

Matrix Algorithms

Volume II: Eigensystems

G. W. Stewart

University of Maryland
College Park, Maryland

siam

Society for Industrial and Applied Mathematics
Philadelphia

CONTENTS

Algorithms	xv
Preface	xvii
1 Eigensystems	1
1 The Algebra of Eigensystems	1
1.1 Eigenvalues and eigenvectors	2
Definitions. Existence of eigenpairs: Special cases. The characteristic equation and the existence of eigenpairs. Matrices of order two. Block triangular matrices. Real matrices.	
1.2 Geometric multiplicity and defective matrices	6
Geometric multiplicity. Defectiveness. Simple eigenvalues.	
1.3 Similarity transformations	8
1.4 Schur Decompositions	10
Unitary similarities. Schur form. Nilpotent matrices. Hermitian matrices. Normal matrices.	
1.5 Block diagonalization and Sylvester's equation	15
From block triangular to block diagonal matrices. Sylvester's equation. An algorithm. Block diagonalization redux.	
1.6 Jordan form	20
1.7 Notes and references	22
General references. History and Nomenclature. Schur form. Sylvester's equation. Block diagonalization. Jordan canonical form.	
2 Norms, Spectral Radii, and Matrix Powers	25
2.1 Matrix and vector norms	25
Definition. Examples of norms. Operator norms. Norms and rounding error. Limitations of norms. Consistency. Norms and convergence.	
2.2 The spectral radius	30
Definition. Norms and the spectral radius.	
2.3 Matrix powers	33
Asymptotic bounds. Limitations of the bounds.	

2.4	Notes and references	36
	Norms. Norms and the spectral radius. Matrix powers.	
3	Perturbation Theory	37
3.1	The perturbation of eigenvalues	37
	The continuity of eigenvalues. Gerschgorin theory. Hermitian matrices.	
3.2	Simple eigenpairs	44
	Left and right eigenvectors. First-order perturbation expansions. Rigorous bounds. Qualitative statements. The condition of an eigenvalue. The condition of an eigenvector. Properties of sep. Hermitian matrices.	
3.3	Notes and references	52
	General references. Continuity of eigenvalues. Gerschgorin theory. Eigenvalues of Hermitian matrices. Simple eigenpairs. Left and right eigenvectors. First-order perturbation expansions. Rigorous bounds. Condition numbers. Sep. Relative and structured perturbation theory.	
2	The QR Algorithm	55
1	The Power and Inverse Power Methods	56
1.1	The power method	56
	Convergence. Computation and normalization. Choice of a starting vector. Convergence criteria and the residual. Optimal residuals and the Rayleigh quotient. Shifts and spectral enhancement. Implementation. The effects of rounding error. Assessment of the power method.	
1.2	The inverse power method	66
	Shift-and-invert enhancement. The inverse power method. An example. The effects of rounding error. The Rayleigh quotient method.	
1.3	Notes and references	69
	The power method. Residuals and backward error. The Rayleigh quotient. Shift of origin. The inverse power and Rayleigh quotient methods.	
2	The Explicitly Shifted QR Algorithm	71
2.1	The QR algorithm and the inverse power method	72
	Schur from the bottom up. The QR choice. Error bounds. Rates of convergence. General comments on convergence.	
2.2	The unshifted QR algorithm	76
	The QR decomposition of a matrix polynomial. The QR algorithm and the power method. Convergence of the unshifted QR algorithm.	
2.3	Hessenberg form	80

	Householder transformations. Reduction to Hessenberg form.	
	Plane rotations. Invariance of Hessenberg form.	
2.4	The explicitly shifted algorithm	94
	Detecting negligible subdiagonals. Deflation. Back searching.	
	The Wilkinson shift. Reduction to Schur form. Eigenvectors.	
2.5	Bits and pieces	105
	Ad hoc shifts. Aggressive deflation. Cheap eigenvalues.	
	Balancing. Graded matrices.	
2.6	Notes and references	111
	Historical. Variants of the QR algorithm. The QR algorithm, the	
	inverse power method, and the power method. Local	
	convergence. Householder transformations and plane rotations.	
	Hessenberg form. The Hessenberg QR algorithm. Deflation	
	criteria. The Wilkinson shift. Aggressive deflation.	
	Preprocessing. Graded matrices.	
3	The Implicitly Shifted QR Algorithm	114
3.1	Real Schur form	115
	Real Schur form. A preliminary algorithm.	
3.2	The uniqueness of Hessenberg reduction	117
3.3	The implicit double shift	119
	A general strategy. Getting started. Reduction back to Hessenberg	
	form. Deflation. Computing the real Schur form. Eigenvectors.	
3.4	Notes and references	129
	Implicit shifting. Processing 2×2 blocks. The multishifted QR	
	algorithm.	
4	The Generalized Eigenvalue Problem	130
4.1	The theoretical background	131
	Definitions. Regular pencils and infinite eigenvalues. Equivalence	
	transformations. Generalized Schur form. Multiplicity of	
	eigenvalues. Projective representation of eigenvalues.	
	Generalized shifting. Left and right eigenvectors of a simple	
	eigenvalue. Perturbation theory. First-order expansions:	
	Eigenvalues. The chordal metric. The condition of an eigenvalue.	
	Perturbation expansions: Eigenvectors. The condition of an	
	eigenvector.	
4.2	Real Schur and Hessenberg-triangular forms	144
	Generalized real Schur form. Hessenberg-triangular form.	
4.3	The doubly shifted QZ algorithm	148
	Overview. Getting started. The QZ step.	
4.4	Important miscellanea	153
	Balancing. Back searching. Infinite eigenvalues. The 2×2	
	problem. Eigenvectors.	

4.5	Notes and References	156
	The algebraic background. Perturbation theory. The QZ algorithm.	
3	The Symmetric Eigenvalue Problem	159
1	The QR Algorithm	160
1.1	Reduction to tridiagonal form	160
	The storage of symmetric matrices. Reduction to tridiagonal form. Making Hermitian tridiagonal matrices real.	
1.2	The symmetric tridiagonal QR algorithm	165
	The implicitly shifted QR step. Choice of shift. Local convergence. Deflation. Graded matrices. Variations.	
1.3	Notes and references	171
	General references. Reduction to tridiagonal form. The tridiagonal QR algorithm.	
2	A Clutch of Algorithms	173
2.1	Rank-one updating	173
	Reduction to standard form. Deflation: Small components of z . Deflation: Nearly equal d_i . When to deflate. The secular equation. Solving the secular equation. Computing eigenvectors. Concluding comments.	
2.2	A Divide-and-conquer algorithm	183
	Generalities. Derivation of the algorithm. Complexity.	
2.3	Eigenvalues and eigenvectors of band matrices	188
	The storage of band matrices. Tridiagonalization of a symmetric band matrix. Inertia. Inertia and the LU decomposition. The inertia of a tridiagonal matrix. Calculation of a selected eigenvalue. Selected eigenvectors.	
2.4	Notes and References	203
	Updating the spectral decomposition. The divide-and-conquer algorithm. Reduction to tridiagonal form. Inertia and bisection. Eigenvectors by the inverse power method. Jacobi's method.	
3	The Singular Value Decomposition	206
3.1	Background	206
	Existence and nomenclature. Uniqueness. Relation to the spectral decomposition. Characterization and perturbation of singular values. First-order perturbation expansions. The condition of singular vectors.	
3.2	The cross-product algorithm	213
	Inaccurate singular values. Inaccurate right singular vectors. Inaccurate left singular vectors. Assessment of the algorithm.	
3.3	Reduction to bidiagonal form	217
	The reduction. Real bidiagonal form.	

3.4	The QR algorithm	220
	The bidiagonal QR step. Computing the shift. Negligible superdiagonal elements. Back searching. Final comments.	
3.5	A hybrid QRD-SVD algorithm	228
3.6	Notes and references	228
	The singular value decomposition. Perturbation theory. The cross-product algorithm. Reduction to bidiagonal form and the QR algorithm. The QRD-SVD algorithm. The differential qd algorithm. Divide-and-conquer algorithms. Downdating a singular value decomposition. Jacobi methods.	
4	The Symmetric Positive Definite (S/PD) Generalized Eigenvalue Problem	231
4.1	Theory	231
	The fundamental theorem. Condition of eigenvalues.	
4.2	Wilkinson's algorithm	233
	The algorithm. Computation of $R^{-T}AR^{-1}$. Ill-conditioned B .	
4.3	Notes and references	237
	Perturbation theory. Wilkinson's algorithm. Band matrices. The definite generalized eigenvalue problem. The generalized singular value and CS decompositions.	
4	Eigenspaces and Their Approximation	241
1	Eigenspaces	242
1.1	Definitions	242
	Eigenbases. Existence of eigenspaces. Deflation.	
1.2	Simple eigenspaces	246
	Definition. Block diagonalization and spectral representations. Uniqueness of simple eigenspaces.	
1.3	Notes and references	249
	Eigenspaces. Spectral projections. Uniqueness of simple eigenspaces. The resolvent.	
2	Perturbation Theory	250
2.1	Canonical angles	250
	Definitions. Computing canonical angles. Subspaces of unequal dimensions. Combinations of subspaces.	
2.2	Residual analysis	253
	Optimal residuals. The Rayleigh quotient. Backward error. Residual bounds for eigenvalues of Hermitian matrices. Block deflation. The quantity sep. Residual bounds.	
2.3	Perturbation theory	260
	The perturbation theorem. Choice of subspaces. Bounds in terms of E . The Rayleigh quotient and the condition of L . Angles between the subspaces.	
2.4	Residual bounds for Hermitian matrices	264

	Residual bounds for eigenspaces. Residual bounds for eigenvalues.	
2.5	Notes and references	266
	General references. Canonical angle. Optimal residuals and the Rayleigh quotient. Backward error. Residual eigenvalue bounds for Hermitian matrices. Block deflation and residual bounds. Perturbation theory. Residual bounds for eigenspaces and eigenvalues of Hermitian matrices.	
3	Krylov Subspaces	268
3.1	Krylov sequences and Krylov spaces	268
	Introduction and definition. Elementary properties. The polynomial connection. Termination.	
3.2	Convergence	271
	The general approach. Chebyshev polynomials. Convergence redux. Multiple eigenvalues. Assessment of the bounds. Non-Hermitian matrices.	
3.3	Block Krylov sequences	279
3.4	Notes and references	281
	Sources. Krylov sequences. Convergence (Hermitian matrices). Convergence (non-Hermitian matrices). Block Krylov sequences.	
4	Rayleigh–Ritz Approximation	282
4.1	Rayleigh–Ritz methods	283
	Two difficulties. Rayleigh–Ritz and generalized eigenvalue problems. The orthogonal Rayleigh–Ritz procedure.	
4.2	Convergence	286
	Setting the scene. Convergence of the Ritz value. Convergence of Ritz vectors. Convergence of Ritz values revisited. Hermitian matrices. Convergence of Ritz blocks and bases. Residuals and convergence.	
4.3	Refined Ritz vectors	291
	Definition. Convergence of refined Ritz vectors. The computation of refined Ritz vectors.	
4.4	Harmonic Ritz vectors	294
	Computation of harmonic Ritz pairs.	
4.5	Notes and references	297
	Historical. Convergence. Refined Ritz vectors. Harmonic Ritz vectors.	
5	Krylov Sequence Methods	301
1	Krylov Decompositions	301
1.1	Arnoldi decompositions	302
	The Arnoldi decomposition. Uniqueness. The Rayleigh quotient. Reduced Arnoldi decompositions. Computing Arnoldi	

	decompositions. Reorthogonalization. Practical considerations. Orthogonalization and shift-and-invert enhancement.	
1.2	Lanczos decompositions	310
	Lanczos decompositions. The Lanczos recurrence.	
1.3	Krylov decompositions	313
	Definition. Similarity transformations. Translation. Equivalence to an Arnoldi decomposition. Reduction to Arnoldi form.	
1.4	Computation of refined and Harmonic Ritz vectors	317
	Refined Ritz vectors. Harmonic Ritz vectors.	
1.5	Notes and references	319
	Lanczos and Arnoldi. Shift-and-invert enhancement and orthogonalization. Krylov decompositions.	
2	The Restarted Arnoldi Method	320
2.1	The implicitly restarted Arnoldi method	321
	Filter polynomials. Implicitly restarted Arnoldi. Implementation. The restarted Arnoldi cycle. Exact shifts. Forward instability.	
2.2	Krylov–Schur restarting	330
	Exchanging eigenvalues and eigenblocks. The Krylov–Schur cycle. The equivalence of Arnoldi and Krylov–Schur. Comparison of the methods.	
2.3	Stability, convergence, and deflation	337
	Stability. Stability and shift-and-invert enhancement. Convergence criteria. Convergence with shift-and-invert enhancement. Deflation. Stability of deflation. Nonorthogonal bases. Deflation in the Krylov–Schur method. Deflation in an Arnoldi decomposition. Choice of tolerance.	
2.4	Rational Krylov Transformations	347
	Krylov sequences, inverses, and shifts. The rational Krylov method.	
2.5	Notes and references	349
	Arnoldi’s method, restarting, and filter polynomials. ARPACK. Reverse communication. Exchanging eigenvalues. Forward instability. The Krylov–Schur method. Stability. Shift-and-invert enhancement and the Rayleigh quotient. Convergence. Deflation. The rational Krylov transformation.	
3	The Lanczos Algorithm	352
3.1	Reorthogonalization and the Lanczos algorithm	354
	Lanczos with reorthogonalization.	
3.2	Full reorthogonalization and restarting	356
	Implicit restarting. Krylov-spectral restarting. Convergence and deflation.	
3.3	Semiorthogonal methods	358

	Semiorthogonal bases. The QR factorization of a semiorthogonal basis. The size of the reorthogonalization coefficients. The effects on the Rayleigh quotient. The effects on the Ritz vectors. Estimating the loss of orthogonality. Periodic reorthogonalization. Updating $\mathbf{H}_k$. Computing residual norms. An example.	
3.4	Notes and references	370
	The Lanczos algorithm. Full reorthogonalization. Filter polynomials. Semiorthogonal methods. No reorthogonalization. The singular value decomposition. Block Lanczos algorithms. The bi-Lanczos algorithm.	
4	The Generalized Eigenvalue Problem	372
4.1	Transformation and convergence	373
	Transformation to an ordinary eigenproblem. Residuals and backward error. Bounding the residual.	
4.2	Positive definite $\mathbf{B}$	375
	The $\mathbf{B}$ inner product. Orthogonality. $\mathbf{B}$ -Orthogonalization. The $\mathbf{B}$ -Arnoldi method. The restarted $\mathbf{B}$ -Lanczos method. The $\mathbf{B}$ -Lanczos method with periodic reorthogonalization. Semidefinite $\mathbf{B}$.	
4.3	Notes and references	384
	The generalized shift-and-invert transformation and the Lanczos algorithm. Residuals and backward error. Semidefinite $\mathbf{B}$.	
6	Alternatives	387
1	Subspace Iteration	387
1.1	Theory	388
	Convergence. The QR connection. Schur–Rayleigh–Ritz refinement.	
1.2	Implementation	392
	A general algorithm. Convergence. Deflation. When to perform an SRR step. When to orthogonalize. Real matrices.	
1.3	Symmetric matrices	397
	Economization of storage. Chebyshev acceleration.	
1.4	Notes and references	400
	Subspace iteration. Chebyshev acceleration. Software.	
2	Newton-Based Methods	401
2.1	Approximate Newton methods	402
	A general approximate Newton method. The correction equation. Orthogonal corrections. Analysis. Local convergence. Three approximations.	
2.2	The Jacobi–Davidson method	410
	The basic Jacobi–Davidson method. Extending Schur decompositions. Restarting. Harmonic Ritz vectors. Hermitian	

matrices. Solving projected systems. The correction equation: Exact solution. The correction equation: Iterative solution.	
2.3 Notes and references	424
Newton's method and the eigenvalue problem. Inexact Newton methods. The Jacobi–Davidson method. Hermitian matrices.	
Appendix: Background	427
1 Scalars, vectors, and matrices	427
2 Linear algebra	430
3 Positive definite matrices	431
4 The LU decomposition	431
5 The Cholesky decomposition	432
6 The QR decomposition	432
7 Projectors	433
References	435
Index	457

ALGORITHMS

Chapter 1. Eigensystems

1.1 Solution of Sylvester's Equation	18
--	----

Chapter 2. The QR Algorithm

1.1 The shifted power method	64
1.2 The inverse power method	67
2.1 Generation of Householder transformations	82
2.2 Reduction to upper Hessenberg form	85
2.3 Generation of a plane rotation	89
2.4 Application of a plane rotation	90
2.5 Basic QR step for a Hessenberg matrix	93
2.6 Finding deflation rows in an upper Hessenberg matrix	97
2.7 Computation of the Wilkinson shift	99
2.8 Schur form of an upper Hessenberg matrix	100
2.9 Right eigenvectors of an upper triangular matrix	104
3.1 Starting an implicit QR double shift	121
3.2 Doubly shifted QR step	123
3.3 Finding deflation rows in a real upper Hessenberg matrix	125
3.4 Real Schur form of a real upper Hessenberg matrix	126
4.1 Reduction to Hessenberg-triangular form	147
4.2 The doubly shifted QZ step	152

Chapter 3. The Symmetric Eigenvalue Problem

1.1 Reduction to tridiagonal form	163
1.2 Hermitian tridiagonal to real tridiagonal form	166
1.3 The symmetric tridiagonal QR step	168
2.1 Rank-one update of the spectral decomposition	174
2.2 Eigenvectors of a rank-one update	182
2.3 Divide-and-conquer eigensystem of a symmetric tridiagonal matrix	186
2.4 Counting left eigenvalues	195
2.5 Finding a specified eigenvalue	197
2.6 Computation of selected eigenvectors	202
3.1 The cross-product algorithm	213
3.2 Reduction to bidiagonal form	219

3.3	Complex bidiagonal to real bidiagonal form	220
3.4	Bidiagonal QR step	223
3.5	Back searching a bidiagonal matrix	227
3.6	Hybrid QR-SVD algorithm	228
4.1	Solution of the S/PD generalized eigenvalue problem	234
4.2	The computation of $C = R^{-T}AR^{-1}$	236
Chapter 5. Krylov Sequence Methods		
1.1	The Arnoldi step	308
1.2	The Lanczos recurrence	312
1.3	Krylov decomposition to Arnoldi decomposition	318
2.1	Filtering an Arnoldi decomposition	326
2.2	The restarted Arnoldi cycle	327
2.3	The Krylov–Schur cycle	335
2.4	Deflating in a Krylov–Schur decomposition	346
2.5	The rational Krylov transformation	349
3.1	Lanczos procedure with orthogonalization	355
3.2	Estimation of $u_{k+1}^T u_j$	363
3.3	Periodic orthogonalization I: Outer loop	365
3.4	Periodic reorthogonalization II: Orthogonalization step	366
Chapter 6. Alternatives		
1.1	Subspace iteration	393
2.1	The basic Jacobi–Davidson algorithm	411
2.2	Extending a partial Schur decomposition	416
2.3	Harmonic extension of a partial Schur decomposition	419
2.4	Solution of projected equations	421
2.5	Davidson’s method	426