

Contents

Preface to the second edition — V

1 Introduction — 1

- 1.1 Relationships between mathematical subjects and data science — 2
- 1.2 Structure of the book — 4
 - 1.2.1 Part one — 4
 - 1.2.2 Part two — 4
 - 1.2.3 Part three — 5
- 1.3 Our motivation for writing this book — 5
- 1.4 Examples and listings — 6
- 1.5 How to use this book — 7

Part I: Introduction to R

2 Overview of programming paradigms — 11

- 2.1 Introduction — 11
- 2.2 Imperative programming — 12
- 2.3 Functional programming — 13
- 2.4 Object-oriented programming — 15
- 2.5 Logic programming — 17
- 2.6 Other programming paradigms — 18
 - 2.6.1 The multiparadigm language R — 18
- 2.7 Compiler versus interpreter languages — 20
- 2.8 Semantics of programming languages — 21
- 2.9 Further reading — 21
- 2.10 Summary — 22

3 Setting up and installing the R program — 23

- 3.1 Installing R on Linux — 23
- 3.2 Installing R on MAC OS X — 24
- 3.3 Installing R on Windows — 24
- 3.4 Using R — 24
- 3.5 Summary — 24

4 Installation of R packages — 26

- 4.1 Installing packages from CRAN — 26
- 4.2 Installing packages from Bioconductor — 26
- 4.3 Installing packages from GitHub — 27
- 4.4 Installing packages manually — 27

4.4.1	Terminal and unix commands —	27
4.4.2	Package installation —	28
4.5	Activation of a package in an R session —	29
4.6	Summary —	29
5	Introduction to programming in R —	30
5.1	Basic elements of R —	30
5.1.1	Navigating directories —	31
5.1.2	System functions —	31
5.1.3	Getting help —	32
5.2	Basic programming —	33
5.2.1	If-clause —	33
5.2.2	Switch —	34
5.2.3	Loops —	35
5.2.4	For-loop —	35
5.2.5	While-loop —	35
5.2.6	Logic behind a For-loop —	36
5.2.7	Break —	39
5.2.8	Repeat-loop —	39
5.3	Data structures —	39
5.3.1	Vector —	39
5.3.2	Matrix —	42
5.3.3	List —	45
5.3.4	Array —	46
5.3.5	Data frame —	47
5.3.6	Environment —	48
5.3.7	Removing variables from the workspace —	49
5.3.8	Factor —	49
5.3.9	Date and Time —	50
5.3.10	Information about R objects —	50
5.4	Handling character strings —	51
5.4.1	The function <i>nchar()</i> —	51
5.4.2	The function <i>paste()</i> —	52
5.4.3	The function <i>substr()</i> —	52
5.4.4	The function <i>strsplit()</i> —	53
5.4.5	Regular expressions —	53
5.5	Sorting vectors —	56
5.6	Writing functions —	57
5.6.1	One input argument and one output value —	57
5.6.2	Scope of variables —	59
5.6.3	One input argument, many output values —	60
5.6.4	Many input arguments, many output values —	61

5.7	Writing and reading data — 61
5.7.1	Writing data to a file — 61
5.7.2	Reading data from a file — 63
5.7.3	Low level reading functions — 64
5.7.4	Summary of writing and reading functions — 67
5.7.5	Other data formats — 67
5.8	Useful commands — 68
5.8.1	The function <i>which()</i> — 68
5.8.2	The function <i>apply()</i> — 69
5.8.3	Set commands — 70
5.8.4	The function <i>unique()</i> — 70
5.8.5	Testing arguments and converting variables — 71
5.8.6	The function <i>sample()</i> — 71
5.8.7	The function <i>try()</i> — 73
5.8.8	The function <i>system()</i> — 74
5.9	Practical usage of R — 74
5.9.1	Advantage over GUI software — 75
5.10	Summary — 75
6	Creating R packages — 76
6.1	Requirements — 76
6.1.1	R base packages — 76
6.1.2	R repositories — 77
6.1.3	Rtools — 77
6.2	R code optimization — 77
6.2.1	Profiling an R script — 78
6.2.2	Byte code compilation — 78
6.2.3	GPU library, code, and others — 79
6.2.4	Exception handling — 79
6.3	S3, S4, and RC object-oriented systems — 80
6.3.1	The S3 class — 80
6.3.2	The S4 class — 82
6.3.3	Reference class (RC) system — 83
6.4	Creating an R package based on the S3 class system — 84
6.4.1	R program file — 84
6.4.2	Building an R package — 86
6.5	Checking the package — 87
6.6	Installation and usage of the package — 87
6.7	Loading and using a package — 88
6.7.1	Content of the files edited when generating the package — 88
6.8	Summary — 91

Part II: Graphics in R

7	Basic plotting functions — 95
7.1	Plot — 95
7.1.1	Adding multiple curves in one plot — 97
7.1.2	Adding horizontal and vertical lines — 99
7.1.3	Opening a new figure window — 100
7.2	Histograms — 100
7.3	Bar plots — 101
7.4	Pie charts — 102
7.5	Dot plots — 102
7.6	Strip and rug plots — 105
7.7	Density plots — 107
7.8	Combining a scatterplot with histograms: the layout function — 110
7.9	Three-dimensional plots — 111
7.10	Contour and image plots — 112
7.11	Summary — 113
8	Advanced plotting functions: ggplot2 — 114
8.1	Introduction — 114
8.2	<i>qplot()</i> — 114
8.3	<i>ggplot()</i> — 117
8.3.1	Simple examples — 118
8.3.2	Multiple data sets — 120
8.3.3	<i>geoms()</i> — 122
8.3.4	Smoothing — 125
8.4	Summary — 128
9	Visualization of networks — 129
9.1	Introduction — 129
9.2	<i>igraph</i> — 129
9.2.1	Generation of regular and complex networks — 131
9.2.2	Basic network attributes — 132
9.2.3	Layout styles — 135
9.2.4	Plotting networks — 136
9.2.5	Analyzing and manipulating networks — 137
9.3	<i>NetBioV</i> — 137
9.3.1	Global network layout — 138
9.3.2	Modular network layout — 138
9.3.3	Layered network (multiroot) layout — 140
9.3.4	Further features — 140
9.3.5	Examples: Visualization of networks using <i>NetBioV</i> — 141

9.4 Summary — 144

Part III: Mathematical basics of data science

10 Mathematics as a language for science — 149

- 10.1 Introduction — 149
- 10.2 Numbers and number operations — 151
- 10.3 Sets and set operations — 153
- 10.4 Boolean logic — 155
- 10.5 Sum, product, and Binomial coefficients — 157
- 10.6 Further symbols — 161
- 10.7 Importance of definitions and theorems — 164
- 10.8 Summary — 165

11 Computability and complexity — 166

- 11.1 Introduction — 166
- 11.2 A brief history of computer science — 167
- 11.3 Turing machines — 168
- 11.4 Computability — 169
- 11.5 Complexity of algorithms — 170
- 11.5.1 Bounds — 171
- 11.5.2 Examples — 172
- 11.5.3 Important properties of the O -notation — 174
- 11.5.4 Known complexity classes — 174
- 11.6 Summary — 175

12 Linear algebra — 176

- 12.1 Vectors and matrices — 176
- 12.1.1 Vectors — 176
- 12.1.2 Vector representations in other coordinates systems — 189
- 12.1.3 Matrices — 197
- 12.2 Operations with matrices — 201
- 12.3 Special matrices — 204
- 12.4 Trace and determinant of a matrix — 205
- 12.5 Subspaces, dimension, and rank of a matrix — 206
- 12.6 Eigenvalues and eigenvectors of a matrix — 209
- 12.7 Matrix norms — 212
- 12.8 Matrix factorization — 213
- 12.8.1 LU factorization — 213
- 12.8.2 Cholesky factorization — 215
- 12.8.3 QR factorization — 216

- 12.8.4 Singular value decomposition — **218**
- 12.9 Systems of linear equations — **221**
- 12.10 Exercises — **224**

13 Analysis — 225

- 13.1 Introduction — **225**
- 13.2 Limiting values — **225**
- 13.3 Differentiation — **228**
- 13.4 Extrema of a function — **233**
- 13.5 Taylor series expansion — **235**
- 13.6 Integrals — **239**
- 13.6.1 Properties of definite integrals — **240**
- 13.6.2 Numerical integration — **240**
- 13.7 Polynomial interpolation — **241**
- 13.8 Root finding methods — **243**
- 13.9 Further reading — **247**
- 13.10 Exercises — **247**

14 Differential equations — 249

- 14.1 Ordinary differential equations (ODE) — **249**
- 14.1.1 Initial value ODE problems — **249**
- 14.2 Partial differential equations (PDE) — **254**
- 14.2.1 First-order PDE — **255**
- 14.2.2 Second-order PDE — **255**
- 14.2.3 Boundary and initial conditions — **256**
- 14.2.4 Well-posed PDE problems — **256**
- 14.3 Exercises — **260**

15 Dynamical systems — 262

- 15.1 Introduction — **262**
- 15.2 Population growth models — **264**
- 15.2.1 Exponential population growth model — **264**
- 15.2.2 Logistic population growth model — **264**
- 15.2.3 Logistic map — **266**
- 15.3 The Lotka–Volterra or predator–prey system — **270**
- 15.4 Cellular automata — **273**
- 15.5 Random Boolean networks — **276**
- 15.6 Case studies of dynamical system models with complex attractors — **283**
- 15.6.1 The Lorenz attractor — **283**
- 15.6.2 Clifford attractor — **285**
- 15.6.3 Ikeda attractor — **286**
- 15.6.4 The Peter de Jong attractor — **286**

15.6.5	Rössler attractor —	288
15.7	Fractals —	289
15.7.1	The Sierpiński carpet and triangle —	289
15.7.2	The Barnsley fern —	291
15.7.3	Julia sets —	293
15.7.4	Mandelbrot set —	294
15.8	Exercises —	296
16	Graph theory and network analysis —	299
16.1	Introduction —	299
16.2	Basic types of networks —	300
16.2.1	Undirected networks —	300
16.2.2	Geometric visualization of networks —	301
16.2.3	Directed and weighted networks —	302
16.2.4	Walks, paths, and distances in networks —	304
16.3	Quantitative network measures —	305
16.3.1	Degree and degree distribution —	305
16.3.2	Clustering coefficient —	306
16.3.3	Path-based measures —	306
16.3.4	Centrality measures —	307
16.4	Graph algorithms —	308
16.4.1	Breadth-first search —	309
16.4.2	Depth-first search —	309
16.4.3	Shortest paths —	311
16.4.4	Minimum spanning tree —	315
16.5	Network models and graph classes —	317
16.5.1	Trees —	317
16.5.2	Generalized trees —	318
16.5.3	Random networks —	319
16.5.4	Small-world networks —	320
16.5.5	Scale-free networks —	322
16.6	Further reading —	323
16.7	Summary —	324
16.8	Exercises —	324
17	Probability theory —	325
17.1	Events and sample space —	325
17.2	Set theory —	326
17.3	Definition of probability —	328
17.4	Conditional probability —	329
17.5	Conditional probability and independence —	330
17.6	Random variables and their distribution function —	331

17.7	Discrete and continuous distributions —	333
17.7.1	Uniform distribution —	334
17.8	Expectation values and moments —	334
17.8.1	Expectation values —	334
17.8.2	Variance —	335
17.8.3	Moments —	336
17.8.4	Covariance and correlation —	336
17.9	Bivariate distributions —	337
17.10	Multivariate distributions —	338
17.11	Important discrete distributions —	339
17.11.1	Bernoulli distribution —	339
17.11.2	Binomial distribution —	340
17.11.3	Geometric distribution —	342
17.11.4	Negative binomial distribution —	343
17.11.5	Poisson distribution —	343
17.12	Important continuous distributions —	344
17.12.1	Exponential distribution —	345
17.12.2	Beta distribution —	345
17.12.3	Gamma distribution —	346
17.12.4	Normal distribution —	347
17.12.5	Chi-square distribution —	349
17.12.6	Student's t -distribution —	350
17.12.7	Log-normal distribution —	351
17.12.8	Weibull distribution —	352
17.13	Bayes' theorem —	353
17.14	Information theory —	356
17.14.1	Entropy —	356
17.14.2	Kullback–Leibler divergence —	358
17.14.3	Mutual information —	359
17.15	Law of large numbers —	361
17.16	Central limit theorem —	364
17.17	Concentration inequalities —	364
17.17.1	Hoeffding's inequality —	365
17.17.2	Cauchy–Schwartz inequality —	365
17.17.3	Chernoff bounds —	366
17.18	Further reading —	366
17.19	Summary —	367
17.20	Exercises —	367

18 Optimization — 369

18.1	Introduction —	369
18.2	Formulation of an optimization problem —	370

18.3	Unconstrained optimization problems —	371
18.3.1	Gradient-based methods —	371
18.3.2	Derivative-free methods —	379
18.4	Constrained optimization problems —	384
18.4.1	Constrained linear optimization problems —	384
18.4.2	Constrained nonlinear optimization problems —	388
18.4.3	Lagrange multiplier method —	388
18.5	Some applications in statistical machine learning —	390
18.5.1	Maximum likelihood estimation —	391
18.5.2	Support vector classification —	392
18.6	Further reading —	393
18.7	Summary —	394
18.8	Exercises —	394

Bibliography — 397

Index — 405