Contents

• • • • • • •

	List of Figures				
	Ack	nowled	gments	xxi	
0	Intr	oducti	ion: Building a Computing Toolbox	1	
	0.1	The P	hilosophy	2	
			tructure of the Book	4	
			How to Read the Book	6	
		0.2.2	Exercises and Further Reading	6	
	0.3		n the Classroom	8	
	0.4	Forma	atting of the Book	10	
	0.5	Setup		10	
1	Unix			12	
	1.1	What	Is Unix?	12	
	1.2	Why I	Use Unix and the Shell?	13	
	1.3	Gettir	ng Started with Unix	14	
		1.3.1	Installation	14	
		1.3.2	Directory Structure	15	
	1.4	Gettir	ng Started with the Shell	17	
		1.4.1	Invoking and Controlling Basic Unix Commands	18	
		1.4.2	How to Get Help in Unix	19	
		1.4.3	Navigating the Directory System	20	
	1.5	Basic	Unix Commands	22	
		1.5.1	Handling Directories and Files	22	
		1.5.2	Viewing and Processing Text Files	24	
	1.6		nced Unix Commands	27	
			Redirection and Pipes	27	
		1.6.2	e	29	
		1.6.3	Substituting Characters Using tr	32	

		1.6.4 Wildcards	35
		1.6.5 Selecting Lines Using grep	36
		1.6.6 Finding Files with find	39
		1.6.7 Permissions	41
	1.7	Basic Scripting	43
	1.8	Simple for Loops	47
	1.9	Tips, Tricks, and Going beyond the Basics	49
		1.9.1 Setting a PATH in .bash_profile	49
		1.9.2 Line Terminators	50
		1.9.3 Miscellaneous Commands	50
	1.10	Exercises	5]
		1.10.1 Next Generation Sequencing Data	51
		1.10.2 Hormone Levels in Baboons	51
		1.10.3 Plant–Pollinator Networks	52
		1.10.4 Data Explorer	53
	1.11	References and Reading	53
2	Vers	sion Control	55
	2 1	What Is Version Control?	55
		Why Use Version Control?	55
	2.3	·	56
		2.3.1 Installing Git	57
		2.3.2 Configuring Git after Installation	57
		2.3.3 How to Get Help in Git	58
	2.4	Everyday Git	58
		2.4.1 Workflow	58
		2.4.2 Showing Changes	64
		2.4.3 Ignoring Files and Directories	65
		2.4.4 Moving and Removing Files	66
		2.4.5 Troubleshooting Git	66
	2.5	Remote Repositories	68
		Branching and Merging	70
	2.7	Contributing to Public Repositories	78
	2.8	References and Reading	79
3	Bas	ic Programming	81
J			
	3.1	Why Programming?	81
	3.2	Choosing a Programming Language	81
	3.3	Getting Started with Python	83

				Contents	•	xi
		3.3.1	Installing Python and Jupyter			83
		3.3.2	How to Get Help in Python			84
		3.3.3	Simple Calculations with Basic Data Types			85
		3.3.4	Variable Assignment			87
		3.3.5	Built-In Functions			89
		3.3.6	Strings			90
	3.4	Data S	Structures			93
		3.4.1	Lists			93
		3.4.2	Dictionaries			96
		3.4.3	Tuples			100
		3.4.4	Sets			101
	3.5	Comr	non, General Functions			103
	3.6	The F	low of a Program			105
		3.6.1	Conditional Branching			105
		3.6.2	Looping			107
	3.7	Work	ing with Files			112
		3.7.1	Text Files			112
		3.7.2	Character-Delimited Files		1	115
	3.8	Exerc	ises			117
		3.8.1	Measles Time Series			117
		3.8.2	Red Queen in Fruit Flies		1	118
	3.9	Refere	ences and Reading			118
4	Wri	ting G	iood Code		1	20
		•				120
			ng Code for Science			120
	4.2		lles and Program Structure			121
			Writing Functions			121
			Importing Packages and Modules			126
	4.2	4.2.3	e			127
			ng Style			133
	4.4		on from the Command Line			135
	4.5		s and Exceptions			137
	1.0	4.5.1	Handling Exceptions			138
	4.6	Debu				139
	4.7	Unit 7	•			146
			Writing the Tests			147
		4.7.2	Executing the Tests Handling More Complex Tests			149 150
		4./.3	Trancing wore Complex Tests			เอบ

	4.8	Profiling	153
	4.9	Beyond the Basics	155
		4.9.1 Arithmetic of Data Structures	155
		4.9.2 Mutable and Immutable Types	156
		4.9.3 Copying Objects	158
		4.9.4 Variable Scope	160
	4.10	Exercises	161
		4.10.1 Assortative Mating in Animals	161
		4.10.2 Human Intestinal Ecosystems	162
	4.11	References and Reading	163
5	Reg	ular Expressions	165
	5.1	What Are Regular Expressions?	165
	5.2	Why Use Regular Expressions?	165
	5.3	Regular Expressions in Python	166
		5.3.1 The re Module in Python	166
	5.4	0 0 1	167
		5.4.1 Literal Characters	168
		5.4.2 Metacharacters	168
		5.4.3 Sets	169
		5.4.4 Quantifiers	170
		5.4.5 Anchors	171
		5.4.6 Alternations	172
		5.4.7 Raw String Notation and Escaping	
		Metacharacters	173
	5.5	Functions of the re Module	175
		Groups in Regular Expressions	179
	5.7	Verbose Regular Expressions	181
	5.8	The Quest for the Perfect Regular Expression	181
	5.9	Exercises	182
		5.9.1 Bee Checklist	182
		5.9.2 A Map of Science	182
	5.10	References and Reading	184
6	Scie	entific Computing	185
	6.1	Programming for Science	185
		6.1.1 Installing the Packages	185

				Contents	•	xiii
	6.2	Scient	tific Programming with NumPy and SciPy			185
		6.2.1				186
		6.2.2	Random Numbers and Distributions			194
		6.2.3	Linear Algebra			196
			Integration and Differential Equations			197
		6.2.5	Optimization			200
	6.3	Work	ing with pandas			202
	6.4	Віору	thon			208
		6.4.1	Retrieving Sequences from NCBI			208
		6.4.2	Input and Output of Sequence Data			
			Using SeqI0			210
		6.4.3	Programmatic BLAST Search			212
		6.4.4	Querying PubMed for Scientific Literature			
			Information			214
	6.5	Other	Scientific Python Modules			216
	6.6	Exerc	ises			216
		6.6.1	Lord of the Fruit Flies			216
		6.6.2	Number of Reviewers and Rejection Rate			217
		6.6.3	The Evolution of Cooperation			217
	6.7	Refere	ences and Reading			219
7	Scie	entific	Typesetting			220
	7.1	What	Is LaTeX.			220
			Use LATEXS			220
		•	ling LATEX			223
			tructure of LaTeX Documents			223
			Document Classes			224
			₽T _E X Packages			224
			The Main Body			225
			Document Sections			227
	7.5		etting Text with LATEX			228
		7.5.1	Spaces, New Lines, and Special Characters			228
		7.5.2	Commands and Environments			228
		7.5.3	Typesetting Math			229
		7.5.4	, ,			231
		7.5.5				232
		7.5.6	Long Documents			232
		7.5.7	•			233
		7.5.8	Typesetting Matrices			236

		7.5.9 Figures	237
		7.5.10 Labels and Cross-References	240
		7.5.11 Itemized and Numbered Lists	241
		7.5.12 Font Styles	241
		7.5.13 Bibliography	242
	7.6	LATEX Packages for Biologists	244
		7.6.1 Sequence Alignments with LATEX	245
		7.6.2 Creating Chemical Structures with LATEX	246
	7.7	Exercises	246
		7.7.1 Typesetting Your Curriculum Vitae	246
	7.8	References and Reading	247
8	Sta	tistical Computing	249
	8.1	Why Statistical Computing?	249
		What Is R?	249
	8.3	Installing R and RStudio	250
	8.4	Why Use R and RStudio?	250
	8.5	Finding Help	251
	8.6	Getting Started with R	251
	8.7	Assignment and Data Types	253
	8.8	Data Structures	255
		8.8.1 Vectors	255
		8.8.2 Matrices	257
		8.8.3 Lists	261
		8.8.4 Strings	262
		8.8.5 Data Frames	263
	8.9	Reading and Writing Data	264
	8.10	Statistical Computing Using Scripts	267
		8.10.1 Why Write a Script?	267
		8.10.2 Writing Good Code	267
	8.11	The Flow of the Program	270
		8.11.1 Branching	270
		8.11.2 Loops	272
	8.12	Functions	275
		Importing Libraries	278
		Random Numbers	279
	8.15	Vectorize It!	280
		Debugging	283
	8.17	Interfacing with the Operating System	284

			Contents	•	χv
	8.18	Running R from the Command Line		2	285
	8.19	Statistics in R		2	287
	8.20	Basic Plotting		2	90
		8.20.1 Scatter Plots		2	290
		8.20.2 Histograms		2	91
		8.20.3 Bar Plots		2	92
		8.20.4 Box Plots		2	92
		8.20.5 3D Plotting (in 2D)		2	93
	8.21	Finding Packages for Biological Research		2	93
	8.22	Documenting Code		2	94
	8.23	Exercises		2	295
		8.23.1 Self-Incompatibility in Plants		2	95
		8.23.2 Body Mass of Mammals		2	296
		8.23.3 Leaf Area Using Image Processing		2	296
		8.23.4 Titles and Citations		2	297
	8.24	References and Reading		2	297
9	Dat	a Wrangling and Visualization		3	00
	9.1	Efficient Data Analysis and Visualization		3	800
	9.2	·			800
		9.2.1 Reading Data			801
		9.2.2 Tibbles			302
	9.3	Selecting and Manipulating Data			04
		9.3.1 Subsetting Data		3	05
		9.3.2 Pipelines			807
		9.3.3 Renaming Columns			808
		9.3.4 Adding Variables		3	809
	9.4	Counting and Computing Statistics		3	310
		9.4.1 Summarize Data		3	310
		9.4.2 Grouping Data		3	310
	9.5	Data Wrangling			313
		9.5.1 Gathering		3	313
		9.5.2 Spreading		3	315
		9.5.3 Joining Tibbles		3	316
	9.6	Data Visualization		3	318
		9.6.1 Philosophy of ggplot2		3	319
		9.6.2 The Structure of a Plot			320
		9.6.3 Plotting Frequency Distribution of One			
		Continuous Variable		3	321

		9.6.4 Box Plots and Violin Plots	322
		9.6.5 Bar Plots	323
		9.6.6 Scatter Plots	324
		9.6.7 Plotting Experimental Errors	325
		9.6.8 Scales	326
		9.6.9 Faceting	328
		9.6.10 Labels	329
		9.6.11 Legends	330
		9.6.12 Themes	331
		9.6.13 Setting a Feature	332
		9.6.14 Saving	332
	9.7	Tips & Tricks	333
	9.8	Exercises	335
		9.8.1 Life History in Songbirds	335
		9.8.2 Drosophilidae Wings	335
		9.8.3 Extinction Risk Meta-Analysis	335
	9.9	References and Reading	336
10	Rela	ational Databases	337
	10.1	What Is a Relational Database?	337
		Why Use a Relational Database?	338
		Structure of Relational Databases	340
	10.4	Relational Database Management Systems	341
		10.4.1 Installing SQLite	341
		10.4.2 Running the SQLite RDBMS	341
	10.5	Getting Started with SQLite	342
		10.5.1 Comments	342
		10.5.2 Data Types	342
		10.5.3 Creating and Importing Tables	343
		10.5.4 Basic Queries	344
	10.6	Designing Databases	352
	10.7	Working with Databases	355
		10.7.1 Joining Tables	355
		10.7.2 Views	358
		10.7.3 Backing Up and Restoring a Database	359
		10.7.4 Inserting, Updating, and Deleting Records	360
		10.7.5 Exporting Tables and Views	361
	10.8	Scripting	362
	10.9	Graphical User Interfaces (GUIs)	362

			Contents	•	xvii	
	10.10	Accessing Databases Programmatically			362	
		10.10.1 In Python			363	
		10.10.2 In R			363	
	10.11	Exercises			364	
		10.11.1 Species Richness of Birds in Wetland	ls		364	
		10.11.2 Gut Microbiome of Termites			364	
	10.12	References and Reading			365	
11	Wrap	oping Up			366	
	11.1	How to Be a More Efficient Computational Bio	logist		367	
	11.2	What Next?	-		368	
	11.3	Conclusion			371	
	Intermezzo Solutions					
	Bibliography					
	Indexes					
	Index of Symbols					
	Index of Unix Commands					
	Ind	Index of Git Commands				
	Index of Python Functions, Methods, Properties,					
	a	and Libraries				
	Ind	Index of MEX Commands and Libraries				
	Ind	Index of R Functions and Libraries				
	Ind	ex of SQLite Commands			405	
	Ge	neral Index			407	