近年来矩阵计算领域的飞速发展。

本书可作为高等院校数学系高年级本科生和研究生教材，亦可作为计算数学和工程技术人员参考书。

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To

Alston S. Householder

And

Janes H. Wilkinson

Preface

My thirty-year book collaboration with Gene Golub began in 1977 at a matrix computation workshop held at Johns Hopkins University. His interest in my work at the start of my academic career prompted the writing of GVL1. Sadly, Gene died on November 16, 2007. At the time we had only just begun to talk about GVL4. While writing these pages, I was reminded every day of his far-reaching impact and professional generosity. This edition is a way to thank Gene for our collaboration and the friendly research community that his unique personality helped create.

It has been sixteen years since the publication of the third edition—a power-of-two reminder that what we need to know about matrix computations is growing exponentially! Naturally, it is impossible to provide in-depth coverage of all the great new advances and research trends. However, with the relatively recent publication of so many excellent textbooks and specialized volumes, we are able to complement our brief treatments with useful pointers to the literature. That said, here are the new features of GVL4:

Content

The book is about twenty-five percent longer. There are new sections on fast transforms (§1.4), parallel LU (§3.6), fast methods for circulant systems and discrete Poisson systems (§4.8), Hamiltonian and product eigenvalue problems (§7.8), pseudospectra (§7.9), the matrix sign, square root, and logarithm functions (§9.4), Lanczos and quadrature (§10.2), large-scale SVD (§10.4), Jacobi-Davidson (§10.6), sparse direct methods (§11.1), multigrid (§11.6), low displacement rank systems (§12.1), structured-rank systems (§12.2), Kronecker product problems (§12.3), tensor contractions (§12.4), and tensor decompositions (§12.5).

New topics at the subsection level include recursive block LU (§3.2.11), rook pivoting (§3.4.7), tournament pivoting (§3.6.3), diagonal dominance (§4.1.1), recursive block structures (§4.2.10), band matrix inverse properties (§4.3.8), divide-and-conquer strategies for block tridiagonal systems (§4.5.4), the cross product and various point/plane least squares problems (§5.3.9), the polynomial eigenvalue problem (§7.7.9), and the structured quadratic eigenvalue problem (§8.7.9).

Substantial upgrades include our treatment of floating-point arithmetic (§2.7), LU roundoff error analysis (§3.3.1), LS sensitivity analysis (§5.3.6), the generalized singular value decomposition (§6.1.6 and §8.7.4), and the CS decomposition (§8.7.6).

References

The annotated bibliographies at the end of each section remain. Because of space limitations, the master bibliography that was included in previous editions is now available through the book website. References that are historically important have been retained because old ideas have a way of resurrecting themselves. Plus, we must never forget the 1950's and 1960's! As mentioned above, we have the luxury of being able to draw upon an expanding library of books on matrix computations. A mnemonic-based citation system has been incorporated that supports these connections to the literature.

Examples

Non-illuminating, small-n numerical examples have been removed from the text. In their place is a modest suite of MATLAB demo scripts that can be run to provide insight into critical theorems and algorithms. We believe that this is a much more effective way to build intuition. The scripts are available through the book website.

Algorithmic Detail

It is important to have an algorithmic sense and an appreciation for high-performance matrix computations. After all, it is the clever exploitation of advanced architectures that account for much of the field's soaring success. However, the algorithms that we "formally" present in the book must never be considered as even prototype implementations. Clarity and communication of the big picture are what determine the level of detail in our presentations. Even though specific strategies for specific machines are beyond the scope of the text, we hope that our style promotes an ability to reason about memory traffic overheads and the importance of data locality.

Acknowledgements

I would like to thank everybody who has passed along typographical errors and suggestions over the years. Special kudos to the Cornell students in CS 4220, CS 6210, and CS 6220, where I used preliminary versions of GVL4. Harry Terkelson earned big bucks through through my ill-conceived $5-per-typo program!

A number of colleagues and students provided feedback and encouragement during the writing process. Others provided inspiration through their research and books. Thank you all: Diego Accame, David Bindel, Åke Björck, Laura Bolzano, Jim Demmel, Jack Dongarra, Mark Embree, John Gilbert, David Gleich, Joseph Grcar, Anne Greenbaum, Nick Higham, Ilse Ipsen, Bo Kågström, Vel Kahan, Tammy Kolda, Amy Langville, Julian Langou, Lek-Heng Lim, Nicola Mastronardi, Steve McCormick, Mike McCourt, Volker Mehrmann, Cleve Moler, Dianne O'Leary, Michael Overton, Chris Paige, Beresford Parlett, Stefan Ragnarsson, Lothar Reichel, Yousef Saad, Mike Saunders, Rob Schreiber, Danny Sorensen, Pete Stewart, Gil Strang, Francoise Tisseur, Nick Trefethen, Raf Vandebril, and Jianlin Xia.

Chris Paige and Mike Saunders were especially helpful with the editing of Chapters 10 and 11.

Vincent Burke, Jennifer Mallet, and Juliana McCarthy at Johns Hopkins University Press provided excellent support during the production process. Jennifer Slater did a terrific job of copy-editing. Of course, I alone am responsible for all mistakes and oversights.

Finally, this book would have been impossible to produce without my great family and my 4AM writing companion: Henry the Cat!

Charles F. Van Loan
Ithaca, New York
July, 2012

Global References

A number of books provide broad coverage of the field and are cited multiple times. We identify these global references using mnemonics. Bibliographic details are given in the Other Books section that follows.

AEP	**Wilkinson:** *Algebraic Eigenvalue Problem*
ANLA	**Demmel:** *Applied Numerical Linear Algebra*
ASNA	**Higham:** *Accuracy and Stability of Numerical Algorithms,* second edition
EOM	**Chatelin:** *Eigenvalues of Matrices*
FFT	**Van Loan:** *Computational Frameworks for the Fast Fourier Transform*
FOM	**Higham:** *Functions of Matrices*
FMC	**Watkins:** *Fundamentals of Matrix Computations*
IMC	**Stewart:** *Introduction to Matrix Computations*
IMK	**van der Vorst:** *Iterative Krylov Methods for Large Linear Systems*
IMSL	**Greenbaum:** *Iterative Methods for Solving Linear Systems*
ISM	**Axelsson:** *Iterative Solution Methods*
IMSLE	**Saad:** *Iterative Methods for Sparse Linear Systems,* second edition
LCG	**Meurant:** *The Lanczos and Conjugate Gradient Algorithms ...*
MA	**Horn and Johnson:** *Matrix Analysis*
MABD	**Stewart:** *Matrix Algorithms: Basic Decompositions*
MAE	**Stewart:** *Matrix Algorithms Volume II: Eigensystems*
MEP	**Watkins:** *The Matrix Eigenvalue Problem: GR and Krylov Subspace Methods*
MPT	**Stewart and Sun:** *Matrix Perturbation Theory*
NLA	**Trefethen and Bau:** *Numerical Linear Algebra*
NMA	**Ipsen:** *Numerical Matrix Analysis: Linear Systems and Least Squares*
NMLE	**Saad:** *Numerical Methods for Large Eigenvalue Problems,* revised edition
NMLS	**Björck:** *Numerical Methods for Least Squares Problems*
NMSE	**Kressner:** *Numerical Methods for General and Structured Eigenvalue Problems*
SAP	**Trefethen and Embree:** *Spectra and Pseudospectra*
SEP	**Parlett:** *The Symmetric Eigenvalue Problem*
SLAS	**Forsythe and Moler:** *Computer Solution of Linear Algebraic Systems*
SLS	**Lawson and Hanson:** *Solving Least Squares Problems*
TMA	**Horn and Johnson:** *Topics in Matrix Analysis*

`LAPACK` *LAPACK Users' Guide,* third edition
E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen.

`scaLAPACK` *ScaLAPACK Users' Guide*
L.S. Blackford, J. Choi, A. Cleary, E. D'Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, and R. C. Whaley.

`LIN_TEMPLATES` *Templates for the Solution of Linear Systems ...*
R. Barrett, M.W. Berry, T.F. Chan, J. Demmel, J. Donato, J. Dongarra, V. Eijkhout, R. Pozo, C. Romine, and H. van der Vorst.

`EIG_TEMPLATES` *Templates for the Solution of Algebraic Eigenvalue Problems ...*
Z. Bai, J. Demmel, J. Dongarra, A. Ruhe, and H. van der Vorst.

Other Books

The following volumes are a subset of a larger, ever-expanding library of textbooks and monographs that are concerned with matrix computations and supporting areas. The list of references below captures the evolution of the field and its breadth. Works that are more specialized are cited in the annotated bibliographies that appear at the end of each section in the chapters.

Early Landmarks

V.N. Faddeeva (1959). *Computational Methods of Linear Algebra*, Dover, New York.

E. Bodewig (1959). *Matrix Calculus*, North-Holland, Amsterdam.

J.H. Wilkinson (1963). *Rounding Errors in Algebraic Processes*, Prentice-Hall, Englewood Cliffs, NJ.

A.S. Householder (1964). *Theory of Matrices in Numerical Analysis*, Blaisdell, New York. Reprinted in 1974 by Dover, New York.

L. Fox (1964). *An Introduction to Numerical Linear Algebra*, Oxford University Press, Oxford.

J.H. Wilkinson (1965). *The Algebraic Eigenvalue Problem,* Clarendon Press, Oxford.

General Textbooks on Matrix Computations

G.W. Stewart (1973). *Introduction to Matrix Computations,* Academic Press, New York.

R.J. Goult, R.F. Hoskins, J.A. Milner, and M.J. Pratt (1974). *Computational Methods in Linear Algebra*, John Wiley and Sons, New York.

W.W. Hager (1988). *Applied Numerical Linear Algebra,* Prentice-Hall, Englewood Cliffs, NJ.

P.G. Ciarlet (1989). *Introduction to Numerical Linear Algebra and Optimisation*, Cambridge University Press, Cambridge.

P.E. Gill, W. Murray, and M.H. Wright (1991). *Numerical Linear Algebra and Optimization, Vol. 1*, Addison-Wesley, Reading, MA.

A. Jennings and J.J. McKeowen (1992). *Matrix Computation,*second edition, John Wiley and Sons, New York.

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J.W. Demmel (1997). *Applied Numerical Linear Algebra*, SIAM Publications, Philadelphia, PA.

A.J. Laub (2005). *Matrix Analysis for Scientists and Engineers*, SIAM Publications, Philadelphia, PA.

B.N. Datta (2010). *Numerical Linear Algebra and Applications,* second edition, SIAM Publications, Philadelphia, PA.

D.S. Watkins (2010). *Fundamentals of Matrix Computations*, John Wiley and Sons, New York.

A.J. Laub (2012). *Computational Matrix Analysis*, SIAM Publications, Philadelphia, PA.

Linear Equation and Least Squares Problems

G.E. Forsythe and C.B. Moler (1967). *Computer Solution of Linear Algebraic Systems,* Prentice-Hall, Englewood Cliffs, NJ.

A. George and J.W-H. Liu (1981). *Computer Solution of Large Sparse Positive Definite Systems.* Prentice-Hall, Englewood Cliffs, NJ.

I.S. Duff, A.M. Erisman, and J.K. Reid (1986). *Direct Methods for Sparse Matrices,* Oxford University Press, New York.

R.W. Farebrother (1987). *Linear Least Squares Computations*, Marcel Dekker, New York.

C.L. Lawson and R.J. Hanson (1995). *Solving Least Squares Problems*, SIAM Publications, Philadelphia, PA.

Å. Björck (1996). *Numerical Methods for Least Squares Problems,* SIAM Publications, Philadelphia, PA.

G.W. Stewart (1998). *Matrix Algorithms: Basic Decompositions*, SIAM Publications, Philadelphia, PA.

N.J. Higham (2002). *Accuracy and Stability of Numerical Algorithms,* second edition, SIAM Publications, Philadelphia, PA.

T.A. Davis (2006). *Direct Methods for Sparse Linear Systems*, SIAM Publications, Philadelphia, PA.

I.C.F. Ipsen (2009). *Numerical Matrix Analysis: Linear Systems and Least Squares*, SIAM Publications, Philadelphia, PA.

Eigenvalue Problems

A.R. Gourlay and G.A. Watson (1973). *Computational Methods for Matrix Eigenproblems*, John Wiley & Sons, New York.

F. Chatelin (1993). *Eigenvalues of Matrices*, John Wiley & Sons, New York.

B.N. Parlett (1998). *The Symmetric Eigenvalue Problem*, SIAM Publications, Philadelphia, PA.

G.W. Stewart (2001). *Matrix Algorithms Volume II: Eigensystems*, SIAM Publications, Philadelphia, PA.

L. Komzsik (2003). *The Lanczos Method: Evolution and Application*, SIAM Publications, Philadelphia, PA.

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Y. Saad (2011). *Numerical Methods for Large Eigenvalue Problems,* revised edition, SIAM Publications, Philadelphia, PA.

Iterative Methods

R.S. Varga (1962). *Matrix Iterative Analysis*, Prentice-Hall, Englewood Cliffs, NJ.

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J. Cullum and R.A. Willoughby (1985). *Lanczos Algorithms for Large Symmetric Eigenvalue Computations, Vol. II Programs,* Birkhaüser, Boston.

W. Hackbusch (1994). *Iterative Solution of Large Sparse Systems of Equations*, Springer-Verlag, New York.

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Y. Saad (2003). *Iterative Methods for Sparse Linear Systems,* second edition, SIAM Publications, Philadelphia, PA.

H. van der Vorst (2003). *Iterative Krylov Methods for Large Linear Systems*, Cambridge University Press, Cambridge, UK.

G. Meurant (2006). *The Lanczos and Conjugate Gradient Algorithms: From Theory to Finite Precision Computations*, SIAM Publications, Philadelphia, PA.

Special Topics/Threads

L.N. Trefethen and M. Embree (2005). *Spectra and Pseudospectra—The Behavior of Nonnormal Matrices and Operators*, Princeton University Press, Princeton and Oxford.

R. Vandebril, M. Van Barel, and N. Mastronardi (2007). *Matrix Computations and Semiseparable Matrices I: Linear Systems*, Johns Hopkins University Press, Baltimore, MD.

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Collected Works

R.H. Chan, C. Greif, and D.P. O'Leary, eds. (2007). *Milestones in Matrix Computation: Selected Works of G.H. Golub, with Commentaries*, Oxford University Press, Oxford.

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MATLAB

D.J. Higham and N.J. Higham (2005). *MATLAB Guide,* second edition, SIAM Publications, Philadelphia, PA.

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C.F. Van Loan and D. Fan (2009). *Insight Through Computing: A Matlab Introduction to Computational Science and Engineering,* SIAM Publications, Philadelphia, PA.

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C.B. Moler (2008) *Numerical Computing with MATLAB,* revised reprint, SIAM Publications, Philadelphia, PA.

G. Dahlquist and Å. Björck (2008). *Numerical Methods in Scientific Computing,* Vol. 1, SIAM Publications, Philadelphia, PA.

U. Ascher and C. Greif (2011). *A First Course in Numerical Methods,* SIAM Publications, Philadelphia, PA.

Useful URLs

GVL4

MATLAB demo scripts and functions, master bibliography, list of errata.

`http://www.cornell.edu/cv/GVL4`

Netlib

Huge repository of numerical software including LAPACK.

`http://www.netlib.org/index.html`

Matrix Market

Test examples for matrix algorithms.

`http://math.nist.gov/MatrixMarket/`

Matlab Central

Matlab functions, demos, classes, toolboxes, videos.

`http://www.mathworks.com/matlabcentral/`

University of Florida Sparse Matrix Collections

Thousands of sparse matrix examples in several formats.

`http://www.cise.ufl.edu/research/sparse/matrices/`

Pseudospectra Gateway

Grapical tools for pseudospectra.

`http://www.cs.ox.ac.uk/projects/pseudospectra/`

ARPACK

Software for large sparse eigenvalue problems

`http://www.caam.rice.edu/software/ARPACK/`

Innovative Computing Laboratory

State-of-the-art high performance matrix computations.

`http://icl.cs.utk.edu/`

Common Notation

$\mathbb{R}$, $\mathbb{R}^n$, $\mathbb{R}^{m\times n}$	set of real numbers, vectors, and matrices (p. 2)
$\mathbb{C}$, $\mathbb{C}^n$, $\mathbb{C}^{m\times n}$	set of complex numbers, vectors, and matrices (p. 13)
a_{ij}, $A(i,j)$, $[A]_{ij}$	(i,j) entry of a matrix (p. 2)
$\mathbf{u}$	unit roundoff (p. 96)
$\mathsf{fl}(\cdot)$	floating point operator (p. 96)
$\Vert x \Vert_p$	p-norm of a vector (p. 68)
$\Vert A \Vert_p$, $\Vert A \Vert_F$	p-norm and Frobenius norm of a matrix (p. 71)
$\mathsf{length}(x)$	dimension of a vector (p. 236)
$\kappa_p(A)$	p-norm condition (p. 87)
$\vert A \vert$	absolute value of a matrix (p. 91)
A^T, A^H	transpose and conjugate transpose (p. 2, 13)
$\mathsf{house}(x)$	Householder vector (p. 236)
$\mathsf{givens}(a,b)$	cosine-sine pair (p. 240)
$x_{\rm LS}$	minimum-norm least squares solution (p. 260)
$\mathsf{ran}(A)$	range of a matrix (p. 64)
$\mathsf{null}(A)$	nullspace of a matrix (p. 64)
$\mathsf{span}\{v_1,\ldots,v_n\}$	span defined by vectors (p. 64)
$\mathsf{dim}(S)$	dimension of a subspace (p. 64)
$\mathsf{rank}(A)$	rank of a matrix (p. 65)
$\mathsf{det}(A)$	determinant of a matrix (p. 66)
$\mathsf{tr}(A)$	trace of a matrix (p. 327)
$\mathsf{vec}(A)$	vectorization of a matrix (p. 28)
$\mathsf{reshape}(A,p,q)$	reshaping a matrix (p. 28)
$\mathsf{Re}(A)$, $\mathsf{Im}(A)$	real and imaginary parts of a matrix (p. 13)
$\mathrm{diag}(d_1,\ldots,d_n)$	diagonal matrix (p. 18)
I_n	n-by-n identity matrix (p. 19)
e_i	ith column of the identity matrix (p. 19)
$\mathcal{E}_n$, $\mathcal{D}_n$, $\mathcal{P}_{p,q}$	exchange, downshift, and perfect shuffle permutations (p. 20)
$\sigma_i(A)$	ith largest singular value (p. 77)
$\sigma_{\max}(A)$, $\sigma_{\min}(A)$	largest and smallest singular value (p. 77)
$\mathsf{dist}(S_1,S_2)$	distance between two subspaces (p. 82)
$\mathsf{sep}(A_1,A_2)$	separation between two matrices (p. 360)
$\lambda(A)$	set of eigenvalues (p. 66)
$\lambda_i(A)$	ith largest eigenvalue of a symmetric matrix (p. 66)
$\lambda_{\max}(A)$, $\lambda_{\min}(A)$	largest and smallest eigenvalue of a symmetric matrix (p. 66)
$\rho(A)$	spectral radius (p. 349)
$\mathcal{K}(A,q,j)$	Krylov subspace (p. 548)

Contents