



Numerical Methods for Large Eigenvalue Problems

REVISED EDITION



Yousef Saad

University of Minnesota
Twin Cities

siam.

Society for Industrial and Applied Mathematics
Philadelphia

Contents

Preface to the Classics Edition	xiii
Preface	xv
1 Background in Matrix Theory and Linear Algebra	1
1.1 Matrices	1
1.2 Square Matrices and Eigenvalues	2
1.3 Types of Matrices	4
1.3.1 Matrices with Special Structures	4
1.3.2 Special Matrices	5
1.4 Vector Inner Products and Norms	6
1.5 Matrix Norms	8
1.6 Subspaces	9
1.7 Orthogonal Vectors and Subspaces	11
1.8 Canonical Forms of Matrices	12
1.8.1 Reduction to the Diagonal Form	14
1.8.2 The Jordan Canonical Form	14
1.8.3 The Schur Canonical Form	18
1.9 Normal and Hermitian Matrices	21
1.9.1 Normal Matrices	21
1.9.2 Hermitian Matrices	23
1.10 Nonnegative Matrices	25
2 Sparse Matrices	29
2.1 Introduction	29
2.2 Storage Schemes	30
2.3 Basic Sparse Matrix Operations	34
2.4 Sparse Direct Solution Methods	35
2.5 Test Problems	36
2.5.1 Random Walk Problem	36
2.5.2 Chemical Reactions	38
2.5.3 The Harwell-Boeing Collection	40
2.6 SPARSKIT	40
2.7 The New Sparse Matrix Repositories	43

2.8	Sparse Matrices in MATLAB	43
3	Perturbation Theory and Error Analysis	47
3.1	Projectors and their Properties	47
3.1.1	Orthogonal Projectors	48
3.1.2	Oblique Projectors	50
3.1.3	Resolvent and Spectral Projector	51
3.1.4	Relations with the Jordan form	53
3.1.5	Linear Perturbations of A	55
3.2	A-Posteriori Error Bounds	59
3.2.1	General Error Bounds	59
3.2.2	The Hermitian Case	61
3.2.3	The Kahan-Parlett-Jiang Theorem	66
3.3	Conditioning of Eigen-problems	70
3.3.1	Conditioning of Eigenvalues	70
3.3.2	Conditioning of Eigenvectors	72
3.3.3	Conditioning of Invariant Subspaces	75
3.4	Localization Theorems	77
3.5	Pseudo-eigenvalues	79
4	The Tools of Spectral Approximation	85
4.1	Single Vector Iterations	85
4.1.1	The Power Method	85
4.1.2	The Shifted Power Method	88
4.1.3	Inverse Iteration	88
4.2	Deflation Techniques	90
4.2.1	Wielandt Deflation with One Vector	91
4.2.2	Optimality in Wielandt's Deflation	92
4.2.3	Deflation with Several Vectors.	94
4.2.4	Partial Schur Decomposition.	95
4.2.5	Practical Deflation Procedures	96
4.3	General Projection Methods	96
4.3.1	Orthogonal Projection Methods	97
4.3.2	The Hermitian Case	100
4.3.3	Oblique Projection Methods	106
4.4	Chebyshev Polynomials	108
4.4.1	Real Chebyshev Polynomials	108
4.4.2	Complex Chebyshev Polynomials	109
5	Subspace Iteration	115
5.1	Simple Subspace Iteration	115
5.2	Subspace Iteration with Projection	118
5.3	Practical Implementations	121
5.3.1	Locking	121
5.3.2	Linear Shifts	123

5.3.3	Preconditioning	123
6	Krylov Subspace Methods	125
6.1	Krylov Subspaces	125
6.2	Arnoldi's Method	128
6.2.1	The Basic Algorithm	128
6.2.2	Practical Implementations	131
6.2.3	Incorporation of Implicit Deflation	134
6.3	The Hermitian Lanczos Algorithm	136
6.3.1	The Algorithm	137
6.3.2	Relation with Orthogonal Polynomials	138
6.4	Non-Hermitian Lanczos Algorithm	138
6.4.1	The Algorithm	139
6.4.2	Practical Implementations	143
6.5	Block Krylov Methods	145
6.6	Convergence of the Lanczos Process	147
6.6.1	Distance between $\mathcal{K}_m$ and an Eigenvector	147
6.6.2	Convergence of the Eigenvalues	149
6.6.3	Convergence of the Eigenvectors	150
6.7	Convergence of the Arnoldi Process	151
7	Filtering and Restarting Techniques	163
7.1	Polynomial Filtering	163
7.2	Explicitly Restarted Arnoldi's Method	165
7.3	Implicitly Restarted Arnoldi's Method	166
7.3.1	Which Filter Polynomials?	169
7.4	Chebyshev Iteration	169
7.4.1	Convergence Properties.	173
7.4.2	Computing an Optimal Ellipse	174
7.5	Chebyshev Subspace Iteration	177
7.5.1	Getting the Best Ellipse.	178
7.5.2	Parameters k and m	178
7.5.3	Deflation	178
7.6	Least Squares - Arnoldi	179
7.6.1	The Least Squares Polynomial	179
7.6.2	Use of Chebyshev Bases	181
7.6.3	The Gram Matrix	182
7.6.4	Computing the Best Polynomial	184
7.6.5	Least Squares Arnoldi Algorithms	188
8	Preconditioning Techniques	193
8.1	Shift-and-invert Preconditioning	193
8.1.1	General Concepts	194
8.1.2	Dealing with Complex Arithmetic	195
8.1.3	Shift-and-Invert Arnoldi	197

8.2	Polynomial Preconditioning	200
8.3	Davidson's Method	203
8.4	The Jacobi-Davidson approach	206
8.4.1	Olsen's Method	206
8.4.2	Connection with Newton's Method	207
8.4.3	The Jacobi-Davidson Approach	208
8.5	The CMS – AMLS connection	209
8.5.1	AMLS and the Correction Equation	212
8.5.2	Spectral Schur Complements	213
8.5.3	The Projection Viewpoint	215
9	Non-Standard Eigenvalue Problems	219
9.1	Introduction	219
9.2	Generalized Eigenvalue Problems	220
9.2.1	General Results	220
9.2.2	Reduction to Standard Form	225
9.2.3	Deflation	226
9.2.4	Shift-and-Invert	227
9.2.5	Projection Methods	228
9.2.6	The Hermitian Definite Case	229
9.3	Quadratic Problems	231
9.3.1	From Quadratic to Generalized Problems	232
10	Origins of Matrix Eigenvalue Problems	235
10.1	Introduction	235
10.2	Mechanical Vibrations	236
10.3	Electrical Networks.	241
10.4	Electronic Structure Calculations	242
10.4.1	Quantum descriptions of matter	242
10.4.2	The Hartree approximation	244
10.4.3	The Hartree-Fock approximation	246
10.4.4	Density Functional Theory	248
10.4.5	The Kohn-Sham equation	250
10.4.6	Pseudopotentials	250
10.5	Stability of Dynamical Systems	251
10.6	Bifurcation Analysis	252
10.7	Chemical Reactions	253
10.8	Macro-economics	254
10.9	Markov Chain Models	255
	Bibliography	259
	Index	271