Numerical Analysis A Mathematical Introduction

MICHELLE SCHATZMAN

Directeur de Recherche au CNRS Université Claude Bernard Lyon

Translated by
JOHN TAYLOR

Edinburgh Petroleum Services

CLARENDON PRESS · OXFORD 2002

Contents

Ι	\mathbf{Th}	e ent	rance fee	1	
1	Flo	ating r	numbers	3	
	1.1	Count	β in base β	3	
	1.2	Expar	nsion of the rational numbers in base β	5	
	1.3		nachine representation of numbers	5	
	1.4	Summ	nation of series in floating-point numbers	7	
	1.5	Even	the obvious problems are rotten	8	
	1.6	Even	the easy problems are hard	9	
	1.7	A floa	ting conclusion	10	
2	A f	lavour	of numerical analysis	11	
	2.1	Comp	arison of exponentials and powers	12	
	2.2	Conve	ergence and divergence of classic series	13	
	2.3	Discre	ete approximation of the logarithm	13	
	2.4	Comp	arison of means	16	
	2.5	Eleme	entary construction of the exponential	17	
	2.6	Expor	nentials of matrices	20	
3	Algebraic preliminaries				
	3.1		r algebra refresher	25	
		3.1.1	The matrix of a linear mapping	25	
		3.1.2	The determinant	27	
		3.1.3	The fundamental theorem of linear algebra and its		
		-	consequences	29	
		3.1.4	Eigenvalues and eigenvectors	30	
		3.1.5	1 , 0 , 1 0	31	
		3.1.6	Triangular matrices	34	
	3.2	Block	matrices	34	
		3.2.1	1	34	
		3.2.2		36	
	3.3	\mathbf{Exerc}	ises from Chapter 3	37	
		3.3.1	Elementary algebra	37	
		222	Block decomposition	38	

xii CONTENTS

		3.3.3	Graphs and matrices	39
		3.3.4	Functions of matrices	40
		3.3.5	Square roots, cosines, and sines of matrices	41
		3.3.6	Companion matrices and bounds of matrix powers	42
		3.3.7	The Kantorovich inequality	44
II	Pe	olyno	mial and trigonometric approximation	47
4	Inte	erpolat	ion and divided differences	51
	4.1	Lagra	nge interpolation	51
		4.1.1	The Lagrange interpolation problem	51
	4.2	Newto	on's interpolation	54
		4.2.1	Newton's basis is better than Lagrange's basis	54
		4.2.2	Integral representation of divided differences	57
	4.3	Interp	polation error	59
	4.4	Hermi	ite and osculating interpolation	64
	4.5	Divide	ed differences as operators	67
		4.5.1	Finite differences on uniform grids	70
	4.6	Exerc	ises from Chapter 4	72
		4.6.1	More on divided differences	72
		4.6.2	Boundary value problem for an ODE	74
		4.6.3	Extrapolation to the limit	75
5	Lea	_	ares approximation for polynomials	77
	5.1	Posing	g the problem	77
		5.1.1		77
		5.1.2	Is it really calculable?	80
	5.2		gonal polynomials	81
		5.2.1	Construction of orthogonal polynomials	82
		5.2.2	Examples of orthogonal polynomials	83
		5.2.3	Revival of special functions	87
		5.2.4	Orthogonal polynomials and least-squares	88
	5.3	Polyn	omial density: Bernstein polynomials	88
		5.3.1	Modulus of continuity	89
		5.3.2	Bernstein polynomials and Bernstein approximation	90
		5.3.3	Application of Bernstein polynomials to graphics software:	
			the Bézier curves	94
	5.4		-squares convergence	96
	5.5	-	tative properties	97
	5.6		ises from Chapter 5	99
		5.6.1	Laguerre polynomials	99
		5.6.2	Padé type and Padé approximations	101

ENTS	xiii
ENTS	

6	Spli	ines		106
	6.1	Natur	ral splines: the functional approach	107
		6.1.1	Weak equality of functions	107
		6.1.2	Weak integrals of functions	108
		6.1.3	The space of natural splines	110
>	6.2	Nume	erics for cubic natural splines	116
	6.3	Space	s of splines, B-splines	119
		6.3.1	Splines with distinct knots	119
		6.3.2	The beautiful properties of B-splines	120
		6.3.3	Numerics with B -splines	125
		6.3.4	Using B-splines to understand natural splines	127
		6.3.5	B-splines in CAGD	128
	6.4	Exerc	ises from Chapter 6	130
		6.4.1	Varied exercises on splines	130
		6.4.2	Approximation by splines	131
		6.4.3	Coincident knots	132
7	Fou	rier's	world	133
	7.1	Trigo	nometric approximation and Fourier series	133
		7.1.1	Trigonometric polynomials	134
		7.1.2	Integration of periodic functions	134
		7.1.3	Least-squares approximation for trigonometric	
			polynomials	135
		7.1.4	Density of trigonometric polynomials in the space of	
		42	continuous periodic functions	136
		7.1.5	Convergence in the mean square of trigonometric	
			approximation to continuous functions	139
		7.1.6	Asymptotic behaviour of Fourier coefficients	140
		7.1.7	Convergence of trigonometric approximation to L^2_{\sharp} functions	142
		7.1.8	Uniform convergence of Fourier series	144
	7.2		olution and pointwise convergence	146
	2	7.2.1	Convolution	146
		7.2.2	Regularization	148
		7.2.3	Constructive density results	150
		7.2.4	Convolution and Fourier series	151
		7.2.5	Convergence of Fourier series as a local phenomenon	152
		7.2.6	Pointwise convergence of partial Fourier sums of	10-
			absolutely continuous functions	153
	•	7.2.7	Pointwise convergence of partial Fourier sums of piecewise	
			absolutely continuous functions	156
		7.2.8	Gibbs phenomenon	157
	7.3		rises from Chapter 7	159
		7.3.1	Elementary exercises on Fourier series	159

xiv CONTENTS

		7.3.2	Féjer, La Vallée Poussin, and Poisson kernels	160
		7.3.3	There exists an integrable function whose Fourier	
			coefficients decrease arbitrarily slowly to 0	162
		7.3.4	The existence of sequences of numbers a_k tending to 0 as	
		5	k tends to infinity which are not the Fourier coefficients	
	8		of any integrable function	162
		7.3.5	Discrete least-squares approximation by trigonometric	
			polynomials	163
3	Qua	dratu	re	165
	8.1	Nume	rical integration	166
		8.1.1	Numerical integration for dummies	166
	8.2	The a	nalysis of quadrature formulae	169
		8.2.1	Order of a quadrature formula	169
		8.2.2	On the practical interest of weighted formulae	171
		8.2.3	Examples of simple formulae	172
		8.2.4	Composite formulae	173
	8.3	The P	Peano kernel and error estimates	174
		8.3.1	Definition of the Peano kernel	174
		8.3.2	Quadrature error in composite formulae	179
	8.4	Gauss	ian quadrature	180
	8.5	Period	dic numerical integration	183
	8.6	Berno	ulli, Euler–MacLaurin	184
		8.6.1	Detailed analysis of the trapezium formula	185
		8.6.2	The Bernoulli polynomials	187
		8.6.3	The Euler-MacLaurin formula	189
	8.7	Discre	ete Fourier and fast Fourier transforms	189
,		8.7.1	Discrete Fourier transforms	190
		8.7.2	Principle of the fast Fourier transform algorithm	191
	•	8.7.3	FFT algorithm: decimation-in-frequency	193
	8.8	Exerc	ises from Chapter 8	197
		8.8.1	Summation of series with Bernoulli numbers and	
			polynomials	197
		8.8.2	The Fredholm integral equation of the first kind	200
		8.8.3	Towards Franklin's periodic wavelets	202
ΙΙ	I N	Vume:	rical linear algebra	205
9	Gau	ıss's w	orld	207
	9.1	Elimi	nation without pivoting	207
		9.1.1	Just elimination	207
		9.1.2	Matrix interpretation of Gaussian elimination	209
	9.2	Puttir	ng it into practice: operation counts	212

CONTENTS xv

		9.2.1	The madness of Cramer's rule	212
		9.2.2	Putting elimination into practice	214
		9.2.3	Operation counts for elimination	214
		9.2.4	Inverting a matrix: putting it into practice and the	
			operation count	215
		9.2.5	Do we need to invert matrices?	216
	9.3	Elimin	ation with pivoting	217
		9.3.1	The effect of a small pivot	217
		9.3.2	Partial pivoting and total pivoting: general description	
			and cost	219
		9.3.3	Aside: permutation matrices	221
		9.3.4	Matrix interpretation of partial and total pivoting	222
		9.3.5	The return of the determinant	224
		9.3.6	Banded matrices	224
	9.4	Other	decompositions: LDU and Cholesky	227
		9.4.1	The LDU decomposition	227
		9.4.2	· ·	228
		9.4.3	Putting the Cholesky method into practice and operation counts	231
	9.5	Evoroi	ses from Chapter 9	$\frac{231}{231}$
	9.0	9.5.1	Exercises on the rank of systems of vectors	231
		9.5.1	Echelon matrices and least-squares	$\frac{231}{232}$
		9.5.2 $9.5.3$	The conditioning of a linear system	$\frac{232}{235}$
	•	9.5.3	Inverting persymmetric matrices	$\frac{233}{237}$
		9.0.4	inverting persymmetric matrices	201
10	The	oretica	al interlude	240
	10.1	The R	ayleigh quotient	240
	10.2	Spectr	al radius and norms	242
		10.2.1	Spectral radius	242
		10.2.2	Norms of vectors, operators, and matrices	243
	10.3	Topolo	ogy and norms	244
		10.3.1	Topology refresher	244
		10.3.2	Equivalence of norms	244
		10.3.3	Linear mappings: continuity, norm	247
		10.3.4	Subordinate norms	248
		10.3.5	Examples of subordinate norms	250
		10.3.6	The Frobenius norm is not subordinate	252
	10.4	Exerci	ses from Chapter 10	254
		10.4.1	Continuity of the eigenvalues of a matrix with respect to	
			itself	254
		10.4.2	Various questions on norms	255

vi 2 CONTENTS

11	Itera	ations and recurrence	257
	11.1	Iterative solution of linear systems	258
	11.2	Linear recurrence and powers of matrices	270
		11.2.1 The spectrum of a finite difference matrix	273
	11.3	Exercises from Chapter 11	276
		11.3.1 Finite difference matrix of the Laplacian in a rectangle	276
		11.3.2 Richardson's and pre-conditioned Richardson's methods	277
		11.3.3 Convergence rate of the gradient method	280
		11.3.4 The conjugate gradient	282
		11.3.5 Introduction to multigrid methods	285
12	Pyt	nagoras' world	290
	12.1	About orthogonalization	290
		12.1.1 The Gram-Schmidt orthonormalization revisited	290
		12.1.2 Paths of inertia	293
		12.1.3 Topology for QR and Cholesky	295
		12.1.4 Operation counts and numeric strategies	296
		12.1.5 Hessenberg form	297
		12.1.6 Householder transformations	298
		12.1.7 QR decomposition by Householder transformations	299
		12.1.8 Hessenberg form by Householder transformations	302
	12.2	Exercises from Chapter 12	303
		12.2.1 The square root of a Hermitian positive definite matrix	303
÷			
IV	N	onlinear problems	305
13	Spe	etra	307
	13.1	Eigenvalues: the naïve approach 13.1.1 Seeking eigenvalues and polynomial equations	311
		13.1.1 Seeking eigenvalues and polynomial equations	311
	•	13.1.2 The bisection method	312
	13.2	Resonance and vibration	313
		13.2.1 Galloping Gertie	313
		13.2.2 Small vibrations	314
	13.3	Power method	316
		13.3.1 The straightforward case	316
		13.3.2 Modification of the power method	319
		13.3.3 Inverse power method	321
	13.4	QR method	322
		13.4.1 The algorithm and its basic properties	322
		13.4.2 Convergence in a special case	324
		13.4.3 Effectiveness of QR	327
	13.5	Exercises from Chapter 13	328
		13.5.1 Spectral pathology	328

CO	NTE	NTS		xvii
		13.5.2	QR flow and Lax pairs	328
14	Non	linear	equations and systems	331
	14.1	From	existence to construction	331
		14.1.1	Existence and non-existence of solutions	331
		14.1.2	Existence proofs translate into algorithms	333
		14.1.3	A long and exciting history	333
		14.1.4	An overview of existence proofs	334
	14.2	Consti	ruction of several methods	336
		14.2.1	The strictly contracting fixed point theorem	336
		14.2.2	Newton's method: geometric interpretation and examples	338
		14.2.3	Convergence of Newton's method	341
		14.2.4	The secant method	344
		14.2.5	The golden ratio and Fibonacci's rabbits	348
		14.2.6	Order of an iterative method	351
		14.2.7	Ideas on the solution of vector problems	352
	14.3	Exerci	ses from Chapter 14	353
		14.3.1	The Cardano formulae	353
		14.3.2	Brouwer's fixed point theorem in dimension 2	354
		14.3.3	Comparison of two methods for calculating square roots	355
		14.3.4	Newton's method for finding the square roots of matrices	357
15	Solv	ing di	fferential systems	362
	15.1	Cauch	y-Lipschitz theory	362
		15.1.1	Idea of the proof of existence for ODEs	362
		15.1.2	Cauchy–Lipschitz existence theorem	363
		15.1.3	Systems of order 1 and of order p	366
		15.1.4	Autonomous and non-autonomous systems	367
	15.2	Linear	differential equations	367
		15.2.1	Constant coefficient linear systems	367
		15.2.2	Matrix exponentials	369
		15.2.3	Duhamel's formula	371
		15.2.4	Linear equations and systems with variable coefficients	372
		15.2.5	Gronwall's lemma	377
		15.2.6	Applications of Gronwall's lemma	379
		15.2.7	Smoother solutions	380
	15.3	Exerci	ses from Chapter 15	382
		15.3.1	Lyapunov function for a 2×2 linear system	382

15.3.2 A delay differential equation

15.3.3 A second-order ordinary differential equation

382

384

xviii CONTENTS

16	Single-step schemes			
	16.1	Single-	step schemes: the basics	386
		16.1.1	Convergence, stability, consistency	387
		16.1.2	Necessary and sufficient condition of consistency	389
		16.1.3	Sufficient condition for stability	390
	16.2	${\rm Order}$	of a one-step scheme	392
	16.3	Explic	it and implicit Euler schemes	395
		16.3.1	The forward Euler scheme	395
		16.3.2	Backwards Euler scheme	396
		16.3.3	θ -method	398
	16.4	Runge	-Kutta formulae	399
		16.4.1	Examples of Runge–Kutta schemes	400
	16.5	Exerci	ses from Chapter 16	403
		16.5.1	Detailed study of the θ -scheme	403
		16.5.2	Euler scheme with variable step size and asymptotic error	
			estimates	404
-			Numerical schemes for a delay differential equation	407
			Alternate directions	409
		16.5.5	Numerical analysis of a second-order differential equation	412
17	Line	ar mu	lltistep schemes	414
	17.1	Consti	ructing multistep methods	414
		17.1.1	Adams methods	415
		17.1.2	The multistep methods of Adams	416
		17.1.3	Backward differentiation	419
		17.1.4	Other multistep methods	420
	17.2	Order	of multistep methods	421
		17.2.1	The order is nice and easy for multistep methods	421
		17.2.2	Order of some multistep methods	423
	17.3	Stabili	ty of multistep methods	424
		17.3.1	Multistep methods can be very unstable	424
		17.3.2	The stability theory for multistep methods	426
		17.3.3	Stability of some multistep schemes	432
	17.4	Conve	rgence of multistep schemes	432
		17.4.1	Initializing multistep methods	432
		17.4.2	Solving in the implicit case	433
	17.5	Exerci	ses from Chapter 17	433
		17.5.1	Short exercises	433
			An alternative formulation of the order condition	43 4
		17.5.3	Weak instability	434
		17.5.4	Predictor-corrector methods	435
		17.5.5	One-leg methods	437

CONTENTS	xix
ONIENIS	AIA

- 18	Tow	ards p	artial differential equations	439
	18.1	The ac	lvection equation	439
		18.1.1	The advection equation and its physical origin	439^{-}
		18.1.2	Solving the advection equation	442
		18.1.3	More general advection equations and systems	444
	18.2	Numer	rics for the advection equation	446
	•	18.2.1	Definition of some good and some bad schemes	446
		18.2.2	Convergence of the scheme (18.2.6)	450
	18.3	The wa	ave equation in one dimension	455
		18.3.1	Masses and springs	455
		18.3.2	Elementary facts about the wave equation	458
		18.3.3	A numerical scheme for the wave equation	459
	18.4	The he	eat equation and separation of variables	461
		18.4.1	Derivation of the heat equation	461
		18.4.2	Seeking a particular solution by separation of variables	465
		18.4.3	Solution by Fourier series	467
		18.4.4	Relation between the heat equation and the discrete	
			model	469
	18.5	Exerci	ses from Chapter 18	471
		18.5.1	The eigenvectors of a strictly hyperbolic matrix	471
		18.5.2	More on the upwind scheme	472
		18.5.3	Fourier analysis of difference schemes for the advection	
			equation	474
		18.5.4	The Lax–Friedrichs scheme	474
	*	18.5.5	The Lax-Wendroff scheme	475
		18.5.6	Stability of the leap-frog scheme	475
		18.5.7	Elementary questions on the wave equation	476
		18.5.8	Generalized solutions for the advection equation	476
		18.5.9	Advection-diffusion equation	478
\mathbf{Re}	ferer	ices	/	479
Inc	lex			485