

# L A P A C K

---

## Users' Guide

Second Edition

E. Anderson

Z. Bai

C. Bischof

J. Demmel

J. Dongarra

J. Du Croz

A. Greenbaum

S. Hammarling

A. McKenney

S. Ostrouchov

D. Sorensen

# Contents

Preface to the Second Edition	xiii
Preface to the First Edition	xvii
<b>1 Guide</b>	<b>1</b>
<b>1 Essentials</b>	<b>3</b>
1.1 LAPACK	3
1.2 Problems that LAPACK can Solve	3
1.3 Computers for which LAPACK is Suitable	3
1.4 LAPACK Compared with LINPACK and EISPACK	4
1.5 LAPACK and the BLAS	4
1.6 Documentation for LAPACK	4
1.7 Availability of LAPACK	5
1.8 Installation of LAPACK	5
1.9 Support for LAPACK	6
1.10 Known Problems in LAPACK	6
1.11 Other Related Software	6
1.11.1 LAPACK++	6
1.11.2 CLAPACK	7
1.11.3 ScaLAPACK	9
1.11.4 LAPACK routines exploiting IEEE arithmetic	9

<b>2</b>	<b>Contents of LAPACK</b>	<b>11</b>
2.1	Structure of LAPACK	11
2.1.1	Levels of Routines	11
2.1.2	Data Types and Precision	12
2.1.3	Naming Scheme	12
2.2	Driver Routines	14
2.2.1	Linear Equations	14
2.2.2	Linear Least Squares (LLS) Problems	15
2.2.3	Generalized Linear Least Squares (LSE and GLM) Problems	16
2.2.4	Standard Eigenvalue and Singular Value Problems	17
2.2.4.1	Symmetric Eigenproblems (SEP)	17
2.2.4.2	Nonsymmetric Eigenproblems (NEP)	18
2.2.4.3	Singular Value Decomposition (SVD)	19
2.2.5	Generalized Eigenvalue and Singular Value Problems	20
2.2.5.1	Generalized Symmetric Definite Eigenproblems (GSEEP)	20
2.2.5.2	Generalized Nonsymmetric Eigenproblems (GNEP)	21
2.2.5.3	Generalized Singular Value Decomposition (GSVD)	22
2.3	Computational Routines	24
2.3.1	Linear Equations	24
2.3.2	Orthogonal Factorizations and Linear Least Squares Problems	29
2.3.2.1	<i>QR</i> Factorization	29
2.3.2.2	<i>LQ</i> Factorization	30
2.3.2.3	<i>QR</i> Factorization with Column Pivoting	30
2.3.2.4	Complete Orthogonal Factorization	31
2.3.2.5	Other Factorizations	32
2.3.3	Generalized Orthogonal Factorizations and Linear Least Squares Problems	33
2.3.3.1	Generalized <i>QR</i> Factorization	33
2.3.3.2	Generalized <i>RQ</i> factorization	34
2.3.4	Symmetric Eigenproblems	36

2.3.5	Nonsymmetric Eigenproblems . . . . .	39
2.3.5.1	Eigenvalues, Eigenvectors and Schur Factorization . . . . .	39
2.3.5.2	Balancing . . . . .	39
2.3.5.3	Invariant Subspaces and Condition Numbers . . . . .	40
2.3.6	Singular Value Decomposition . . . . .	41
2.3.7	Generalized Symmetric Definite Eigenproblems . . . . .	43
2.3.8	Generalized Nonsymmetric Eigenproblems . . . . .	45
2.3.9	Generalized (or Quotient) Singular Value Decomposition . . . . .	47
<b>3</b>	<b>Performance of LAPACK</b> . . . . .	<b>48</b>
3.1	Factors that Affect Performance . . . . .	48
3.1.1	Vectorization . . . . .	49
3.1.2	Data Movement . . . . .	49
3.1.3	Parallelism . . . . .	49
3.2	The BLAS as the Key to Portability . . . . .	49
3.3	Block Algorithms and their Derivation . . . . .	50
3.4	Examples of Block Algorithms in LAPACK . . . . .	53
3.4.1	Factorizations for Solving Linear Equations . . . . .	54
3.4.2	<i>QR</i> Factorization . . . . .	55
3.4.3	Eigenvalue Problems . . . . .	55
3.5	LAPACK Benchmark . . . . .	58
<b>4</b>	<b>Accuracy and Stability</b> . . . . .	<b>65</b>
4.1	Sources of Error in Numerical Calculations . . . . .	66
4.1.1	Further Details: Floating point arithmetic . . . . .	66
4.2	How to Measure Errors . . . . .	68
4.2.1	Further Details: How to Measure Errors . . . . .	71
4.3	Further Details: How Error Bounds Are Derived . . . . .	73
4.3.1	Standard Error Analysis . . . . .	73
4.3.2	Improved Error Bounds . . . . .	74

4.4	Error Bounds for Linear Equation Solving . . . . .	75
4.4.1	Further Details: Error Bounds for Linear Equation Solving . . . . .	77
4.5	Error Bounds for Linear Least Squares Problems . . . . .	78
4.5.1	Further Details: Error Bounds for Linear Least Squares Problems . . . . .	80
4.6	Error Bounds for Generalized Least Squares Problems . . . . .	81
4.7	Error Bounds for the Symmetric Eigenproblem . . . . .	82
4.7.1	Further Details: Error Bounds for the Symmetric Eigenproblem . . . . .	83
4.8	Error Bounds for the Nonsymmetric Eigenproblem . . . . .	84
4.8.1	Further Details: Error Bounds for the Nonsymmetric Eigenproblem . . . . .	85
4.8.1.1	Overview . . . . .	85
4.8.1.2	Balancing and Conditioning . . . . .	88
4.8.1.3	Computing $s$ and $\text{sep}$ . . . . .	89
4.9	Error Bounds for the Singular Value Decomposition . . . . .	90
4.9.1	Further Details: Error Bounds for the Singular Value Decomposition . . . . .	91
4.10	Error Bounds for the Generalized Symmetric Definite Eigenproblem . . . . .	93
4.10.1	Further Details: Error Bounds for the Generalized Symmetric Definite Eigenproblem . . . . .	96
4.11	Error Bounds for the Generalized Nonsymmetric Eigenproblem . . . . .	98
4.12	Error Bounds for the Generalized Singular Value Decomposition . . . . .	98
4.12.1	Further Details: Error Bounds for the Generalized Singular Value Decomposition . . . . .	100
4.13	Error Bounds for Fast Level 3 BLAS . . . . .	101
<b>5</b>	<b>Documentation and Software Conventions</b> . . . . .	<b>102</b>
5.1	Design and Documentation of Argument Lists . . . . .	102
5.1.1	Structure of the Documentation . . . . .	102
5.1.2	Order of Arguments . . . . .	102
5.1.3	Argument Descriptions . . . . .	103
5.1.4	Option Arguments . . . . .	104
5.1.5	Problem Dimensions . . . . .	104
5.1.6	Array Arguments . . . . .	104

5.1.7	Work Arrays	105
5.1.8	Error Handling and the Diagnostic Argument INFO	105
5.2	Determining the Block Size for Block Algorithms	106
5.3	Matrix Storage Schemes	107
5.3.1	Conventional Storage	107
5.3.2	Packed Storage	108
5.3.3	Band Storage	109
5.3.4	Tridiagonal and Bidiagonal Matrices	110
5.3.5	Unit Triangular Matrices	110
5.3.6	Real Diagonal Elements of Complex Matrices	111
5.4	Representation of Orthogonal or Unitary Matrices	111
<b>6</b>	<b>Installing LAPACK Routines</b>	<b>113</b>
6.1	Points to Note	113
6.2	Installing ILAENV	114
<b>7</b>	<b>Troubleshooting</b>	<b>117</b>
7.1	Common Errors in Calling LAPACK Routines	117
7.2	Failures Detected by LAPACK Routines	117
7.2.1	Invalid Arguments and XERBLA	118
7.2.2	Computational Failures and INFO > 0	118
7.3	Wrong Results	119
7.4	Poor Performance	119
<b>A</b>	<b>Index of Driver and Computational Routines</b>	<b>121</b>
<b>B</b>	<b>Index of Auxiliary Routines</b>	<b>132</b>
<b>C</b>	<b>Quick Reference Guide to the BLAS</b>	<b>140</b>
<b>D</b>	<b>Converting from LINPACK or EISPACK</b>	<b>145</b>
<b>E</b>	<b>LAPACK Working Notes</b>	<b>154</b>

<b>2 Specifications of Routines</b>	<b>161</b>
<b>Bibliography</b>	<b>305</b>
<b>Index by Keyword</b>	<b>311</b>
<b>Index by Routine Name</b>	<b>316</b>