

Contents

Part I Linear Algebra

1	Linear Equations	3
1.1	Row Reduction Methods	4
1.1.1	Gaussian Elimination	5
1.1.2	Pivoting	7
1.1.3	R Code: Gaussian Elimination and Backward Substitution	8
1.1.4	Gauss-Jordan Elimination	9
1.1.5	LU Decomposition	10
1.1.6	R Code: LU Decomposition	14
1.1.7	Cholesky Decomposition	15
1.1.8	R Code: Cholesky Decomposition of a Symmetric Matrix	18
1.2	Matrix Methods	19
1.2.1	Determinant	19
1.2.2	R Code: Determinant	21
1.2.3	Determinants and Linear Dependencies	21
1.2.4	R Code: Reduced Row Echelon Form and Linear Dependencies	22
1.2.5	Using the Determinant to Solve Linear Equations	23
1.2.6	R Code: Cramer's Rule	24
1.2.7	Matrix Inverse	24
1.2.8	R Code: Calculate Inverse Using Reduced Row Echelon Form	26
1.2.9	Norms, Errors, and the Condition Number of a Matrix	26
1.2.10	R Code: Condition Number and Norm Ratio	33

1.3	Iterative Methods	34
1.3.1	Jacobi's Method	34
1.3.2	Gauss-Seidel Method	35
1.3.3	Convergence	36
1.3.4	R Code: Gauss-Seidel	37
1.4	Chapter Summary	38
	References	38
2	Least Squares Estimation	39
2.1	Line of Best Fit	39
2.1.1	Deriving a Line of Best Fit	39
2.1.2	Minimizing the Sum of Squared Differences	41
2.1.3	Normal Equations	42
2.1.4	Analytic Solution	42
2.2	Solving the Normal Equations	43
2.2.1	The QR Decomposition	43
2.2.2	Advantages of an Orthonormal System	44
2.2.3	Hat Matrix	45
2.2.4	Coefficients	47
2.2.5	Summary	48
2.2.6	R Code: QR Solver	49
2.3	Performing the QR Decomposition	49
2.3.1	Gram-Schmidt Orthogonalization	49
2.3.2	R Code: QR Decomposition; Gram-Schmidt Orthogonalization	53
2.3.3	Givens Rotations	54
2.3.4	R Code: QR Decomposition; Givens Rotations	58
2.3.5	Householder Reflections	58
2.3.6	R Code: QR Decomposition; Householder Reflectors	61
2.3.7	Comparing the Decompositions	61
2.3.8	R Code: QR Decomposition Comparison	62
2.4	Linear Regression and its Assumptions	62
2.4.1	Linearity	63
2.4.2	Nature of the Variables	64
2.4.3	Errors and their Distribution	65
2.4.4	Regression Coefficients	67
2.5	OLS Estimation and the Gauss-Markov Theorem	67
2.5.1	Proving the OLS Estimates are Unbiased	68
2.5.2	Proving the OLS Estimates are Efficient	69
2.6	Maximum Likelihood Estimation	71
2.6.1	Log Likelihood Function	71
2.6.2	R Code: Maximum Likelihood Estimation	74
2.7	Beyond OLS Estimation	74
2.8	Chapter Summary	75
	References	76

3	Linear Regression	77
3.1	Simple Linear Regression	77
3.1.1	Inspecting the Residuals	79
3.1.2	Describing the Model's Fit to the Data	80
3.1.3	Testing the Model's Fit to the Data	80
3.1.4	Variance Estimates	81
3.1.5	Tests of Significance	82
3.1.6	Confidence Intervals	83
3.1.7	R Code: Confidence Interval Simulation	83
3.1.8	Confidence Regions	83
3.1.9	Forecasting	84
3.1.10	R Code: Simple Linear Regression	87
3.1.11	R Code: Simple Linear Regression: Graphs	88
3.2	Multiple Regression	89
3.2.1	Regression Model	90
3.2.2	Regression Coefficients	92
3.2.3	Variance Estimates, Significance Tests, and Confidence Intervals	94
3.2.4	Model Comparisons and Changes in R^2	95
3.2.5	Comparing Predictors	97
3.2.6	Forecasting	98
3.2.7	R Code: Multiple Regression	99
3.3	Polynomials, Cross-Products, and Categorical Predictors	99
3.3.1	Polynomial Regression	100
3.3.2	R Code: Polynomial Regression	105
3.3.3	Cross-Product Terms	105
3.3.4	R Code: Cross-Product Terms and Simple Slopes	109
3.3.5	Johnson-Neyman Procedure	110
3.3.6	R Code: Johnson-Neyman Procedure	111
3.3.7	Categorical Predictors	111
3.3.8	R Code: Contrast Codes for Categorical Predictors	113
3.3.9	Summary	114
3.4	Chapter Summary	114
	References	115
4	Eigen Decomposition	117
4.1	Diagonalization	117
4.1.1	Eigenvector Multiplication	117
4.1.2	The Characteristic Equation	119
4.1.3	R Code: Eigen Decomposition of a 2×2 Matrix with Real Eigenvalues	121
4.1.4	Properties of a Diagonalized Matrix	121
4.2	Eigenvalue Calculation	122
4.2.1	Basic QR Algorithm	122
4.2.2	R Code: QR Algorithm Using Gram-Schmidt Orthogonalization	124

4.2.3	Improving the QR Algorithm	124
4.2.4	R Code: Hessenberg Form	126
4.2.5	R Code: Shifted QR Algorithm	129
4.2.6	Francis (Implicitly-Shifted QR) Algorithm	129
4.2.7	R Code: Francis Bulge Chasing Algorithm (Single-Shift)	133
4.3	Eigenvector Calculation	133
4.3.1	R Code: Eigenvector Calculation Using LU Decomposition	135
4.4	Dynamical Systems	135
4.4.1	Matrix Power	135
4.4.2	R Code: Matrix Power Using Eigen Decomposition	136
4.4.3	Power Method for Dominant Eigen Pair	136
4.4.4	Population Ecology	137
4.4.5	Predator-Prey Model	139
4.4.6	Markov Chains	141
4.4.7	R Code: Power Method and Applications	144
4.5	Schur Decomposition	144
4.5.1	Compute an Initial Eigenvector	145
4.5.2	Create an Orthonormal Basis	145
4.5.3	Rotate	146
4.5.4	Deflate and Continue Iterating	146
4.5.5	R Code: Schur Decomposition	147
4.6	Chapter Summary	148
	Reference	148
5	Singular Value Decomposition	149
5.1	Introduction	149
5.1.1	Illustration	150
5.1.2	Geometric Interpretation	151
5.1.3	R Code: Singular Value Decomposition	154
5.1.4	Matrix Properties	155
5.1.5	Pseudoinverse	155
5.1.6	Solving Linear Equations	155
5.1.7	R Code: Matrix Rank and Pseudoinverse	156
5.2	Calculating the SVD	157
5.2.1	Description	157
5.2.2	Calculations	157
5.2.3	R Code: One-Sided Jacobi Algorithm	160
5.3	Data Reduction and Image Compression	161
5.3.1	R Code: Image Compression Using Singular Value Decomposition	162
5.4	Principal Components Analysis	163
5.4.1	Mechanics	163

5.4.2	R Code: Principal Components Analysis	166
5.4.3	Total Least Squares	167
5.4.4	R Code: Total Least Squares	170
5.4.5	Dimension Reduction	170
5.4.6	R Code: Principal Components Analysis of Cereal Data	176
5.4.7	Data Construction	176
5.4.8	R Code: Data Construction	177
5.5	Collinearity	177
5.5.1	Using the SVD to Detect Collinearity	178
5.5.2	R Code: Collinearity Detection	182
5.5.3	Principal Components Regression	182
5.5.4	R Code: Principal Components Regression of (Fictitious) NFL Data	183
5.6	Chapter Summary	185
	References	186

Part II Bias and Efficiency

6	Generalized Least Squares Estimation	189
6.1	Gauss–Markov Violations	189
6.1.1	R Code: Simulations for Fig. 6.1	191
6.2	Generalized Least Squares	192
6.2.1	R Code: OLS Estimation as GLS Estimation	193
6.2.2	OLS and GLS	195
6.2.3	R Code: Generalized Least Squares Estimation	196
6.3	Heteroscedasticity and Feasible Weighted Least Squares	196
6.3.1	Assessing Heteroscedasticity	196
6.3.2	R Code: Breusch–Pagan Test of Heteroscedasticity	198
6.3.3	Feasible Weighted Least Squares	198
6.3.4	R Code: Feasible Weighted Least Squares	199
6.3.5	Heteroscedasticity Consistent Covariance Matrix	201
6.3.6	Summary	202
6.3.7	R Code: Heteroscedasticity Consistent Covariance Matrix	202
6.3.8	Confidence Interval Simulation	203
6.3.9	R Code: Heteroscedasticity Confidence Interval Simulation	204
6.4	Autocorrelated Errors	204
6.4.1	Mathematical Representation	205
6.4.2	Covariance Matrix	206
6.4.3	Detecting Autocorrelations	206
6.4.4	R Code: Detecting Autocorrelations	208
6.4.5	Accommodating Autocorrelated Errors	208
6.4.6	Feasible Generalized Least Squares	210
6.4.7	R Code: Feasible Generalized Least Squares	211

6.4.8	Autocorrelation Consistent Covariance Matrix	212
6.4.9	Summary	212
6.4.10	R Code: Autocorrelation Consistent Covariance Matrix	215
6.5	Chapter Summary	216
	References	217
7	Robust Regression	219
7.1	Assessing Normality	220
7.1.1	Tests of Normality	221
7.1.2	R Code: Assessing the Normality of the Residuals	222
7.1.3	Influence and Normality	222
7.1.4	Leverage and Influence	223
7.1.5	Cook's D	224
7.1.6	Illustration	226
7.1.7	Handling Influential Observations	227
7.1.8	R Code: Cook's D	228
7.2	Robust Estimators and Influential Observations	228
7.2.1	Breakdown Point	229
7.2.2	Efficiency	229
7.2.3	R Code: Robust Regression Simulation	230
7.3	Resistant Estimation	231
7.3.1	Least Absolute Regression	231
7.3.2	R Code: Least Absolute Regression	232
7.3.3	Least Median of Squares	233
7.3.4	R Code: Least Median of Squares	235
7.4	M Estimation	236
7.4.1	Weighting Methods	236
7.4.2	Algorithm	237
7.4.3	R Code: Robust Regression with M Estimation	239
7.5	Bootstrapped Confidence Intervals	239
7.5.1	Case Resampling vs. Residual Resampling	240
7.5.2	Confidence Intervals	241
7.5.3	R Code: Bootstrapping with Robust Regression (M Estimation)	243
7.6	MM Estimation	244
7.6.1	S Estimation	244
7.6.2	R Code: S Estimation (Part 1)	246
7.6.3	R Code: MM Estimation (compact form with sub functions)	247
7.6.4	Application	248
7.6.5	R Code: Robust Regression of Star Data	250
7.7	Concluding Remarks	251
7.8	Chapter Summary	251
	References	252

8	Model Selection and Biased Estimation	253
8.1	Prediction Error and Model Complexity	253
8.1.1	Prediction Errors and the Bias-Variance Tradeoff	254
8.1.2	Cross-Validation	255
8.1.3	Information Criteria Measures and Model Selection	257
8.1.4	R Code: Cross Validation and Information Criteria Measures	258
8.2	Subset Selection Methods	259
8.2.1	Stepwise Regression	259
8.2.2	R Code: Fictitious Data Predicting College Performance	261
8.2.3	R Code: Stepwise Regression	265
8.2.4	Best Subset Regression	266
8.2.5	R Code: Sweep Operator	268
8.2.6	R Code: Sweep Operator for Best Subset Regression	270
8.2.7	Branch and Bound Algorithm	271
8.2.8	R Code: Branch and Bound (Compact Form)	273
8.2.9	Comparing the Models	274
8.2.10	R Code: Model Comparison	274
8.3	Shrinkage Estimators and Regularized Regression	276
8.3.1	Ridge Regression	276
8.3.2	R Code: Ridge Regression: Augmented Matrix Method	279
8.3.3	R Code: Ridge Regression	281
8.3.4	Lasso	281
8.3.5	R Code: LASSO	284
8.4	Comparing the Methods	285
8.5	Chapter Summary	286
	References	287
9	Cubic Splines and Additive Models	289
9.1	Piecewise Polynomials and Regression Splines	289
9.1.1	Truncated Power Basis	291
9.1.2	Natural Cubic Spline	293
9.1.3	R Code: Truncated Power Series and Natural Cubic Spline Bases	294
9.1.4	B Spline Basis	294
9.1.5	R Code: B-Spline Basis	298
9.1.6	Bias-Variance Trade-Off	299
9.2	Penalized Smoothing Splines	299
9.2.1	Reinsch Form	300

9.2.2	R Code: Penalized Smoothing Spline: Reinsch Form	302
9.2.3	P-Splines	302
9.2.4	Statistical Inference and Confidence Intervals	305
9.2.5	Comparing Penalized Smoothing Splines and Regression Splines	307
9.2.6	R Code: P-Spline	309
9.3	Additive Models	309
9.3.1	Fitting an Additive Model	310
9.3.2	Backfitting	311
9.3.3	Partial Slopes	312
9.3.4	Model Selection and Inference	313
9.3.5	R Code: Additive Model: Backfitting	314
9.3.6	Penalized Least Squares	315
9.3.7	R Code: Additive Model: Penalized Least Squares	317
9.4	Chapter Summary	318
	References	319

Part III Nonlinear Models

10	Nonlinear Regression and Optimization	323
10.1	Comparing Linear and Nonlinear Models	323
10.1.1	Model Representation	323
10.1.2	Partial Derivatives	325
10.1.3	Parameter Estimation	325
10.1.4	Standard Errors, Parameter Interpretation, and Degrees of Freedom	325
10.1.5	Variety	326
10.2	Root Finding Algorithms	326
10.2.1	Newton's Method	328
10.2.2	Secant Method	329
10.2.3	R Code: Root-Finding Algorithms	330
10.3	Optimization	331
10.3.1	Exponential Growth Model	331
10.3.2	Newton-Raphson	333
10.3.3	R Code: Newton-Raphson	335
10.3.4	Fisher's Method of Scoring	335
10.3.5	R Code: Fisher's Method of Scoring	337
10.3.6	Gauss-Newton	338
10.3.7	R Code: Gauss-Newton	340
10.3.8	BFGS Algorithm	340
10.3.9	R Code: BFGS	343
10.3.10	Nelder-Mead	344
10.3.11	R Code: Nelder-Mead (Compact Form)	348
10.3.12	Summary	349

10.4	Missing Observations	349
10.4.1	Classifying Missing Data	349
10.4.2	Maximum Likelihood Estimation and the Expectation-Maximization Algorithm	350
10.4.3	Bivariate Example	351
10.4.4	Multivariate Illustration	354
10.4.5	R Code: EM Algorithm for Multivariate Normal with Missing Data	356
10.4.6	Multiple Regression with Missing Observations	357
10.4.7	R Code: EM Regression with Bootstrapped Standard Errors	358
10.5	Chapter Summary	359
	References	359
11	Generalized Linear Models	361
11.1	Generalized Linear Models	361
11.1.1	Log Likelihood Functions	362
11.1.2	Components of a Generalized Linear Model	364
11.1.3	Iteratively Reweighted Least Squares Estimation	365
11.1.4	Canonical Link	367
11.1.5	R Code: IRLS Estimation for GLM with Canonical Links	368
11.2	Poisson Distribution	369
11.2.1	Estimation	370
11.2.2	Deviance and Goodness of Fit	371
11.2.3	Goodness of Fit	372
11.2.4	Regression Coefficients and Fitted Values	373
11.2.5	Standard Errors, Tests of Significance, and Confidence Intervals	374
11.2.6	R Code: GLM Fit	376
11.2.7	R-Code: GLM: Profile Likelihood	377
11.2.8	Diagnostics	378
11.2.9	Overdispersion and Quasi-Likelihood Estimation	379
11.2.10	R-Code: GLM Residuals	381
11.3	Binomial Distribution	381
11.3.1	Overview	381
11.3.2	GLM with a Binomial Distribution	382
11.3.3	Goodness of Fit	382
11.3.4	Interpreting the Fitted Values and Regression Coefficients	384
11.3.5	Standard Errors and Confidence Intervals	386
11.3.6	Extensions	386
11.3.7	R Code: GLM: Binomial Distribution with Logit Link	387

11.4	Gamma Distribution	387
11.4.1	Properties of a Gamma Distribution	387
11.4.2	R Code: Gamma Distribution Maximum Likelihood Estimation	391
11.4.3	Gamma GLM with Canonical Link	392
11.4.4	R Code: GLM: Gamma Distribution	394
11.4.5	Gamma GLM with Non Canonical Links	395
11.4.6	R Code: GLM: Gamma Distribution	396
11.5	Chapter Summary	397
	References	398
12	Survival Analysis	399
12.1	Overview	399
12.1.1	Censoring	399
12.1.2	Statistical Functions	400
12.1.3	Statistical Models	402
12.2	Nonparametric Model	403
12.2.1	Kaplan-Meier Estimator	404
12.2.2	Standard Errors	405
12.2.3	Confidence Intervals	405
12.2.4	Median Survival	406
12.2.5	Hazard Rate	407
12.2.6	R Code: Kaplan-Meier Estimator (Log-Log Confidence Intervals)	408
12.2.7	Log-Rank Test	409
12.2.8	R Code: Log Rank Test	412
12.2.9	R Code: Log Rank Test cont.	413
12.3	Semiparametric Model	413
12.3.1	Hazard Function	413
12.3.2	Preliminary Example Without Ties	414
12.3.3	Interpreting the Hazard Ratio	415
12.3.4	Partial Likelihood Function	415
12.3.5	Goodness of Fit	416
12.3.6	Diagnostics	419
12.3.7	R Code: Cox Regression—No Ties/Single Predictor	421
12.3.8	Handling Ties	421
12.3.9	R Code: Cox Regression (Compact Form)	426
12.3.10	Residuals When Ties are Present	427
12.3.11	Interpretation	428
12.3.12	R Code: Cox Regression Residuals (Compact Form)	429
12.4	Parametric Model	430
12.4.1	Properties of a Weibull Distribution	430
12.4.2	Assessing the Appropriateness of a Weibull Distribution	432

12.4.3	R Code: Weibull MLE	433
12.4.4	Weibull Regression	433
12.4.5	Interpreting the AFT Coefficients	434
12.4.6	Model Fit and Standard Errors	437
12.4.7	R Code: Weibull Regression Single Predictor	438
12.4.8	Conversions to Proportional Hazard	439
12.4.9	R Code: Weibull AFT and PH Conversion	440
12.4.10	Diagnostics	440
12.4.11	Diagnostic Plots	441
12.4.12	R Code: Weibull AFT Diagnostics	445
12.5	For Further Reading	446
12.6	Chapter Summary	446
	References	447
13	Time Series Analysis	449
13.1	Overview	449
13.1.1	Dynamics of a Time Series	450
13.1.2	Stationarity and Differencing	452
13.1.3	From ARIMA to ARMA	456
13.1.4	R Code: Stationarity and Differencing	456
13.2	Autocorrelations	457
13.2.1	Autocorrelation Function	457
13.2.2	Partial Autocorrelations	458
13.2.3	R Code: Autocorrelation and Partial Autocorrelation Function	459
13.3	Moving Averages and Autoregressive Processes	459
13.3.1	Moving Averages	460
13.3.2	Autoregressive Processes	461
13.3.3	Wold Representation	462
13.3.4	ARMA(p,q)	463
13.3.5	Simulations and Filters	465
13.3.6	R Code: ARMA Simulations and Wold Representation	467
13.4	Model Identification	468
13.4.1	Moving Averages	468
13.4.2	Autoregressive Processes	471
13.4.3	Mixed Models	473
13.4.4	R Code: Stationarity, Invertibility, and Redundancy	477
13.5	Model Estimation	477
13.5.1	State-Space Representation	478
13.5.2	Kalman Filter	479
13.5.3	R Code: State Space Representation and Kalman Filter	482
13.5.4	R Code: ARMA Estimation	483

13.6	Model Adequacy	484
13.6.1	Test Residuals for Dependencies	484
13.6.2	R Code: Box-Pierce & Ljung-Box Tests of Model Fit	484
13.6.3	Models Comparisons	485
13.6.4	R Code: Tests of Model Fit	485
13.7	Forecasting	486
13.7.1	Generating Predicted Values	486
13.7.2	R Code: Forecasting (Mean-Centered) Observations	487
13.8	Integregation	488
13.8.1	Model Identification	488
13.8.2	Model Estimation	488
13.8.3	R Code: Dyads	492
13.9	Chapter Summary	493
	References	494
14	Mixed-Effects Models	495
14.1	Overview	495
14.1.1	Mixed-Effects Models in Matrix Form	496
14.1.2	Estimation and Prediction	498
14.1.3	Mixed Model Equations	498
14.1.4	Variance Components Estimation	499
14.1.5	Modeling the Random Terms	499
14.1.6	R Code: Preliminary Functions for Mixed Modeling	501
14.2	Understanding Mixed-Effects Models	502
14.2.1	Creating a Simulation	502
14.2.2	Plotting the Data	503
14.2.3	Testing Hierarchical Models	503
14.2.4	Intraclass Correlation	505
14.2.5	Fixed Effects and Random Effects	507
14.2.6	Interpreting the Random Coefficients	507
14.2.7	Standard Errors	510
14.2.8	Adding a Random Slope	511
14.2.9	Diagnostics	512
14.2.10	Summary	512
14.2.11	R Code: Mixed Model Simulations	513
14.3	Estimation	514
14.3.1	R Code: Mixed Model Fit	515
14.3.2	Illustration	516
14.3.3	R Code: Mixed Model Estimation	517
14.4	Repeated Measures and Growth Curve Models	518
14.4.1	Growth Curve Model	518
14.4.2	Reshaping the Data	519

14.4.3	Slopes and Intercepts	519
14.4.4	Model Comparisons	520
14.4.5	R Code: Growth Curve Analysis	524
14.5	Chapter Summary	525
	References	526