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2

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Scientific Computing with MATLAB and Octave

Fourth Edition



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The picture on the cover shows a re-entrant electrical wave on a slab of homogeneous excitable medium, exhibiting spiral turbulence and spatiotemporal chaos. Computation by Ricardo Ruiz-Baier, IST, University of Lausanne, CH.

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To the memory of Fausto Saleri

Preface

Preface to the First Edition

This textbook is an introduction to Scientific Computing. We will illustrate several numerical methods for the computer solution of certain classes of mathematical problems that cannot be faced by paper and pencil. We will show how to compute the zeros or the integrals of continuous functions, solve linear systems, approximate functions by polynomials and construct accurate approximations for the solution of differential equations.

With this aim, in Chapter 1 we will illustrate the rules of the game that computers adopt when storing and operating with real and complex numbers, vectors and matrices.

In order to make our presentation concrete and appealing we will adopt the programming environment MATLAB $^{\circledR}$ 1 as a faithful companion. We will gradually discover its principal commands, statements and constructs. We will show how to execute all the algorithms that we introduce throughout the book. This will enable us to furnish an immediate quantitative assessment of their theoretical properties such as stability, accuracy and complexity. We will solve several problems that will be raised through exercises and examples, often stemming from specific applications.

Several graphical devices will be adopted in order to render the reading more pleasant. We will report in the margin the MATLAB command along side the line where that command is being introduced for the first time. The symbol will be used to indicate the presence of exercises, the symbol to indicate the presence of a MATLAB program, while

¹ MATLAB is a trademark of TheMathWorks Inc., 24 Prime Park Way, Natick, MA 01760, Tel: 001+508-647-7000, Fax: 001+508-647-7001.

the symbol will be used when we want to attract the attention of the reader on a critical or surprising behavior of an algorithm or a procedure. The mathematical formulae of special relevance are put within a frame. Finally, the symbol indicates the presence of a display panel summarizing concepts and conclusions which have just been reported and drawn.

At the end of each chapter a specific section is devoted to mentioning those subjects which have not been addressed and indicate the bibliographical references for a more comprehensive treatment of the material that we have carried out.

Quite often we will refer to the textbook [QSS07] where many issues faced in this book are treated at a deeper level, and where theoretical results are proven. For a more thorough description of MATLAB we refer to [HH05]. All the programs introduced in this text can be downloaded from the web address

mox.polimi.it/qs

No special prerequisite is demanded of the reader, with the exception of an elementary course of Calculus.

However, in the course of the first chapter, we recall the principal results of Calculus and Geometry that will be used extensively throughout this text. The less elementary subjects, those which are not so necessary for an introductory educational path, are highlighted by the special

symbol .

We express our thanks to Thanh-Ha Le Thi from Springer-Verlag Heidelberg, and to Francesca Bonadei and Marina Forlizzi from Springer-Italia for their friendly collaboration throughout this project. We gratefully thank Prof. Eastham of Cardiff University for editing the language of the whole manuscript and stimulating us to clarify many points of our text.

Milano and Lausanne May 2003 Alfio Quarteroni Fausto Saleri

Preface to the Second Edition

In this second edition we have enriched all the Chapters by introducing several new problems. Moreover, we have added new methods for the numerical solution of linear and nonlinear systems, the eigenvalue computation and the solution of initial-value problems. Another relevant improvement is that we also use the Octave programming environment. Octave is a reimplementation of part of MATLAB which

includes many numerical facilities of MATLAB and is freely distributed under the GNU General Public License.

Throughout the book, we shall often make use of the expression "MATLAB command": in this case, MATLAB should be understood as the *language* which is the common subset of both programs MATLAB and Octave. We have striven to ensure a seamless usage of our codes and programs under both MATLAB and Octave. In the few cases where this does not apply, we shall write a short explanation notice at the end of each corresponding section.

For this second edition we would like to thank Paola Causin for having proposed several problems, Christophe Prud´homme, John W. Eaton and David Bateman for their help with Octave, and Silvia Quarteroni for the translation of the new sections. Finally, we kindly acknowledge the support of the Poseidon project of the Ecole Polytechnique Fédérale de Lausanne.

Lausanne and Milano May 2006 Alfio Quarteroni Fausto Saleri

Preface to the Third Edition

This third edition features a complete revisitation of the whole book, many improvements in style and content to all the chapters, as well as a substantial new development of those chapters devoted to the numerical approximation of boundary-value problems and initial-boundary-value problems. We remind the reader that all the programs introduced in this text can be downloaded from the web address

mox.polimi.it/qs

Lausanne, Milano and Brescia March 2010

Alfio Quarteroni Paola Gervasio

Preface to the Fourth Edition

The fourth edition features the addition of a new chapter on numerical optimization of both univariate and multivariate functions in which several methods are presented, discussed and analyzed.

For unconstrained minimization, we consider derivative free methods, descent (or line search) methods, and trust region methods.

For constrained minimization we restrict our discussion to penalization methods and augmented Lagrangian methods.

X Preface

As for the other chapters of this book, also this new chapter is supported by examples, exercises and programs written in both MATLAB and Octave environments.

The addition of this chapter made it necessary a renumbering of several other chapters with respect to the previous editions. Moreover, new sections have been added in some other chapters.

Finally we remind the reader that all programs presented in this book can be downloaded from the web address

http://mox.polimi.it/qs

Lausanne, Milano and Brescia December 2013 Alfio Quarteroni Paola Gervasio

Contents

1	$\mathbf{W}\mathbf{h}$	nat can't be ignored	1
	1.1	The MATLAB and Octave environments	1
	1.2	Real numbers	3
		1.2.1 How we represent them	3
		1.2.2 How we operate with floating-point numbers	6
	1.3	Complex numbers	8
	1.4	Matrices	0
		1.4.1 Vectors	4
	1.5	Real functions	6
		1.5.1 The zeros	9
		1.5.2 Polynomials	0
		1.5.3 Integration and differentiation	2
	1.6	To err is not only human	5
		1.6.1 Talking about costs	8
	1.7	The MATLAB language 3	0
		1.7.1 MATLAB statements	2
		1.7.2 Programming in MATLAB 3	4
		1.7.3 Examples of differences between MATLAB	
		and Octave languages	8
	1.8	What we haven't told you	8
	1.9	Exercises	9
2	Noı	nlinear equations 4	1
	2.1	Some representative problems 4	1
	2.2	The bisection method 4	3
	2.3	The Newton method	7
		2.3.1 How to terminate Newton's iterations 5	0
	2.4	The secant method	1
	2.5	Systems of nonlinear equations	2

	2.6	Fixed point iterations	56
		2.6.1 How to terminate fixed point iterations	62
	2.7	Acceleration using Aitken method	63
	2.8	Algebraic polynomials	67
		2.8.1 Hörner's algorithm	68
		2.8.2 The Newton-Hörner method	70
	2.9	What we haven't told you	72
	2.10	Exercises	74
3	App	proximation of functions and data	77
	3.1	Some representative problems	77
	3.2	Approximation by Taylor's polynomials	79
	3.3	Interpolation	80
		3.3.1 Lagrangian polynomial interpolation	81
		3.3.2 Stability of polynomial interpolation	86
		3.3.3 Interpolation at Chebyshev nodes	87
		3.3.4 Barycentric interpolation formula	90
		3.3.5 Trigonometric interpolation and FFT	93
	3.4	Piecewise linear interpolation	98
	3.5	Approximation by spline functions	
	3.6	The least-squares method	
	3.7	What we haven't told you	
	3.8	Exercises	110
4		nerical differentiation and integration	
	4.1	Some representative problems	
	4.2	Approximation of function derivatives	
	4.3	Numerical integration	
		4.3.1 Midpoint formula	
		4.3.2 Trapezoidal formula	
		4.3.3 Simpson formula	
	4.4	Interpolatory quadratures	
	4.5	Simpson adaptive formula	
	4.6	Monte Carlo Methods for Numerical Integration	
	4.7	What we haven't told you	
	4.8	Exercises	134
5	Line	ear systems	137
	5.1	Some representative problems	137
	5.2	Linear system and complexity	
	5.3	The LU factorization method	143
	5.4	The pivoting technique	154
		5.4.1 The <i>fill-in</i> of a matrix	
	5.5	How accurate is the solution of a linear system?	158
	5.6	How to solve a tridiagonal system	162

			Contents	XIII
	5.7	Overdetermined systems		163
	5.8	What is hidden behind the MATLAB command	d \	166
	5.9	Iterative methods		
		5.9.1 How to construct an iterative method		169
	5.10	Richardson and gradient methods		174
	5.11	The conjugate gradient method		177
	5.12	When should an iterative method be stopped? .		180
		To wrap-up: direct or iterative?		
	5.14	What we haven't told you		188
	5.15	Exercises		188
6	Eige	envalues and eigenvectors		193
	6.1	Some representative problems		194
	6.2	The power method		196
		6.2.1 Convergence analysis		199
	6.3	Generalization of the power method		201
	6.4	How to compute the shift		203
	6.5	Computation of all the eigenvalues		206
	6.6	What we haven't told you		209
	6.7	Exercises		210
7	Nun	nerical optimization		213
	7.1	Some representative problems		214
	7.2	Unconstrained optimization		217
	7.3	Derivative free methods		219
		7.3.1 Golden section and quadratic interpolation	on	
		methods		
		7.3.2 Nelder and Mead method		
	7.4	The Newton method		
	7.5	Descent (or line search) methods		
		7.5.1 Descent directions		
		7.5.2 Strategies for choosing the steplength α_k		
		7.5.3 The descent method with Newton's direct		
		7.5.4 Descent methods with quasi-Newton dire	ctions	238
		7.5.5 Gradient and conjugate gradient descent methods		240
	7.6	Trust region methods		
	7.7	The nonlinear least squares method		
	1.1	7.7.1 Gauss-Newton method		
		7.7.2 Levenberg-Marquardt's method		
	7.8	Constrained optimization		
	0	7.8.1 The penalty method		
		7.8.2 The augmented Lagrangian method		
	7.9	What we haven't told you		
		Exercises		

8	Ord	inary	differential equations	. 271
	8.1	Some	representative problems	. 271
	8.2	The C	Cauchy problem	. 274
	8.3	Euler	methods	. 275
		8.3.1	Convergence analysis	. 278
	8.4	The C	Crank-Nicolson method	. 282
	8.5	Zero-s	stability	. 284
	8.6	Stabil	ity on unbounded intervals	. 286
		8.6.1	The region of absolute stability	. 289
		8.6.2	Absolute stability controls perturbations	. 290
		8.6.3	1 1	
			method	
	8.7		order methods	
	8.8		oredictor-corrector methods	
	8.9		ms of differential equations	
	8.10		examples	
			The spherical pendulum	
			The three-body problem	
			Some stiff problems	
			we haven't told you	
	8.12	Exerc	ises	. 326
9	Nur	nerica	d approximation of boundary-value	
				. 329
	9.1	Some	representative problems	. 330
	9.2	Appro	eximation of boundary-value problems	. 332
		9.2.1	Finite difference approximation of the	
			one-dimensional Poisson problem	. 333
		9.2.2	Finite difference approximation of a	
			convection-dominated problem	. 336
		9.2.3	Finite element approximation of the	
			one-dimensional Poisson problem	. 337
		9.2.4	Finite difference approximation of the	
			two-dimensional Poisson problem	. 341
		9.2.5	Consistency and convergence of finite difference	
			discretization of the Poisson problem	. 347
		9.2.6	Finite difference approximation of the	
			one-dimensional heat equation	. 348
		9.2.7	Finite element approximation of the	
			one-dimensional heat equation	. 352
	9.3	Hyper	rbolic equations: a scalar pure advection	
			em	. 355
		9.3.1		
			transport equation	357

														Co	$_{ m nte}$	nts	3		XV
		9.3.2	Finite												-				
			equation															•	359
		9.3.3	Finite			-													
			advecti		-														
	9.4	The w	ave equ	ation															367
		9.4.1	Finite	differ	ence	e ap	pro	xim	ati	on	of	$^{\mathrm{th}}$	e v	vav	e				
			equation	n															369
	9.5		we have																
	9.6	Exerci	ises																374
	~ .		0.1																
10	Solu	$_{ m tions}$	of the	exer	cise	s					٠.								377
	10.1	Chapt	$er 1 \dots$																377
	10.2	Chapt	er 2																380
	10.3	Chapt	er 3																385
	10.4	Chapt	er 4																389
	10.5	Chapt	er 5																394
		_	er 6																
	10.7	Chapt	er 7																404
			er 8																
			er 9																
		-																	
$R\epsilon$	eferei	ices																	429

Index of MATLAB and Octave programs

All the programs introduced in this text can be downloaded from http://mox.polimi.it/qs

2.1	bisection : bisection method
2.2	newton : Newton method
2.3	newtonsys : Newton method for nonlinear systems
2.4	aitken: Aitken method
2.5	horner : synthetic division algorithm 69
2.6	newtonhorner : Newton-Hörner method
3.1	barycentric : barycentric interpolation
3.2	${\it cubic spline}$: interpolating cubic spline
4.1	midpointc : composite midpoint quadrature formula 120
4.2	simpsonc : composite Simpson quadrature formula 122
4.3	simpadpt : adaptive Simpson formula
5.1	lugauss: Gauss LU factorization
5.2	itermeth : general iterative method
6.1	eigpower: power method
6.2	invshift : inverse power method with shift $\dots 202$
6.3	gershcircles: Gershgorin circles
6.4	qrbasic : method of QR iterations
7.1	golden : golden section method
7.2	backtrack: backtracking strategy
7.3	descent: descent method
7.4	trustregion: trust region method
7.5	gaussnewton: Gauss-Newton method
7.6	penalty: penalty method
7.7	auglagrange: augmented Lagrangian method
8.1	feuler : forward Euler method
8.2	beuler : backward Euler method

XVIII Index of MATLAB and Octave programs

8.3	$\textbf{cranknic} : Crank-Nicolson \ method \ \ldots \ldots \ 283$
8.4	predcor : predictor-corrector method
8.5	feonestep : one step of the forward Euler method 307
8.6	beonestep : one step of the backward Euler method $\dots 307$
8.7	${\bf cnonestep}$: one step of the Crank-Nicolson method 307
8.8	newmark : Newmark method
8.9	fvinc : forcing term for the spherical pendulum problem $\dots 316$
8.10	threebody: forcing term for the simplified three
	body system $\dots 318$
9.1	bvp: approximation of a two-point
	diffusion-convection-reaction problem by the finite
	difference method $\dots \dots 335$
9.2	poissonfd: approximation of the Poisson problem with
	Dirichlet boundary data by the five-point finite
	difference method $\dots \dots 345$
9.3	heattheta : θ -method for the one-dimensional
	heat equation $\dots \dots 350$
9.4	${\it newmarkwave}$: Newmark method for the wave equation 369
10.1	gausslegendre: Gauss-Legendre composite quadrature
	formula, with $n=1$
	rk2 : Heun (or RK2) method
	${\bf rk3}$: explicit Runge-Kutta method of order $3\ldots\ldots 416$
10.4	neumann: numerical solution of a Neumann boundary-value
	$problem \ \dots \ \ 423$
10.5	hyper : Lax-Friedrichs, Lax-Wendroff and upwind schemes 427