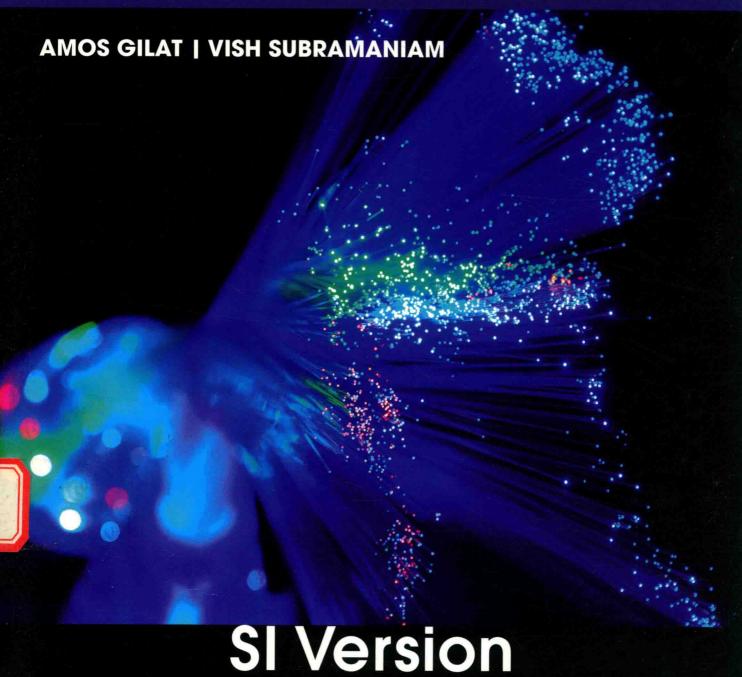
Numerical Methods

An Introduction with Applications Using MATLAB®



Numerical Methods

An Introduction with Applications using MATLAB®

Second Edition SI Version

Amos Gilat Vish Subramaniam

Department of Mechanical Engineering The Ohio State University



JOHN WILEY & SONS, INC. Copyright © 2011 John Wiley & Sons, Inc. All rights reserved

Copyright © 2011 John Wiley & Sons (Asia) Pte Ltd

Cover image from © asharkyu /shutterstock

Founded in 1807, John Wiley & Sons, Inc. has been a valued source of knowledge and understanding for more than 200 years, helping people around the world meet their needs and fulfi II their aspirations. Our company is built on a foundation of principles that include responsibility to the communities we serve and where we live and work. In 2008, we launched a Corporate Citizenship Initiative, a global effort to address the environmental, social, economic, and ethical challenges we face in our business. Among the issues we are addressing are carbon impact, paper specifications and procurement, ethical conduct within our business and among our vendors, and community and charitable support. For more information, please visit our website: www.wiley.com/go/citizenship.

All rights reserved. This book is authorized for sale in Canada, Australia, Europe, Asia, Africa and the Middle East only and may not be exported outside of these territories. Exportation from or importation of this book to another region without the Publisher's authorization is illegal and is a violation of the Publisher's rights. The Publisher may take legal action to enforce its rights. The Publisher may recover damages and costs, including but not limited to lost profits and attorney's fees, in the event legal action is required.

No part of this publication may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronic, mechanical, photocopying, recording, scanning, or otherwise, except as permitted under Section 107 or 108 of the 1976 United States Copyright Act, without either the prior written permission of the Publisher or authorization through payment of the appropriate per-copy fee to the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, website www.copyright.com. Requests to the Publisher for permission should be addressed to the Permissions

Department, John Wiley & Sons, Inc., 111 River Street, Hoboken, NJ 07030, (201) 748-6011, fax (201) 748-6008, website http://www.wiley.com/go/permissions.

ISBN: 978-0-470-87374-8

Printed in Asia

109876543

Preface

This textbook is intended for a first course in numerical methods for students in engineering and science, typically taught in the second year of college. The book covers the fundamentals of numerical methods from an applied point of view. It explains the basic ideas behind the various methods and shows their usefulness for solving problems in engineering and science.

In the past, a numerical methods course was essentially mathematical, emphasizing numerical analysis and theory. More recently, due to the availability of powerful desktop computers and computing software that is both affordable and powerful, the content and nature of a first course in numerical methods for engineering and science students are changing. The emphasis is shifting more and more toward applications and toward implementing numerical methods with ready-to-use tools. In a typical course, students still learn the fundamentals of numerical methods. In addition, however, they learn computer programming (or improve their programming skills if they have already been introduced to programming), and use advanced software as a tool for solving problems. MATLAB is a good example of such software. It can be used by students to write their own programs, and can be used as a tool for solving problems using its built-in functions. One of the objectives of a course in numerical methods is to prepare students in science and engineering for future courses in their areas of specialization (and their future careers) where they will have to use computers for solving problems.

Main objectives of the book

To teach the fundamentals of numerical methods, with emphasis on the most essential methods.

To provide students with the opportunity to enhance their programming skills using the MATLAB environment to implement algorithms.

To teach the use of MATLAB as a tool (using its built-in functions) for solving problems in science and engineering, and for checking the results of any programs students write themselves.

Features/pedagogy of the book

- This book is written in simple, clear, and direct language. Frequently, bullets and a list of steps, rather than lengthy text, are used to list facts and details of a specific subject.
- Numerous illustrations are used for explaining the principles of the numerical methods.
- Many of the examples and end-of-chapter problems involve realistic problems in science and engineering.
- MATLAB is integrated within the text and in the examples. A light colored background is used when MATLAB syntax is displayed.
- Annotating comments that explain the commands are posted alongside the MATLAB syntax.
- MATLAB's built-in functions that are associated with the numerical methods are presented in detail.
- The homework problems at the end of the chapters are divided into three groups:
- (a) <u>Problems to be solved by hand:</u> Problems related to improving understanding of numerical methods. In these problems the students are asked to answer questions related to the fundamentals of numerical methods, and to carry out a few steps of the numerical methods by hand.
- (b) <u>Problems to be programmed in MATLAB:</u> Problems designed to provide the opportunity to improve programming skills. In these problems students are asked to use MATLAB to write computer programs (script files and user-defined functions) implementing various numerical methods.
- (c) <u>Problems in math, science, and engineering:</u> Problems in science and engineering that have to be solved by using numerical methods. The objective is to train the students to use numerical methods for solving problems they can expect to see in future courses or in practice. Students are expected to use the programs that are presented in the book, programs that they write, and the built-in functions in MATLAB.

Organization of the book

Chapter 1: The first chapter gives a general introduction to numerical methods and to the way that computers store numbers and carry out numerical operations. It also includes a section on errors in numerical solutions and a section on computers and programming.

Chapters 2 through 8: The seven chapters present the various numerical methods in an order that is typically followed in a first course on numerical methods. These chapters follow the format explained next.

Organization of a typical chapter

An itemized list of the topics that are covered in the chapter is displayed below the title of the chapter. The list is divided into *core* and *complementary* topics. The *core topics* are the most essential topics related to the subject of the chapter. The *complementary topics* include more advanced topics. Obviously, a division of topics related to one subject into core and complementary is subjective. The intent is to help instructors in the design of their course when there is not enough time to cover all the topics. In practicality, the division can be ignored in courses where all the topics are covered.

The first section of the chapter provides a general background with illustrative examples of situations in the sciences and engineering where the methods described in the chapter are used. This section also explains the basic ideas behind the specific class of numerical methods that are described in the chapter. The following sections cover the core topics of the chapter. Next, a special section discusses the built-in functions in MATLAB that implement the numerical methods described in the chapter, and how they may be used to solve problems. The later sections of the chapter cover the complementary topics.

The order of topics

It is probably impossible to write a text book where all the topics follow an order that is agreed upon by all instructors. In the present book, the main subjects are in an order that is typical in a first course in numerical methods. Chapter 2 covers solution of nonlinear equations. It mostly deals with the solution of a single equation, which is a simple application of numerical methods. The chapter also includes, as a complementary topic, a section on the solution of a system of nonlinear equations. Chapter 3 deals with the solution of a system of linear equations. A complementary topic in this chapter deals with eigenvalue problems. Chapter 4 covers curve fitting and interpolation, and Chapters 5 and 6 cover differentiation and integration, respectively. Finally, solution of ordinary differential equations (ODE) is presented in the last two chapters. Chapter 7 deals with the solution of initial-value problems (first-order, systems, and higher-order) and Chapter 8 considers boundary-value problems.

The order of some of the topics is dictated by the subjects themselves. For example, differentiation and integration need to be covered before ordinary differential equations. It is possible, however, to cover the other subjects in different order than is in the book. The various chapters and sections in the book are written in a self-contained manner that make it easy for the instructor to cover the subjects in a different order, if desired.

MATLAB programs

This book contains many MATLAB programs. The programs are clearly identified as user-defined functions, or as script files. All the programs are listed in Appendix B. The programs, or the scripts, are written in a simple way that is easy to follow. The emphasis of these programs is on the basics and on how to program an algorithm of a specific numerical method. Obviously, the programs are not general, and do not cover all possible circumstances when executed. The programs are not written from the perspective of being shortest, fastest, or most efficient. Rather, they are written such that they are easy to follow. It is assumed that most of the students have only limited understanding of MATLAB and programming, and presenting MATLAB in this manner will advance their computing skills. More advanced users of MATLAB are encouraged to write more sophisticated and efficient programs and scripts, and compare their performance with the ones in the book.

SI Version

MATLAB: The SI version of the book is updated to MATLAB R2009b. All the programs have been modified and use anonymous functions instead of inline functions. In addition, function handles are used for passing functions into functions. Appendix A has been updated to the current version of MATLAB. It includes three new sections (A.8, A.9, and A.10) that cover anonymous functions, function functions, function handles, and subfunction.

Homework problems: Many new homework problems have been added to the SI version. Most are application problems in engineering and science. Most of the Chapters have 40 or more problems. Overall, more than 50% of the problems are new or have been revised.

Support material

The following is available on the instructor companion site at www.wiley.com/go/global/gilat):

- (a) for faculty who have adopted the text for use in their course, a fully worked solution manual, triple checked for accuracy.
- (b) suggested course syllabi with suggested assignments to help quickly integrate the text into your course.
- (c) conversion guides from other major numerical methods titles to show where each section of your current text is covered in this new text, helping you quickly convert from old to new.
- (d) electronic versions of all the figures and tables from the text, for creating lecture slides and quizzes/exams based on images from the book.
- (e) m-files of all the programs in the text.

Many people have assisted during the preparation of the first edi-

tion of the book. We would like to thank the reviewers for the many comments and suggestions they have made.

Lawrence K. Agbezuge, Rochester Institute of Technology

David Alciatore, Colorado State University

Salame Amr, Virginia State University

John R. Cotton, Virginia Polytechnic Institute and State University

David Dux, Purdue University

Venkat Ganesan, University of Texas-Austin

Michael R. Gustafson II, Duke University

Alain Kassab, University of Central Florida

Tribikram Kundu, University of Arizona

Ronald A. Mann, University of Louisville

Peter O. Orono, Indiana University Purdue University Indianapolis

Charles Ritz, California State Polytechnic University-Pomona

Douglas E. Smith, University of Missouri-Columbia

Anatoliy Swishchuk, University of Calgary

Ronald F. Taylor, Wright State University

Brian Vick, Virginia Polytechnic Institute and State University

We would also like to thank Mike McDonald, acquisition editor, and Renata Marchione, editorial assistant, from Wiley. Special thanks to Professor Subramaniam's daughters, Sonya and Priya, for typing early drafts of some chapters and for proofreading them.

Our intention was to write a book that is useful to students and instructors alike. We would like to thank all the users of the first edition of the book who have sent us compliments and suggestions. We would appreciate any comments that will help to improve future editions.

Amos Gilat (gilat.1@osu.edu) Vish Subramaniam (subramaniam.1@osu.edu) Columbus, Ohio December 2010

To Yaela, Taly, and Edan

To my parents, Dr. K. S. Venkateswaran & Seethalakshmy Venkateswaran, and Deepa, Priya, and Sonya

Brief Table of Contents

Preface i	ii
Chapter 1	Introduction 1
Chapter 2	Solving Nonlinear Equations 23
Chapter 3	Solving a System of Linear Equations 65
Chapter 4	Curve Fitting and Interpolation 153
Chapter 5	Numerical Differentiation 211
Chapter 6	Numerical Integration 249
Chapter 7	Ordinary Differential Equations: Initial-Value Problems 293
Chapter 8	Ordinary Differential Equations: Boundary-Value Problems 377
Appendix A	Introductory MATLAB 415
Appendix B	MATLAB Programs 453
Index 457	

Contents

iii

Preface

Chapter 1 Introduction 1
1.1 Background 1
1.2 Representation of Numbers on a Computer 4
1.3 Errors in Numerical Solutions 10
1.3.1 Round-Off Errors 10
1.3.2 Truncation Errors 13 1.3.3 Total Error 14
1.4 Computers and Programming 15
1.5 Problems 18
Chapter 2 Solving Nonlinear Equations 23
2.1 Background 23
2.2 Estimation of Errors in Numerical Solutions 25
2.3 Bisection Method 27
2.4 Regula Falsi Method 30
2.5 Newton's Method 32
2.6 Secant Method 37
2.7 Fixed-Point Iteration Method 40
 2.8 Use of MATLAB Built-In Functions for Solving Nonlinear Equations 43 2.8.1 The fzero Command 44 2.8.2 The roots Command 45
2.9 Equations with Multiple Solutions 45
2.10 Systems of Nonlinear Equations 47
2.10.1 Newton's Method for Solving a System of Nonlinear Equations 48 2.10.2 Fixed-Point Iteration Method for Solving a System of Nonlinear Equations 52
2.11 Problems 54

Chapter 3	Solving	a System	of Linear	Equations	65
-----------	---------	----------	-----------	------------------	----

3.1 Background 65
3.1.1 Overview of Numerical Methods for Solving a System of Linear Algebraic Equations 66
3.2 Gauss Elimination Method 68
3.2.1 Potential Difficulties When Applying the Gauss Elimination Method 76
3.3 Gauss Elimination with Pivoting 78
3.4 Gauss–Jordan Elimination Method 81
3.5 LU Decomposition Method 84
3.5.1 LU Decomposition Using the Gauss Elimination Procedure 86
3.5.2 LU Decomposition Using Crout's Method 87
3.5.3 LU Decomposition with Pivoting 94
3.6 Inverse of a Matrix 94
3.6.1 Calculating the Inverse with the LU Decomposition Method 95
3.6.2 Calculating the Inverse Using the Gauss–Jordan Method 97
3.7 Iterative Methods 98
3.7.1 Jacobi Iterative Method 99
3.7.2 Gauss-Seidel Iterative Method 99
3.8 Use of MATLAB Built-In Functions for Solving a System of Linear Equations 102
3.8.1 Solving a System of Equations Using MATLAB's Left and Right Division 102
3.8.2 Solving a System of Equations Using MATLAB's Inverse Operation 103
3.8.3 MATLAB's Built-In Function for LU Decomposition 104
3.8.4 Additional MATLAB Built-In Functions 105
3.9 Tridiagonal Systems of Equations 107
3.10 Error, Residual, Norms, and Condition Number 112
3.10.1 Error and Residual 112
3.10.2 Norms and Condition Number 114
3.11 Ill-Conditioned Systems 117
3.12 Eigenvalues and Eigenvectors 121
3.12.1 The Basic Power Method 124
3.12.2 The Inverse Power Method 128
3.12.3 The Shifted Power Method 129
3.12.4 The QR Factorization and Iteration Method 129
3.12.5 Use of MATLAB Built-In Functions for Determining Eigenvalues and Eigenvectors 139
3.13 Problems 141

Chapter 4 Curve Fitting and Interpolation 153

- 4.1 Background 153
- 4.2 Curve Fitting with a Linear Equation 155
 - 4.2.1 Measuring How Good Is a Fit 155
 - 4.2.2 Linear Least-Squares Regression 157
- 4.3 Curve Fitting with Nonlinear Equation by Writing the Equation in a Linear Form 16
- 4.4 Curve Fitting with Quadratic and Higher-Order Polynomials 165
- 4.5 Interpolation Using a Single Polynomial 170
 - 4.5.1 Lagrange Interpolating Polynomials 172
 - 4.5.2 Newton's Interpolating Polynomials 176
- 4.6 Piecewise (Spline) Interpolation 183
 - 4.6.1 Linear Splines 183
 - 4.6.2 Quadratic Splines 185
 - 4.6.3 Cubic Splines 189
- 4.7 Use of MATLAB Built-In Functions for Curve Fitting and Interpolation 196
- 4.8 Curve Fitting with a Linear Combination of Nonlinear Functions 198
- 4.9 Problems 201

Chapter 5 Numerical Differentiation 211

- 5.1 Background 211
- 5.2 Finite Difference Approximation of the Derivative 213
- 5.3 Finite Difference Formulas Using Taylor Series Expansion 218
 - 5.3.1 Finite Difference Formulas of First Derivative 218
 - 5.3.2 Finite Difference Formulas for the Second Derivative 223
- 5.4 Summary of Finite Difference Formulas for Numerical Differentiation 225
- 5.5 Differentiation Formulas Using Lagrange Polynomials 227
- 5.6 Differentiation Using Curve Fitting 228
- 5.7 Use of MATLAB Built-In Functions for Numerical Differentiation 228
- 5.8 Richardson's Extrapolation 230
- 5.9 Error in Numerical Differentiation 233
- 5.10 Numerical Partial Differentiation 235
- 5.11 Problems 238

Chapter 6 Numerical Integration 249

- 6.1 Background 249
 6.1.1 Overview of Approaches in Numerical Integration 250
- 6.2 Rectangle and Midpoint Methods 252
- 6.3 Trapezoidal Method 254
 6.3.1 Composite Trapezoidal Method 255
- 6.4 Simpson's Methods 258
 - 6.4.1 Simpson's 1/3 Method 258
 - 6.4.2 Simpson's 3/8 Method 261
- 6.5 Gauss Quadrature 263
- 6.6 Evaluation of Multiple Integrals 269
- 6.7 Use of MATLAB Built-In Functions for Integration 270
- 6.8 Estimation of Error in Numerical Integration 272
- 6.9 Richardson's Extrapolation 274
- 6.10 Romberg Integration 277
- 6.11 Improper Integrals 280
 - 6.11.1 Integrals with Singularities 280
 - 6.11.2 Integrals with Unbounded Limits 281
- 6.12 Problems 282

Chapter 7 Ordinary Differential Equations: Initial-Value Problems 293

- 7.1 Background 293
- 7.2 Euler's Methods 298
 - 7.2.1 Euler's Explicit Method 298
 - 7.2.2 Analysis of Truncation Error in Euler's Explicit Method 302
 - 7.2.3 Euler's Implicit Method 306
- 7.3 Modified Euler's Method 309
- 7.4 Midpoint Method 312
- 7.5 Runge-Kutta Methods 313
 - 7.5.1 Second-Order Runge-Kutta Methods 314
 - 7.5.2 Third-Order Runge-Kutta Methods 318
 - 7.5.3 Fourth-Order Runge–Kutta Methods 319
- 7.6 Multistep Methods 325
 - 7.6.1 Adams–Bashforth Method 326
 - 7.6.2 Adams-Moulton Method 327

- 7.7 Predictor-Corrector Methods 328
- 7.8 System of First-Order Ordinary Differential Equations 330
 - 7.8.1 Solving a System of First-Order ODEs Using Euler's Explicit Method 332
 - 7.8.2 Solving a System of First-Order ODEs Using Second-Order Runge–Kutta Method (Modified Euler Version) 332
 - 7.8.3 Solving a System of First-Order ODEs Using the Classical Fourth-Order Runge–Kutta Method 339
- 7.9 Solving a Higher-Order Initial Value Problem 340
- 7.10 Use of MATLAB Built-In Functions for Solving Initial-Value Problems 345
 - 7.10.1 Solving a Single First-Order ODE Using MATLAB 346
 - 7.10.2 Solving a System of First-Order ODEs Using MATLAB 352
- 7.11 Local Truncation Error in Second-Order Range–Kutta Method 355
- 7.12 Step Size For Desired Accuracy 356
- 7.13 Stability 360
- 7.14 Stiff Ordinary Differential Equations 362
- 7.15 Problems **365**

Chapter 8 Ordinary Differential Equations: Boundary-Value Problems 377

- 8.1 Background 377
- 8.2 The Shooting Method 380
- 8.3 Finite Difference Method 388
- 8.4 Use of MATLAB Built-In Functions for Solving Boundary Value Problems 398
- 8.5 Error and Stability in Numerical Solution of Boundary Value Problems 403
- 8.6 Problems 405

Appendix A Introductory MATLAB 415

- A.1 Background 415
- A.2 Starting with MATLAB 415
- A.3 Arrays 420
- A.4 Mathematical Operations with Arrays 425
- A.5 Script Files 430
- A.6 Plotting 432
- A.7 User-Defined Functions and Function Files 434
- A.8 Anonymous Functions 436
- A.9 Function functions 438

A.10 Subfunctions 441

A.11 Programming in MATLAB 443

A.11.1 Relational and Logical Operators 443

A.11.2 Conditional Statements, if-else Structures 444

A.11.3 Loops 447

A.12 Problems 448

Appendix B MATLAB Programs 453

Index 457

Introduction

Core Topics

Representation of numbers on a computer (1.2).

Errors in numerical solutions, round-off errors and truncation errors (1.3).

Computers and programming (1.4).

1.1 BACKGROUND

Numerical methods are mathematical techniques used for solving mathematical problems that cannot be solved or are difficult to solve analytically. An analytical solution is an exact answer in the form of a mathematical expression in terms of the variables associated with the problem that is being solved. A numerical solution is an approximate numerical value (a number) for the solution. Although numerical solutions are an approximation, they can be very accurate. In many numerical methods, the calculations are executed in an iterative manner until a desired accuracy is achieved.

For example, Fig. 1-1 shows a block of mass m being pulled by a force F applied at an angle θ . By applying equations of equilibrium, the relationship between the force and the angle is given by:

$$F = \frac{\mu mg}{\cos\theta + \mu \sin\theta} \tag{1.1}$$

where μ is the friction coefficient and g is the acceleration due to gravity. For a given value of F, the angle that is required for moving the block can be determined by solving Eq. (1.1) for θ . Equation (1.1), however, cannot be solved analytically for θ . Using numerical methods, an approximate solution can be determined for specified accuracy. This means that when the numerical solution for θ is substituted back in Eq. (1.1), the value of F that is obtained from the expression on the right-hand side is not exactly equal to the given value of F, but is very close.

Numerical techniques for solving mathematical problems were developed and used hundreds and even thousands of years ago. Implementation of the numerical techniques was difficult since the calculations had to be carried out by hand or by use of simple mechanical

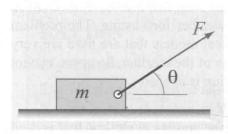


Figure 1-1: Motion of a block on a surface with friction.