

Contents

Preface xv

1	Principles of Mathematical Modeling	1
1.1	A Complex World Needs Models	1
1.2	Systems, Models, Simulations	3
1.2.1	Teleological Nature of Modeling and Simulation	3
1.2.2	Modeling and Simulation Scheme	4
1.2.3	Simulation	6
1.2.4	System	6
1.2.5	Conceptual and Physical Models	7
1.3	Mathematics as a Natural Modeling Language	8
1.3.1	Input–Output Systems	8
1.3.2	General Form of Experimental Data	9
1.3.3	Distinguished Role of Numerical Data	9
1.4	Definition of Mathematical Models	10
1.5	Examples and Some More Definitions	11
1.5.1	State Variables and System Parameters	13
1.5.2	Using Computer Algebra Software	15
1.5.3	The Problem-Solving Scheme	17
1.5.4	Strategies to Set Up Simple Models	18
1.5.4.1	Mixture Problem	21
1.5.4.2	Tank Labeling Problem	24
1.5.4.3	Financial Mathematics	26
1.5.5	Linear Programming	28
1.5.6	Modeling a Black Box System	30
1.6	Even More Definitions	32
1.6.1	Phenomenological and Mechanistic Models	32
1.6.2	Stationary and Instationary Models	35
1.6.3	Distributed and Lumped Models	36
1.7	Classification of Mathematical Models	36
1.7.1	From Black to White Box Models	37
1.7.2	SQM Space Classification: S Axis	38
1.7.3	SQM Space Classification: Q Axis	39

- 1.7.4 SQM Space Classification: M Axis 40
- 1.8 Everything Looks Like a Nail? 41

2 Phenomenological Models 44

- 2.1 Elementary Statistics 45
 - 2.1.1 Descriptive Statistics 45
 - 2.1.1.1 Using *Calc* or *Excel* 46
 - 2.1.1.2 Using R in RStudio 48
 - 2.1.1.3 Roadmap for a First Analysis 49
 - 2.1.1.3.1 Read Example Data 49
 - 2.1.1.3.2 Levels (Scales) of Measurement 49
 - 2.1.1.3.3 One-Dimensional Data 49
 - 2.1.1.3.4 Frequency Analysis 49
 - 2.1.1.3.5 Measures of Location 49
 - 2.1.1.3.6 Measures of Spread 50
 - 2.1.1.3.7 Higher-Dimensional Data 51
 - 2.1.1.3.8 Contingency Tables 51
 - 2.1.1.3.9 Scatter Plots (2D, 3D, and ∞ D) 51
 - 2.1.1.3.10 Correlation Analysis 51
 - 2.1.1.3.11 Regression Analysis 52
 - 2.1.1.3.12 Go on with Your Tour! 52
 - 2.1.2 Random Processes and Probability 52
 - 2.1.2.1 Random Variables 53
 - 2.1.2.2 Probability 53
 - 2.1.2.3 Densities and Distributions 55
 - 2.1.2.4 The Uniform Distribution 56
 - 2.1.2.5 The Normal Distribution 57
 - 2.1.2.6 Expected Value and Standard Deviation 58
 - 2.1.2.7 More on Distributions 59
 - 2.1.2.8 Quantiles and Confidence Intervals 60
 - 2.1.3 Inferential Statistics 62
 - 2.1.3.1 Is Crop A's Yield Really Higher? 62
 - 2.1.3.2 Structure of a Hypothesis Test 62
 - 2.1.3.3 The t -test 63
 - 2.1.3.4 Testing Normality 64
 - 2.1.3.5 Type I/II Errors, Power, and Effect Size 65
 - 2.1.3.6 Testing Regression Parameters 67
 - 2.1.3.7 Analysis of Variance 67
- 2.2 Linear Regression 69
 - 2.2.1 The Linear Regression Problem 70
 - 2.2.2 Solution Using Software 71
 - 2.2.3 The Coefficient of Determination 74
 - 2.2.4 Interpretation of the Regression Coefficients 75
 - 2.2.5 Checking Assumptions 76
 - 2.2.6 Nonlinear Linear Regression 76

2.3	Multiple Linear Regression	79
2.3.1	The Multiple Linear Regression Problem	79
2.3.2	Solution Using Software	80
2.3.3	Cross-Validation	84
2.4	Nonlinear Regression	87
2.4.1	The Nonlinear Regression Problem	87
2.4.2	Solution Using Software	87
2.4.3	Multiple Nonlinear Regression	91
2.4.4	Implicit and Vector-Valued Problems	93
2.5	Smoothing Splines	94
2.6	Neural Networks	97
2.6.1	General Idea	97
2.6.2	Feed-Forward Neural Networks	98
2.6.3	Solution Using Software	100
2.6.4	Interpretation of the Results	102
2.6.5	Generalization and Overfitting	104
2.6.6	Several Inputs Example	106
2.7	Big Data Analysis	109
2.7.1	From Data to Knowledge	109
2.7.2	Artificial Data	110
2.7.3	Influencing Factors and Interactions for z_1	111
2.7.4	Influencing Factors and Interactions for z_2 and z_3	112
2.7.5	Dimensional Reduction and Classification	114
2.7.5.1	Principal Component Analysis, Factor Analysis, and Correspondence Analysis	114
2.7.5.2	Classification	117
2.7.6	Conclusions	119
2.8	Signal Processing	119
2.8.1	Example, Idea, and Useful R Packages	119
2.8.2	Time-Series Classification Using <code>tsfresh</code> , Python and R	121
2.9	Design of Experiments	124
2.9.1	Completely Randomized Design	125
2.9.2	Randomized Complete Block Design	127
2.9.3	Latin Square Design	128
2.9.4	Factorial Designs	130
2.9.5	Optimal Sample Size	132
2.9.6	DOE Workflow	133
2.9.7	Optimal Designs	135
2.10	Other Phenomenological Modeling Approaches	138
2.10.1	Soft Computing	139
2.10.1.1	Fuzzy Model of a Washing Machine	140
2.10.2	Discrete Event Simulation	140

3 Mechanistic Models I: ODEs 142

3.1	Distinguished Role of Differential Equations	142
3.2	Introductory Examples	143

3.2.1	Archaeology Analogy	143
3.2.2	Body Temperature	144
3.2.2.1	Phenomenological Model	144
3.2.2.2	Application	146
3.2.3	Alarm Clock	146
3.2.3.1	Need for a Mechanistic Model	147
3.2.3.2	Applying the Modeling and Simulation Scheme	148
3.2.3.3	Setting Up the Equations	149
3.2.3.4	Comparing Model and Data	150
3.2.3.5	Validation Fails – What Now?	151
3.2.3.6	A Different Way to Explain the Temperature Memory	152
3.2.3.7	Limitations of the Model	153
3.3	General Idea of ODE's	154
3.3.1	Intrinsic Meaning of π	154
3.3.2	e^x Solves an ODE	154
3.3.3	Infinitely Many Degrees of Freedom	155
3.3.4	Intrinsic Meaning of the Exponential Function	156
3.3.5	ODEs as a Function Generator	157
3.4	Setting Up ODE Models	158
3.4.1	Body Temperature Example	158
3.4.1.1	Formulation of an ODE Model	158
3.4.1.2	ODE Reveals the Mechanism	159
3.4.1.3	ODE's Connect Data and Theory	160
3.4.1.4	Three Ways to Set Up ODEs	161
3.4.2	Alarm Clock Example	161
3.4.2.1	A System of Two ODEs	162
3.4.2.2	Parameter Values Based on <i>A Priori</i> Information	163
3.4.2.3	Result of a Hand-Fit	163
3.4.2.4	A Look into the Black Box	164
3.5	Some Theory You Should Know	165
3.5.1	Basic Concepts	165
3.5.2	First-Order ODEs	167
3.5.3	Autonomous, Implicit, and Explicit ODEs	168
3.5.4	The Initial Value Problem	168
3.5.5	Boundary Value Problems	169
3.5.6	Example of Nonuniqueness	170
3.5.7	ODE Systems	171
3.5.8	Linear Versus Nonlinear	173
3.6	Solution of ODE's: Overview	174
3.6.1	Toward the Limits of Your Patience	174
3.6.2	Closed Form Versus Numerical Solutions	175
3.7	Closed Form Solutions	176
3.7.1	Right-Hand Side Independent of the Independent Variable	176
3.7.1.1	General and Particular Solutions	176
3.7.1.2	Solution by Integration	177

3.7.1.3	Using Computer Algebra Software	178
3.7.1.4	Imposing Initial Conditions	179
3.7.2	Separation of Variables	181
3.7.2.1	Application to the Body Temperature Model	183
3.7.2.2	Solution Using <i>Maxima</i> and <i>Mathematica</i>	183
3.7.3	Variation of Constants	185
3.7.3.1	Application to the Body Temperature Model	186
3.7.3.2	Using Computer Algebra Software	187
3.7.3.3	Application to the Alarm Clock Model	188
3.7.3.4	Interpretation of the Result	189
3.7.4	Dust Particles in the ODE Universe	190
3.8	Numerical Solutions	192
3.8.1	Algorithms	192
3.8.1.1	The Euler Method	193
3.8.1.2	Example Application	194
3.8.1.3	Order of Convergence	195
3.8.1.4	Stiffness	196
3.8.2	Solving ODE's Using <i>Maxima</i>	197
3.8.2.1	Heuristic Error Control	198
3.8.2.2	ODE Systems	199
3.8.3	Solving ODEs Using R and <i>lsoda</i>	201
3.8.3.1	Local Error Control in <i>lsoda</i>	203
3.8.3.2	Effect of the Local Error Tolerances	203
3.8.3.3	A Rule of Thumb to Set the Tolerances	204
3.8.3.4	Example Applications	205
3.9	Fitting ODE's to Data	208
3.9.1	Parameter Estimation in the Alarm Clock Model	208
3.9.1.1	Estimating Two Parameters	210
3.9.1.2	Estimating Initial Values	211
3.9.1.3	Sensitivity of the Parameter Estimates	213
3.9.2	The General Parameter Estimation Problem	213
3.9.2.1	One State Variable Characterized by Data	214
3.9.2.2	Several State Variables Characterized by Data	215
3.9.3	Indirect Measurements Using Parameter Estimation	216
3.10	More Examples	216
3.10.1	Predator–Prey Interaction	216
3.10.1.1	Lotka–Volterra Model	217
3.10.1.2	General Dynamical Behavior	218
3.10.1.3	Nondimensionalization	219
3.10.1.4	Phase Plane Plots	220
3.10.2	Wine Fermentation	222
3.10.2.1	Setting Up a Mathematical Model	222
3.10.2.2	Yeast	223
3.10.2.3	Ethanol and Sugar	225
3.10.2.4	Nitrogen	226
3.10.2.5	Using a Hand-Fit to Estimate N_0	227

3.10.2.6	Parameter Estimation	228
3.10.2.7	Problems with Nonautonomous Models	230
3.10.2.8	Converting Data into a Function	231
3.10.2.9	Using Weighting Factors	232
3.10.3	Pharmacokinetics	232
3.10.4	Plant Growth	234
4	Mechanistic Models II: PDEs	237
4.1	Introduction	237
4.1.1	Limitations of ODE Models	237
4.1.2	Overview: Strange Animals, Sounds, and Smells	238
4.1.3	Two Problems You Should Be Able to Solve	239
4.2	The Heat Equation	241
4.2.1	Fourier's Law	241
4.2.2	Conservation of Energy	242
4.2.3	Heat Equation = Fourier's Law + Energy Conservation	243
4.2.4	Heat Equation in Multidimensions	244
4.2.5	Anisotropic Case	245
4.2.6	Understanding Off-diagonal Conductivities	246
4.3	Some Theory You Should Know	247
4.3.1	Partial Differential Equations	247
4.3.1.1	First-Order PDEs	248
4.3.1.2	Second-Order PDEs	249
4.3.1.3	Linear Versus Nonlinear	249
4.3.1.4	Elliptic, Parabolic, and Hyperbolic Equations	250
4.3.2	Initial and Boundary Conditions	252
4.3.2.1	Well Posedness	252
4.3.2.2	A Rule of Thumb	252
4.3.2.3	Dirichlet and Neumann Conditions	253
4.3.3	Symmetry and Dimensionality	254
4.3.3.1	1D Example	255
4.3.3.2	2D Example	256
4.3.3.3	3D Example	256
4.3.3.4	Rotational Symmetry	257
4.3.3.5	Mirror Symmetry	258
4.3.3.6	Symmetry and Periodic Boundary Conditions	258
4.4	Closed-Form Solutions	259
4.4.1	Problem 1	259
4.4.2	Separation of Variables	260
4.4.3	A Particular Solution for Validation	261
4.5	Numerical Solution of PDEs	262
4.6	The Finite Difference Method	263
4.6.1	Replacing Derivatives with Finite Differences	263
4.6.2	Formulating an Algorithm	264
4.6.3	Implementation in R	265
4.6.4	Error and Stability Issues	266

4.6.5	Explicit and Implicit Schemes	266
4.6.6	Computing Electrostatic Potentials	267
4.6.7	Iterative Methods for the Linear Equations	268
4.6.8	Billions of Unknowns	269
4.7	The Finite Element Method	269
4.7.1	Weak Formulation of PDEs	270
4.7.2	Approximation of the Weak Formulation	272
4.7.3	Appropriate Choice of the Basis Functions	273
4.7.4	Generalization to Multidimensions	274
4.7.5	Summary of the Main Steps	274
4.8	The Finite Volume Method	276
4.8.1	Weak Formulations of Conservation Equations	276
4.8.2	Discretization	277
4.8.3	Evaluation of the Fluxes	279
4.8.4	A Simple 1D Finite Volume Method	279
4.8.5	Error and Stability Issues	282
4.8.6	Notes on the Finite Volume Method	282
4.9	Software Packages to Solve PDEs	283
4.10	A Sample Session on the Numerical Solution of Thermal Conduction	285
4.10.1	Geometry Definition Step	286
4.10.1.1	Organization of the GUI	286
4.10.1.2	Constructing the Geometrical Primitives	287
4.10.1.3	Excising the Sphere	288
4.10.1.4	Defining the Boundaries	289
4.10.2	OpenFOAM Terminal	290
4.10.3	Mesh Generation Step	291
4.10.3.1	Blockmesh	292
4.10.3.2	Surface Features	294
4.10.3.3	SnappyHexMesh	295
4.10.4	Case Definition Step	299
4.10.4.1	Transport Properties	299
4.10.4.2	Boundary and Initial Conditions	300
4.10.4.3	Solution Settings	301
4.10.5	Solving the Problem	306
4.10.6	Postprocessing	308
4.10.7	Excursus: Mesh Visualization	312
4.10.8	Excursus: Steady-State Time Discretization with the SIMPLE Algorithm	313
4.10.9	List of Terminal Commands	315
4.11	A Look Beyond the Heat Equation	316
4.11.1	Diffusion and Convection	317
4.11.2	Flow in Porous Media	318
4.11.2.1	Impregnation Processes	319
4.11.2.2	Two-Phase Flow in Porous Media	321
4.11.2.3	Water Retention and Relative Permeability	321

4.11.2.4	Asparagus Drip Irrigation	322
4.11.2.5	Multiphase Flow and Poroelasticity	323
4.11.3	Structural Mechanics	323
4.11.3.1	Linear Static Elasticity	324
4.11.3.2	Example: Eye Tonometry	326
4.12	Computational Fluid Dynamics (CFD)	328
4.12.1	Navier–Stokes Equations	329
4.12.2	Coupled Problems	330
4.13	Numerical Solutions of Example Flow Problems	331
4.13.1	Single-Phase Flow	332
4.13.1.1	Backward-Facing Step Problem	332
4.13.1.2	Creating the Geometry in FreeCAD	333
4.13.1.3	CfdOF Workbench and Mesh Generation	335
4.13.1.4	Physics Model	340
4.13.1.5	Solution Process	341
4.13.1.6	Postprocessing	342
4.13.1.6.1	Streamlines	342
4.13.1.6.2	Line Integral Convolution	343
4.13.1.6.3	Plot Over Line and Data Export	343
4.13.2	Two-Phase Flow	345
4.13.2.1	Problem Description	346
4.13.2.2	Creating and Exporting the Geometry in Salome	346
4.13.2.3	Geometry Import and Boundary Definition	347
4.13.2.4	Physics Model and Phase Definitions	347
4.13.2.5	Mesh Generation	348
4.13.2.6	Solution Process	348
4.13.2.7	Postprocessing	350
4.14	Other Mechanistic Modeling Approaches	352
4.14.1	Difference Equations	352
4.14.2	Cellular Automata	353
4.14.3	Optimal Control Problems	354
4.14.4	Differential-Algebraic Problems	356
4.14.5	Inverse Problems	356
5	Virtualization	358
5.1	Introduction	358
5.2	Virtual Plants	359
5.2.1	Static Models Using 3D-Digitization	360
5.2.1.1	Deriving Geometric Characteristics	362
5.2.1.2	Shape Models for Plant Organs	362
5.2.1.3	Allometric, Growth, and Response Functions	363
5.2.2	Dynamic Models Using Lindenmayer Systems	365
5.2.3	Functional–Structural Plant Models	370
5.3	Examples of Advanced Applications	371
5.3.1	Greenhouse Cucumber	371
5.3.1.1	Light Distribution Within Cucumber Canopies	372

5.3.1.2	Photosynthesis and its Limitations	374
5.3.1.3	Salt Effects	378
5.3.1.4	How to Predict Responses of Plant Architecture to Changing Light Environments	379
5.3.1.5	How to Predict Fruit Growth, While Accounting for Changing Plant Architectures	384
5.3.2	Virtual Riesling Vineyard	386
5.3.2.1	Introduction to the Model <i>Virtual Riesling</i> and Simulation Studies on Vineyard Level	387
5.3.2.2	Learning from Historical Temperature Data	389
5.3.2.3	How to Predict Effects of Leaf Removal on Light Absorption in a Vineyard	390
5.3.2.4	Toward Predicting Sunburn of Grapevine Berries	391
5.3.2.5	Toward Better Understanding How CO ₂ Enrichment Impacts the Growth of Grapevine	392
6	Crashcourses and Book Software	395
6.1	Crashcourse R	395
6.1.1	Preliminaries	395
6.1.1.1	Installation	395
6.1.1.2	Book Software and Course Data	396
6.1.2	Basic Workflow	396
6.1.2.1	Working Directory	396
6.1.2.2	Console Mode	396
6.1.2.3	Programming Mode	397
6.1.2.4	Documentation Mode	397
6.1.2.5	Preprocessing and Analysis of Spreadsheet Data	399
6.1.2.6	Tidyverse and Recommended Default Packages	400
6.1.2.7	Help and Documentation	401
6.1.3	Knowledge Database	401
6.1.3.1	Working Environments	401
6.1.3.1.1	RStudio	401
6.1.3.1.2	RStudio Project Workflow	402
6.1.3.1.3	Alternatives	403
6.1.3.2	Data	403
6.1.3.2.1	Import and Export	403
6.1.3.2.2	Variables	404
6.1.3.2.3	Vectors, Matrices, and Arrays	405
6.1.3.2.4	data.frames	406
6.1.3.2.5	Tibbles	407
6.1.3.2.6	Data Types	408
6.1.3.2.7	Data Operations Using dplyr and forcats	409
6.1.3.2.8	Dates and Times	411
6.1.3.2.9	Logical Data	412
6.1.3.2.10	Lists	413
6.1.3.3	Plots	413

- 6.1.3.3.1 Base R 413
 - 6.1.3.3.2 Colors 415
 - 6.1.3.3.3 The Grammar of Graphics: ggplot2 416
 - 6.1.3.3.4 plotly and rgl 420
 - 6.1.3.4 Programming 421
 - 6.1.3.4.1 Basics 421
 - 6.1.3.4.2 Functions 421
 - 6.1.3.4.3 Conditional Operations 422
 - 6.1.3.4.4 Repeated Operations 422
 - 6.1.3.4.5 Piping 423
 - 6.1.3.4.6 Text (character, string) Operations 424
 - 6.1.3.4.7 Quarto/Markdown 426
 - 6.1.3.4.8 Booksoftware Packages 426
 - 6.2 Crashcourse Maxima 426
 - 6.2.1 Code Examples in the Book Software 426
 - 6.2.2 Software, Documentation, and Interfaces 427
 - 6.2.3 Basics 427
 - 6.2.4 Equations 429
 - 6.2.5 Functions, Derivatives, Integrals 429
 - 6.2.6 Plots 430
 - 6.2.7 Differential Equations 431
 - 6.2.8 Complex Programs and Mixed Topics 431
 - 6.3 CrashCrashcourse Python (and all the rest) 433
 - 6.4 Book Software and GmLinux 434

- References 435**
- Index 455**