

Functions of Matrices: Theory and Computation

Higham, Nicholas J.

2008

MIMS EPrint: **2008.39**

Manchester Institute for Mathematical Sciences
School of Mathematics

The University of Manchester

Reports available from: <http://eprints.maths.manchester.ac.uk/>

And by contacting: The MIMS Secretary
School of Mathematics
The University of Manchester
Manchester, M13 9PL, UK

ISSN 1749-9097

Contents

List of Figures	xiii
List of Tables	xv
Preface	xvii
1 Theory of Matrix Functions	1
1.1 Introduction	1
1.2 Definitions of $f(A)$	2
1.2.1 Jordan Canonical Form	2
1.2.2 Polynomial Interpolation	4
1.2.3 Cauchy Integral Theorem	7
1.2.4 Equivalence of Definitions	8
1.2.5 Example: Function of Identity Plus Rank-1 Matrix	8
1.2.6 Example: Function of Discrete Fourier Transform Matrix	10
1.3 Properties	10
1.4 Nonprimary Matrix Functions	14
1.5 Existence of (Real) Matrix Square Roots and Logarithms	16
1.6 Classification of Matrix Square Roots and Logarithms	17
1.7 Principal Square Root and Logarithm	20
1.8 $f(AB)$ and $f(BA)$	21
1.9 Miscellany	23
1.10 A Brief History of Matrix Functions	26
1.11 Notes and References	27
Problems	29
2 Applications	35
2.1 Differential Equations	35
2.1.1 Exponential Integrators	36
2.2 Nuclear Magnetic Resonance	37
2.3 Markov Models	37
2.4 Control Theory	39
2.5 The Nonsymmetric Eigenvalue Problem	41
2.6 Orthogonalization and the Orthogonal Procrustes Problem	42
2.7 Theoretical Particle Physics	43
2.8 Other Matrix Functions	44
2.9 Nonlinear Matrix Equations	44
2.10 Geometric Mean	46
2.11 Pseudospectra	47
2.12 Algebras	47

2.13	Sensitivity Analysis	48
2.14	Other Applications	48
2.14.1	Boundary Value Problems	48
2.14.2	Semidefinite Programming	48
2.14.3	Matrix Sector Function	48
2.14.4	Matrix Disk Function	49
2.14.5	The Average Eye in Optics	50
2.14.6	Computer Graphics	50
2.14.7	Bregman Divergences	50
2.14.8	Structured Matrix Interpolation	50
2.14.9	The Lambert W Function and Delay Differential Equations .	51
2.15	Notes and References	51
	Problems	52
3	Conditioning	55
3.1	Condition Numbers	55
3.2	Properties of the Fréchet Derivative	57
3.3	Bounding the Condition Number	63
3.4	Computing or Estimating the Condition Number	64
3.5	Notes and References	69
	Problems	70
4	Techniques for General Functions	71
4.1	Matrix Powers	71
4.2	Polynomial Evaluation	72
4.3	Taylor Series	76
4.4	Rational Approximation	78
4.4.1	Best L_∞ Approximation	79
4.4.2	Padé Approximation	79
4.4.3	Evaluating Rational Functions	80
4.5	Diagonalization	81
4.6	Schur Decomposition and Triangular Matrices	84
4.7	Block Diagonalization	89
4.8	Interpolating Polynomial and Characteristic Polynomial	89
4.9	Matrix Iterations	91
4.9.1	Order of Convergence	91
4.9.2	Termination Criteria	92
4.9.3	Convergence	93
4.9.4	Numerical Stability	95
4.10	Preprocessing	99
4.11	Bounds for $\ f(A)\ $	102
4.12	Notes and References	104
	Problems	105
5	Matrix Sign Function	107
5.1	Sensitivity and Conditioning	109
5.2	Schur Method	112
5.3	Newton's Method	113
5.4	The Padé Family of Iterations	115
5.5	Scaling the Newton Iteration	119

5.6	Terminating the Iterations	121
5.7	Numerical Stability of Sign Iterations	123
5.8	Numerical Experiments and Algorithm	125
5.9	Best L_∞ Approximation	128
5.10	Notes and References	129
	Problems	131
6	Matrix Square Root	133
6.1	Sensitivity and Conditioning	133
6.2	Schur Method	135
6.3	Newton's Method and Its Variants	139
6.4	Stability and Limiting Accuracy	144
6.4.1	Newton Iteration	144
6.4.2	DB Iterations	145
6.4.3	CR Iteration	146
6.4.4	IN Iteration	146
6.4.5	Summary	147
6.5	Scaling the Newton Iteration	147
6.6	Numerical Experiments	148
6.7	Iterations via the Matrix Sign Function	152
6.8	Special Matrices	154
6.8.1	Binomial Iteration	154
6.8.2	Modified Newton Iterations	157
6.8.3	M -Matrices and H -Matrices	159
6.8.4	Hermitian Positive Definite Matrices	161
6.9	Computing Small-Normed Square Roots	162
6.10	Comparison of Methods	164
6.11	Involutory Matrices	165
6.12	Notes and References	166
	Problems	168
7	Matrix pth Root	173
7.1	Theory	173
7.2	Schur Method	175
7.3	Newton's Method	177
7.4	Inverse Newton Method	181
7.5	Schur–Newton Algorithm	184
7.6	Matrix Sign Method	186
7.7	Notes and References	187
	Problems	189
8	The Polar Decomposition	193
8.1	Approximation Properties	197
8.2	Sensitivity and Conditioning	199
8.3	Newton's Method	202
8.4	Obtaining Iterations via the Matrix Sign Function	202
8.5	The Padé Family of Methods	203
8.6	Scaling the Newton Iteration	205
8.7	Terminating the Iterations	207
8.8	Numerical Stability and Choice of H	209

8.9	Algorithm	210
8.10	Notes and References	213
	Problems	216
9	Schur–Parlett Algorithm	221
9.1	Evaluating Functions of the Atomic Blocks	221
9.2	Evaluating the Upper Triangular Part of $f(T)$	225
9.3	Reordering and Blocking the Schur Form	226
9.4	Schur–Parlett Algorithm for $f(A)$	228
9.5	Preprocessing	230
9.6	Notes and References	231
	Problems	231
10	Matrix Exponential	233
10.1	Basic Properties	233
10.2	Conditioning	238
10.3	Scaling and Squaring Method	241
10.4	Schur Algorithms	250
	10.4.1 Newton Divided Difference Interpolation	250
	10.4.2 Schur–Fréchet Algorithm	251
	10.4.3 Schur–Parlett Algorithm	251
10.5	Numerical Experiment	252
10.6	Evaluating the Fréchet Derivative and Its Norm	253
	10.6.1 Quadrature	254
	10.6.2 The Kronecker Formulae	256
	10.6.3 Computing and Estimating the Norm	258
10.7	Miscellany	259
	10.7.1 Hermitian Matrices and Best L_∞ Approximation	259
	10.7.2 Essentially Nonnegative Matrices	260
	10.7.3 Preprocessing	261
	10.7.4 The ψ Functions	261
10.8	Notes and References	262
	Problems	265
11	Matrix Logarithm	269
11.1	Basic Properties	269
11.2	Conditioning	272
11.3	Series Expansions	273
11.4	Padé Approximation	274
11.5	Inverse Scaling and Squaring Method	275
	11.5.1 Schur Decomposition: Triangular Matrices	276
	11.5.2 Full Matrices	278
11.6	Schur Algorithms	279
	11.6.1 Schur–Fréchet Algorithm	279
	11.6.2 Schur–Parlett Algorithm	279
11.7	Numerical Experiment	280
11.8	Evaluating the Fréchet Derivative	281
11.9	Notes and References	283
	Problems	284

12 Matrix Cosine and Sine	287
12.1 Basic Properties	287
12.2 Conditioning	289
12.3 Padé Approximation of Cosine	290
12.4 Double Angle Algorithm for Cosine	290
12.5 Numerical Experiment	295
12.6 Double Angle Algorithm for Sine and Cosine	296
12.6.1 Preprocessing	299
12.7 Notes and References	299
Problems	300
13 Function of Matrix Times Vector: $f(A)b$	301
13.1 Representation via Polynomial Interpolation	301
13.2 Krylov Subspace Methods	302
13.2.1 The Arnoldi Process	302
13.2.2 Arnoldi Approximation of $f(A)b$	304
13.2.3 Lanczos Biorthogonalization	306
13.3 Quadrature	306
13.3.1 On the Real Line	306
13.3.2 Contour Integration	307
13.4 Differential Equations	308
13.5 Other Methods	309
13.6 Notes and References	309
Problems	310
14 Miscellany	313
14.1 Structured Matrices	313
14.1.1 Algebras and Groups	313
14.1.2 Monotone Functions	315
14.1.3 Other Structures	315
14.1.4 Data Sparse Representations	316
14.1.5 Computing Structured $f(A)$ for Structured A	316
14.2 Exponential Decay of Functions of Banded Matrices	317
14.3 Approximating Entries of Matrix Functions	318
A Notation	319
B Background: Definitions and Useful Facts	321
B.1 Basic Notation	321
B.2 Eigenvalues and Jordan Canonical Form	321
B.3 Invariant Subspaces	323
B.4 Special Classes of Matrices	323
B.5 Matrix Factorizations and Decompositions	324
B.6 Pseudoinverse and Orthogonality	325
B.6.1 Pseudoinverse	325
B.6.2 Projector and Orthogonal Projector	326
B.6.3 Partial Isometry	326
B.7 Norms	326
B.8 Matrix Sequences and Series	328
B.9 Perturbation Expansions for Matrix Inverse	328

B.10 Sherman–Morrison–Woodbury Formula	329
B.11 Nonnegative Matrices	329
B.12 Positive (Semi)definite Ordering	330
B.13 Kronecker Product and Sum	331
B.14 Sylvester Equation	331
B.15 Floating Point Arithmetic	331
B.16 Divided Differences	332
Problems	334
C Operation Counts	335
D Matrix Function Toolbox	339
E Solutions to Problems	343
Bibliography	379
Index	415