

practical computing for biologists

Steven H. D. Haddock

The Monterey Bay Aquarium Research Institute, and University of California, Santa Cruz

Casey W. Dunn

Department of Ecology and Evolutionary Biology, Brown University



CONTENTS IN BRIEF

Before You Begin 1

PART I: Text	Files 7	
Chapter 1	Getting Set Up 9	
Chapter 2	Regular Expressions: Powerful Search and Replace 17	
Chapter 3	Exploring the Flexibility of Regular Expressions 31	
PART II: The	Shell 45	
Chapter 4	Command-line Operations: The Shell 47	
Chapter 5	Handling Text in the Shell 67	
Chapter 6	Scripting with the Shell 83	
PART III: Programming 103		
Chapter 7	Components of Programming 105	
Chapter 8	Beginning Python Programming 125	
Chapter 9	Decisions and Loops 141	
Chapter 10	Reading and Writing Files 173	
Chapter 11	Merging Files 201	
Chapter 12	Modules and Libraries 215	
Chapter 13	Debugging Strategies 231	
PART IV: Cor	mbining Methods 243	
Chapter 14	Selecting and Combining Tools 245	
Chapter 15	Relational Databases 255	
Chapter 16	Advanced Shell and Pipelines 299	
PART V: Graphics 321		
Chapter 17	Graphical Concepts 323	
Chapter 18	Working with Vector Art 345	
Chapter 19	Working with Pixel Images 363	
PART VI: Adv	vanced Topics 381	
Chapter 20	Working on Remote Computers 383	
Chapter 21	Installing Software 411	
Chapter 22	Electronics: Interacting with the Physical World 425	
Appendices	449	

CONTENTS

Acknowledgments	xviii
-----------------	-------

BEFORE YOU BEGIN 1

Introduction 1
Why this book? 1
Why biologists? 2
Is this about using a particular computer or program? 3

To readers who will use this book on their own 4

To teachers using this book 4

Beyond this book 5

How to use this book 5

PART I Text Files 7

Chapter 1 GETTING SET UP 9

An introduction to text manipulation 9
What are text files? 10
The organization of data within a text file 11

Text editors 12

Installing TextWrangler 12
Optimizing text appearance within a text
editor 13
Line endings 13

The example files 14

Installing the example files 14 Exploring the example files 15

Summary 15

Chapter **2**

REGULAR EXPRESSIONS: POWERFUL SEARCH AND REPLACE 17

A widespread language for search and replace 17

Understanding the components of this new toolbox 18

Setting up the text editor 18

Your first wildcard: \w for letters and digits 20

Capturing text with () 21

Quantifiers: Matching one or more entities

Quantifiers: Matching one or more entities using + 23

Escaping punctuation characters with \ 25 More special search terms: \s \t \r . \d 26

Example: Reformatting molecular data files 28

Comments about generating regular expressions 29

Summary 29

Chapter **3**

EXPLORING THE FLEXIBILITY OF REGULAR EXPRESSIONS 31

Character sets: Making your own wildcards 31

Defining custom character sets with [] 31 Applying custom character sets 32 Negations: Defining custom character sets with [^] 33 Boundaries: ^beginnings and endings\$ 35 Adding more precision to quantifiers 36

Another quantifier: * for zero or more 36

Modifying greediness with? 36

Controlling the number of matches with {} 37

Putting it all together 38

Generating the replacement query 40

Constructing robust searches 41

Summary 42

Moving forward 42

PART II The Shell

45

Chapter 4

COMMAND-LINE OPERATIONS: THE SHELL 47

Getting started: Don't fear the command line 47

Starting the shell and getting oriented 48

Starting the shell 48

A command-line view of the filesystem 50 The path 51

Navigating your computer from the shell 52

Listing files with 1s and figuring out where you are with pwd 52

How to move around with cd 54

Signifying the home directory with ~ 56

Adding and removing directories with mkdir and rmdir 56

Copying files 57

Moving files 58

Command line shortcuts 59

Up arrow 59 *Tab* 60

Modifying command behavior with arguments 61

Viewing file contents with less 62

Viewing help files at the command line with man 63

The command line finally makes your life easier 64

Wildcards in path descriptions 64
Copying and moving multiple files 65

Ending your terminal session 65

Summary 66

Recommended reading 66

Chapter 5

HANDLING TEXT IN THE SHELL 67

Editing text files at the command line with nano 67

Controlling the flow of data in the shell 69
Redirecting output to a file with > 69
Displaying and joining files with cat 70

Regular expressions at the command line with grep 72

Working with a larger dataset 72
Extracting particular rows from a file 73
Redirecting output from one program to another with pipe | 75

Searching across multiple files with grep 76
Refining the behavior of grep 77
Retrieving Web content using curl 78
Other shell commands 81
Summary 81

Chapter **6**

SCRIPTING WITH THE SHELL 83

Combining commands 83 The search path 84

How the command line finds its commands 84
Creating your workspace, the scripts folder 85
Editing your .bash profile settings file 8

Checking your new \$PATH 88

Turning a text file into software 88

Control how the text is interpreted with #! 89
Making the text file executable by adjusting the permissions 90

Generating scripts automatically 91

Copying files in bulk 92

Flexible file renaming 95

Automating curl to retrieve literature references 97

General approaches to curl scripting 99

Aliases 99

Summary 101

Moving forward 101

PART III Programming

103

Chapter **7**

COMPONENTS OF PROGRAMMING 105

What is a program? 105

Goals of the next few chapters 105 Practical programming 106

Variables 108

The anatomy of a variable 108 Basic variable types 108

Variables as containers for other variables 110

Arrays and lists 110

Converting between types 111

Variables in action 112

Mathematical operators 112

Comparative and logical operators 113

Functions 115

Flow control 115

Decisions with the if statement 17

Looping with for and while 116

Using lists and dictionaries 118

Lists 118

Dictionaries 119

Other data types 119

Input and output 120

User interaction 120

Files 120

Libraries and modules 122

Comment statements 122

Objects 122

Summary 124

Chapter **8**

BEGINNING PYTHON PROGRAMMING 125

Why Python 125

Writing a program 126

Getting a program to run 126

x Contents

Constructing the dnacalc.py program 127 Simple print statements 128 The len() function 130 Converting between variable types with str(), int(), and float() 131 The built-in string function .count() 132 Math operations on integers and floating point numbers 132 Adding comments with # 134 Controlling string formatting with the % operator 135 Getting input from the user 137 Gathering user input with raw_input() 137 Sanitizing variables with .replace() and .upper() 137 Reflecting on your program 140	Indexing lists 159 Unpacking more than one value from a list 161 The range() function to define a list 161 A comparison of lists and strings 163 Converting between lists and strings 164 Adding elements to lists 165 Removing elements from lists 166 Checking the contents of lists 166 Sorting lists 167 Identifying unique elements in lists and strings 167 List comprehension 168 Summary 171
Summary 140	Moving forward 172
Chapter 9 DECISIONS AND LOOPS 141 The Python interactive prompt 141 Getting Python help 144 Adding more calculations to dnacalc.py 144 Conditional statements with if 145 Designating code blocks using indentation 145 Logical operators 146 The if statement 147 The else: statement 147 Introducing for loops 149 A brief mention of lists 150 Writing the for loop in proteincalc.py 151 Generating dictionaries 151 Other dictionary functions 157 Applying your looping skills 158	READING AND WRITING FILES 173 Surveying the goal 173 Reading lines from a file 175 Considerations before reading a data file 175 Opening and reading a text file 177 Removing line endings with .strip() 178 Skipping the header line 179 Parsing data from lines 180 Splitting a line into data fields 180 Selecting elements from a list 181 Writing to files 182 Recapping basic file reading and writing 184 Parsing values with regular expressions 184 Importing the re module 185 Using regular expressions with the re module 185

Summary of using re.search() and re.sub() 187 Creating custom Python functions with def 188 Packaging data in a new format 192 Examining markup language 192 Preserving information during conversion 194 Converting to KML format 194 KML file format 194 Generating the KML text 195 Summary 198 Moving forward 199	The urllib module 218 The os module 218 The math module 219 The random module 219 The time module 221 Third-party modules 222 NumPy 223 Biopython 225 Other third-party modules 226 Making your own modules 227 Going further with Python 228 Summary 229 Moving forward 229	
Chapter 11		
MERGING FILES 201	Chapter 13	
Reading from more than one file 201	DEBUGGING STRATEGIES 231	
Getting user input with sys.argv 202 Converting arguments to a file list 204 Providing feedback with sys.stderr.write() 205 Looping through the file list 206 Printing the output and generating a header line 208 Avoiding hardcoded software 209 Other applications of file reading 211 Summary 213 Moving forward 213	Learning by debugging 231 General strategies 232 Build upon working elements 232 Think about your assumptions 233 Specific debugging techniques 234 Isolate the problem 234 Write verbose software 235 Error messages and their meanings 237 Common Python errors 237 Shell errors 238 Making your program more efficient 238 Optimization 238 Try and except to handle errors 239 When you're really stuck 240	
Chapter 12	When you're really stuck 240 Summary 241	
MODULES AND LIBRARIES 215	Moving forward 241	
Importing modules 216	<u> </u>	

More built-in modules from the standard library 218

Combining Methods 243 Chapter 14 Exploring data with SQL 283 Summarizing tables with SELECT and SELECTING AND COMBINING COUNT 283 **TOOLS 245** Collating data with GROUP BY *Mathematical operations in SQL* 286 Your toolkit 245 Refining selections by row with WHERE 286 Categories of data processing tasks 246 Modifying rows with UPDATE Getting digital data 246 Selecting data across tables Reformatting text files 249 Python scripts 251 Generating output using Python 291 General considerations 252 Looking ahead 294 Summary 254 Database users and security 294 Creating a root password Moving forward Adding a new MySQL user 295 Chapter 15 Summary 296 Moving forward 297 **RELATIONAL DATABASES** Recommended reading Spreadsheets and data organization 255 Chapter 16 Data management systems Anatomy of a database 259 ADVANCED SHELL AND Installing MySQL 260 **PIPELINES** 299 Getting started with MySQL and SQL 262 Connecting to the MySQL server at the command Additional useful shell commands 299 line 262 Extract lines with head and tail Creating a database and tables 264 Extract columns with cut. 300 Adding rows of data to tables and displaying table Sorting lines with sort 301 contents 269 Isolating unique lines with uniq 302 Interacting with MySQL from Python Combining advanced shell functions 303 Parsing the input text 271 Approximate searches with agrep

275

Additional grep tips

Functions with user input 313

Looping through all arguments passed to a

A dictionary function 313

Translating characters 313

Remember aliases?

function 314

Functions 309

307

308

279 Bulk-importing text files into a table

Formulating SQL from the data 273

Executing SQL commands from Python

Creating the ctd table 280 Importing data files with the LOAD DATA command 281

Exporting and importing databases as SQL files 283

Removing file extensions 315
Finding files 316
Revisiting piped commands 317
Repeating operations with loops 317

Wrappers 318

Thoughts on pipelines 319
Summary 320
Recommended reading 320

PART V Graphics 321

Chapter **17**GRAPHICAL CONCEPTS

Introduction 323

General image types 324

Vector versus pixel 324

Deciding when to use vector art, pixel art, or both 325

Image resolution and dimensions 326

Image resizing and the DPI misconception 328

Image colors 330

Color models and color space 330
Converting between color models 332
Color gamut and color profiles 333
Color choices 334

Summarizing the decision-making process 335

Layers 337

General considerations for presenting data 337

Eliminate visual clutter 337
Use transparency for overlapping data 338
Make effective use of space 338
Consistency 340

Maintaining data integrity 341
Why you should avoid PowerPoint 342
Summary 342
Moving forward 342
Recommended reading 343

Chapter 18

WORKING WITH VECTOR ART 345

Vector art mechanics 345

File formats 345

Generating vector art 346

Exporting images from another program 346 Drawing new images 347

Tracing photographs 347

Anatomy of vector art 348

Bézier curves 348 Stroke and fill 349

Working with vector art editors 349

Selecting and manipulating entire objects 350
Selecting and manipulating parts of an object 351

Creating Bézier curves with the pen tool 351

Modifying Bézier curves 352

The Join function 353

Stroke and fill 353

Layers 354

Illustrator tips 355

Inkscape tips 357

A typical workflow 358

Creating regularly arranged objects 359

Best practices for composing vector objects 361

Summary 361 Moving forward 362

xiv Contents

Chapter 19	Photosnop shortcuts 370	
WORKING WITH PIXEL	Command-line tools for image processing 370	
IMAGES 363	The sips program 371	
Image compression 363 General principles 363	ImageMagick: convert <i>and</i> mogrify 371 ExifTool 372	
Implications for image workflows 364	Image creation and analysis tools 372	
Pixel image file formats 364 Transparency 366	ImageJ 372 MATLAB 374	
Pixel art editors 366	R 374	
Working with pixel images 366	Animations 375	
Masks and nondestructive editing 366	Photography 375	
Levels adjustment 367	Aperture and exposure time 375 Color balance 378	
Grayscale images 368	Automatic versus manual operation 378	
Antialiasing 368	Summary 379	
Layers 369	Moving forward 379	
Colors in GIMP 369	Woving for ward 377	
PART VI Advanced Topics	381	
Chapter 20	Copying files with scp 392	
WORKING ON REMOTE	Other file transfer programs using SFTP 393	
COMPUTERS 383	Other file sharing protocols 393	
Connecting to a remote computer 383	Full GUI control of a remote computer with VNC 393	
Clients and servers 383	Troubleshooting remote connections 394	
Typical scenarios for remote access 384 Finding computers: IP addresses, hostnames, and	Getting local with a Virtual Private Network (VPN) 394	
DNSs 385 Security 387	Mapping network connections with traceroute 395	
Secure command-line connections with	Configuring the backspace key 395	
ssh 387	Controlling how programs run 396	
The ssh command 388	Terminating a process 397	
Troubleshooting ssh 388	Starting jobs in the background with & 397	
Working on the remote machine 389	Checking job status with ps and top 397	
Transferring files between computers 390 File archiving and compression 390	Suspending jobs and sending them to the background 399	
File transfer with sftp 391	Stopping processes with kill 400	

Keeping jobs alive with nohup 402 Changing program priority with renice 403 High-performance computing 403	Chapter 22 ELECTRONICS: INTERACTING WITH
Parallel programs 404 Job management tools on clusters 405 Setting up a server 405 Configuring the ssh server 406 Finding your addresses 407 Connecting to your own computer with ssh 408 Summary 409 Chapter 21 INSTALLING SOFTWARE 411 Overview 411 Interpreted and compiled programs 412	THE PHYSICAL WORLD 425 Custom electronics in biology 425 Typical scenarios for custom electronics in biology 425 Simple circuits with complex microcontrollers 426 Basic electronics 428 Electricity 428 Basic components 429 Encoding information with electric signals 430 Analog encoding 430 Digitally encoded signals 431 Building circuits 433
Approaches to installing software 414 Readme.txt and Install.txt 414 Installing programs from precompiled binaries 414 Automated installation tools 414 Installing command-line programs from source code 415 Getting your computer ready 416 Unarchiving the source code 416 Compiling and installing binaries 417 Variation 1: Off-the-shelf Makefile 418 Variation 2: Generating a Makefile with ./configure 419 Installing Python modules 420 Troubleshooting 421 What to do when software won't compile or installations don't work 421 Summary 423 Moving forward 423	Schematics 433 Breadboards 433 Translating a schematic to a breadboard 434 Serial communication in practice 435 Baud rate and other settings 436 Null modem 436 Software for serial communication 437 Serial comms through Python 437 Arduino microcontroller boards in practice 438 Where to start 438 Building circuits with Arduino 439 Programming Arduino 440 Other options for data acquisition 443 Common sources of confusion 445 Measuring voltage 445 Current flow versus electron flow 445 Pull-up and pull-down resistors 445 Summary 446 Moving forward 446
vioving for ward 423	Moving forward 446 Recommended reading 447

Appendices 449

Appendix 1

WORKING WITH OTHER OPERATING SYSTEMS 451

Microsoft Windows 451

Should I work in Windows or install Linux? 451
Text editors for text editing and regular
expressions in Chapters 1–3 452
Cygwin for emulating Unix shell operations in
Chapters 4–6 453
Python on Windows for Chapters 8–12 455
Working with MySQL on Windows for
Chapter 15 457

Working with vector and pixel art in Windows for Chapters 17–19 457

Linux 458

Installing Linux 458

Text editing and regular expressions with jEdit for Chapters 1–3 463

Using the Linux shell for shell operations in Chapters 4–6 464

Python on Linux for Chapters 8–12 465

Working with MySQL for Chapter 15 465

Working with vector and pixel art in Linux for Chapters 17–19 466

Appendix 2

REGULAR EXPRESSION SEARCH TERMS 467

Appendix **3**SHELL COMMANDS 471

Appendix 4

PYTHON QUICK REFERENCE 479

Conventions for this appendix 479 Format, syntax, and punctuation in Python 479 The command-line interpreter Command summary 480 Variable types and statistics 480 Strings 480 Gathering user input 481 Building strings 482 Comparisons and logical operators 482 Math operators 483 Decisions 484 Loops 484 Searching with regular expressions 485 Regexp to find matching subsets in a string 485 Regexp to substitute into a string 485 Working with lists 486 List comprehension 488 Dictionaries 488 Creating functions 489 Working with files 490 Using modules and functions 491 Miscellaneous Python operations 493 Presenting warnings and feedback 493 Catching errors 493 Shell operations within Python 493 Reference and getting help 493

Appendix **5 TEMPLATE PROGRAMS 495**

Python 2.7 or earlier 496
Python 3 496
Perl 496
bash shell 497
C 497
C++ 498
Java 498
JavaScript 499
PHP 500
Ruby 500
MATLAB 501
R 501
Arduino 502

Appendix **6 BINARY, HEX, AND ASCII** 503

Alternate base systems 503
Hexadecimal 505
ASCII and Unicode characters 505
Images and color 506
Decimal, hex, binary, and ASCII values 507

Appendix **7**SQL COMMANDS 511
INDEX 515