

# Functions of Matrices

Theory and Computation

Nicholas J. Higham

# Contents

List of Figures	xiii
List of Tables	xv
Preface	xvii
<b>1 Theory of Matrix Functions</b>	<b>1</b>
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
<b>2 Applications</b>	<b>35</b>
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
<b>3</b>	<b>Conditioning</b>	<b>55</b>
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
<b>4</b>	<b>Techniques for General Functions</b>	<b>71</b>
4.1	Matrix Powers . . . . .	71
4.2	Polynomial Evaluation . . . . .	72
4.3	Taylor Series . . . . .	76
4.4	Rational Approximation . . . . .	78
4.4.1	Best $L_\infty$ 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
<b>5</b>	<b>Matrix Sign Function</b>	<b>107</b>
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 $L_\infty$ Approximation . . . . .	128
5.10	Notes and References . . . . .	129
	Problems . . . . .	131
<b>6</b>	<b>Matrix Square Root</b>	<b>133</b>
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
<b>7</b>	<b>Matrix <math>p</math>th Root</b>	<b>173</b>
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
<b>8</b>	<b>The Polar Decomposition</b>	<b>193</b>
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
<b>9</b>	<b>Schur–Parlett Algorithm</b>	<b>221</b>
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
<b>10</b>	<b>Matrix Exponential</b>	<b>233</b>
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 $L_\infty$ Approximation . . . . .	259
	10.7.2 Essentially Nonnegative Matrices . . . . .	260
	10.7.3 Preprocessing . . . . .	261
	10.7.4 The $\psi$ Functions . . . . .	261
10.8	Notes and References . . . . .	262
	Problems . . . . .	265
<b>11</b>	<b>Matrix Logarithm</b>	<b>269</b>
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

<b>12 Matrix Cosine and Sine</b>	<b>287</b>
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
<b>13 Function of Matrix Times Vector: <math>f(A)b</math></b>	<b>301</b>
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
<b>14 Miscellany</b>	<b>313</b>
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
<b>A Notation</b>	<b>319</b>
<b>B Background: Definitions and Useful Facts</b>	<b>321</b>
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
<b>C Operation Counts</b>	<b>335</b>
<b>D Matrix Function Toolbox</b>	<b>339</b>
<b>E Solutions to Problems</b>	<b>343</b>
<b>Bibliography</b>	<b>379</b>
<b>Index</b>	<b>415</b>