

practical computing for biologists

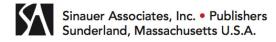
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Appendix 2

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REGULAR EXPRESSION SEARCH TERMS

Regular expressions—ways to perform adaptive searches and replacements—are described in Chapters 2 and 3. Here we provide a quick reference to some of the more common regular expression terms. This table and the text of the book itself do not encompass the entire range of regular expressions. There are many other useful constructs, for example, embedding miniature scripts into your replacement terms, and searching for A or B in a string using the syntax (sword|jelly)fish. If you would like to delve deeper, there are many online references, and there is even an in-depth reference guide built into the Help menu of TextWrangler.

There is some variation in the terms supported from program to program and from language to language. The most widespread terms, which can be used almost anywhere that regular expressions are supported, are the POSIX Extended Regular Expressions. These include \cdot , *, +, {}, (), [], [^], ^, \$, ?, and |. While quite a bit can be accomplished with the POSIX terms, in many implementations the language has been supplemented with some nonstandard terms. Most of these nonstandard terms are based on Perl regular expressions. These include many of the character class wildcards listed in the tables below, such as \d, \w, and \n. These extra wildcards make it easier to write clear regular expressions. Lack of support for Perl-like regular expressions is one of the most common causes of confusion when moving to a new programming context.

If you are using regular expressions in a new context but find that they don't behave as expected, or that they generate errors, check to see which regular expressions are supported by the tool you are using. POSIX does define its own set of wildcards, but the syntax is different from the Perl-style \w format that we use in this book. These wildcards include [:digit:] in place of \d and [:alpa:] instead of \w that we use in this book (though not including the digits). These POSIX character classes can be used in some contexts where Perl classes aren't available, including SQL queries and the command-line tool grep. If you don't want to switch between wildcard types, a more universal solution is to replace character class wildcards with an explicit character range, such as [0-9] or [A-Z].





Wildcards	
\w	Letters, numbers and _
•	Any character except \n \r
\d	Numerical digits
\t	Tab
\r	Return character. Also used as the generic end-of-line character in TextWrangler
\n	Line-feed character. Also used as the generic end-of-line character in Notepad++
\s	Space, tab, or end of line
[A-Z]	A single character of the ranges indicated in square brackets
[^A-Z]	A single character including all characters not in the brackets. Note that this will include \n unless otherwise specified, and may cause you to match across lines
\	Used to escape punctuation characters so they are searched for as themselves, not interpreted as wildcards or special symbols
\\	The \ symbol itself, escaped
Boundaries	
^	Match the start of the line, i.e., the position before the first character
\$	Match the last position before the end-of-line character

Quantifiers, used in combination with characters and wildcards		
+	Look for the longest possible match of one or more occurrences of the character, wildcard, or bracketed character range immediately preceding. The match will extend as far as it can while still allowing the entire expression to match.	
*	As above, matches as many of the previous character to occur, but allows for the character not to occur at all if the match still succeeds	
?	Modifies greediness of + or * to match the shortest possible match instead of longest	
{}	Specify a range of numbers to repeat the match of the previous character. For example: \d{2,4} matches between 2 and 4 digits in a row [AC]{4,} matches 4 or more of the letter A or C in a row	
Capturing a	and replacing	
()	Capture the search results between the parentheses for use in the replacement term	
\1 \$1	Substitute the contents of the matched into the replacement term, in numerical order. Syntax depends on the text editor or language that you are using.	

	ζ	ענ
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SHELL COMMANDS

Terminal operations are described in Chapters 4–6, 16, and 20. Many of the built-in bash shell commands are summarized here for quick reference. To get more information about a command and its options, type man, followed by the name of the command. If you are not sure which command applies, you can also search the contents of the help files using man –k followed by a keyword term.

Command	Description	Usage
ls	List the files in a directory Parameters that follow can be folder names (use * as a wildcard) -a Show hidden files -1 Show dates and permissions -1 List the file names on separate lines. Useful as a starting point for regexp into a list of commands -G Enable color-coding of file types -F Show a slash after directory names	ls -la ls -1 *.txt ls -FG scripts ls ~/Documents ls /etc
cd	Change directory Without a slash, names are relative to the current directory With a preceding slash (/) names start at the root level Tilde (~/) starts at the user's home directory Two dots () goes "up" to the enclosing directory One dot refers to the current directory Minus sign goes to the previously occupied directory Use tab key (see below) to auto-complete partially typed paths Use backslash before spaces or strange characters in the directory name, or put the whole name in quotes	cd scripts cd /User cd ~/scripts cd My\ Documents cd 'My Documents' cd/ cd

Command	Description Usage		
pwd	Print the wo	rking directory (the path to the folder you are in)	
↑	The cursor of and comm	ep back through previously typed commands can be repositioned with the 🕞 and 🗩 keys, nands can then be edited from anywhere in the line to re-execute. On OS also reposition by option -clicking at a cursor	
tab	Auto-compl line	ete file, folder, or script names at the command	cd ~/Doc tab
less		nts of a file, page by page nands also apply to viewing the results of man is running:	less data.txt
	q	Quit viewing	
	space	Next page	
	b	Back a page	
	15 g	Go to line 15	
	G	Go to the end	
	↑ or ↓	Move up or down a line	
	/abc	Search file for text abc	
	n	After an initial search, find next occurrence of the search item	
	?	Find previous occurrence of the search item	
	h	Show help for less	
mkdir	Make a new	directory (a new folder)	mkdir scripts
rmdir	Remove a d	irectory (folder must be empty)	rmdir ~/scripts
rm	Remove file or files Use the -f flag to delete without confirmation (careful!) Use the -r flag to recursively delete the files in a directory and then the directory itself		rm test.txt rm -f *_temp.dat
man	Use -k to se The result is	anual pages for a Unix command earch for a term within all the manuals displayed using the less command above, ne shortcuts allow you to navigate through	man mkdir man -k date man chmod

Command	Description	Usage
ср	Copy file, leaving original intact Does not work on folders themselves Single period as destination copies file to current directory, using same name	<pre>cp test1.txt test1.dat cp temp/temp cp/test.py .</pre>
mv	Move file or folder, renaming or relocating it Unlike cp, this does work on directories	<pre>mv test1.txt test1.dat mv temp/temp2</pre>
l	Pipe output of one command to the input of another command	history grep lucy
>	Send output of a command to a file, overwriting existing files Do not use a destination file that matches a wildcard on the left side	ls -1 *.py > files.txt
>>	Send output of a command to a file, appending to existing files	echo "#Last line" >> data.txt
<	Send contents of a file into command that supports its contents as input	mysql -u root midwater < data.sql
./	Represents the current directory in a path—the same location as pwd Trailing slash is optional Can execute a file in the current directory even when the file directory is not included in the PATH	<pre>cp/*.txt ./ ./myscript.py</pre>
cat	Concatenate (join together) files without any breaks. Streams the contents of the file list across the screen	cat README cat *.fta > fasta.txt
head	Show the first lines of a file or command Use the -n flag to specify the number of lines	head -n 3 *.fasta ls *.txt head
tail	Show the last lines of a file or output stream Use the $-n$ flag to specify the number of lines to show With a plus sign, skip that number of lines and show to the end. Use $-n$ +2 to show from the second line of the file to the end, skipping one header line	tail -n 20 *.fta tail -n +3 data.txt
wc	Count lines, words, and characters in an output stream or file	wc data.txt ls *.txt wc
which	Show the location of executable files in the system path	which man

Command	Description Usage	
grep	Search for phrase in a list of files or pipe and show matching lines: grep -E "searchterm" filelist Often used in conjunction with piped output: command grep searchterm Use quotes around search terms, especially spaces or punctuation like >, &, #, and others To search for tab characters, type ctrl V followed by tab inside the quotes Optional flags:	
	-c Show only a count of the results in the file	
	-v Invert the search and show only lines that do not match	
	-i Match without regard to case	
	-E Use full regular expressions Terms should be enclosed in quotes. Use [] to indicate a character range rather than the wildcards of Chapters 2 and 3 General wildcard equivalents: \s [[:space:]] \w [[:alpha:]] \d [[:digit:]]	
	-1 List only the filenames containing matches	
	-n Show the line numbers of the match	
	-h Hide the filenames in the output	
agrep	Search for approximate matches, allowing insertions, deletions, or mismatched characters. (Must be installed separately.) See Chapter 21 Optional flags include: -d "," Use comma as delimiter between records	ta
	-2 Return results with up to 2 mismatches. Maximum is 8 mismatches	
	-в -y Return the best match without specifying a number of mismatches	
	-1 Only list file names containing matches	
	-i Match without regard to case	
chmod	Change access permissions on a file (usually to make a script executable or Web accessible) First option is one of u, g, o for user, group, other Second option after the plus or minus is r, w, or x, for read, write, or execute. Can also use binary encoding as explained in Appendix 6	

Command	Descriptio	n	Usage
set	Show envir been de	ronmental variables, including functions that have fined	
\$HOME	The enviro directory	nmental variable containing the path user's home	echo \$HOME cd \$HOME
\$РАТН		PATH variable, where the directories to search for ds are stored	export PATH=\$PATH:/usr/local/bin
nano	Invoke the	text editor. Control key sequences include:	nano filename.txt
	ctrl X	Exit nano (will be prompted to save)	
	ctrl O	Save file without exiting	
	ctrl Y	Scroll up a page	
	ctrl V	Scroll down a page	
	ctrl C	Cancel operation	
	ctrl G	Show help and list of commands	
ctrl C	Interrupt the current process		
sort	Sort lines of a file		sort -k 3 data.txt
	-k <i>N</i>	Sort using column number N instead of starting at the first character. Columns are delimited by a series of white space characters	<pre>sort -k 2 -t "," F1.csv sort -nr numbers.txt sort A.txt > A_sort.txt</pre>
	-t ","	In conjunction with —k, use commas as the delimiter to define columns	
	-n	Sort by numerical value instead of alphabetical	
	-r	Sort in reverse order	
	-u	Return only one unique representative from a series of identical sorted lines	
uniq	in a file of anywher to the ur	ngle line for each consecutive instance of that line or output stream. To remove all duplicates from e in the file, it must be sorted before being piped niq command g to return a count along with the repeated	uniq -c records.txt sort names uniq -c

Command	Description	Usage
cut	Extract one or more columns of data from a file	cut -c 5-15 data.txt
	-f 1,3 Return columns 1 and 3, delimited by tabs	cut -f2 -d ":" > Hr.txt
	-d " , " Use commas as the field delimiter instead of tabs. Used in combination with $-\mathbf{f}$	
	-c 3-8 Return characters 3 through 8 from the file or stream of data	
curl	Retrieve the contents of a URL from over the network. URL should be placed in quotes. Without additional parameters, will stream contents to the screen For some Linux versions, wget offers similar functionality See man curl for ways to send user login information at the same time -o Set the name of the output file to save individual files for the data. See #1 below	<pre>curl "www.myloc.edu" > myloc.html curl "http://www.nasa. gov/weather[01-12] {1999,2000}" -m 30 -o weather#1_#2.dat</pre>
	-m 30 Set a time out of 30 seconds	
	[01-25] In the URL, substitute two digit numbers from 01 to 25 into the address in succession	
	$\{22,33\}$ Substitute items in brackets into URL $\{A,C,E\}$	
	#1 The substituted value, for use in generating the filename	
sudo	Run the command that follows as a superuser with privileges to write to system files	<pre>sudo python setup.py install sudo nano /etc/hosts</pre>
alias	Define a shortcut for use at the command line. To make persistent, add to startup settings file .bash_profile or equivalent	alias cx='chmod u+x'
function	Create a shell function—like a small script \$1 is the first user argument supplied after the command is typed \$0 is all the parameters—useful for loops as below Variable names are defined with the format NAME= with no spaces. They are retrieved with \$NAME Save it in .bash_profile to make it permanent	<pre>myfunction() { # insert commands here echo \$1 }</pre>
;	In a command or script, equivalent to pressing return and starting a new line	date; ls

C	Danasia tian	Hanna
Command	Description	Usage
for	Perform a for loop in the shell. Can be useful in the context of a function	for ITEM in *.txt; do echo \$ITEM done
if	An if statement in a shell function: if [test condition] then # insert commands else # alternate command fi Comparison operators are eq for equals, lt for less than and gt for greater than	<pre>if [\$# -lt 1] then echo "Less than" else echo "greater than 1" fi</pre>
` `	Backtick symbols surrounding a command cause the com- mand to be executed and then substitute the output into that place in the shell command or script	<pre>cd `which python`/ nano `which script.py`</pre>
host	Return IP number associated with a hostname, or the hostname associated with an IP address, if available	host www.sinauer.com host 127.0.0.1
ssh	Start a secure remote shell connection	ssh lucy@pcfb.org
scp	Securely copy files to or from a remote location	<pre>scp localfile user@host/path/remotefile scp user@host/home/file.txt localfile.txt</pre>
sftp	Start a file transfer connection to a remote site. The prompt changes to an ftp prompt, at which the following commands can be used: open From the prompt, open a new sftp connection get Bring a remote file to the local server put Place a local file on the remote system cd Change directory on the remote server lcd Change directory on the local machine quit Exit the sftp connection	sftp user@remotemachine
gzip gunzip zip unzip	Compress and uncompress files	gzip files.tar gunzip files.tar.gz unzip archive.zip
tar	Create or expand an archive containing files or folders -cf Create -xvf Expand -xvfz Expand and uncompress gzip	tar -cf archive.tar -/scripts tar -xvfz arch.tar.gz

Command	Description	Usage
&	When placed at the end of a command, runs it in the back- ground	
ps	Show currently running processes. Flags controlling the output vary greatly by system. Usually a good starting point is -ax. See man ps for more	ps -ax grep lucy
top	Show current processes sorted by various parameters, most useful of which is processor usage $-\mathtt{u}$	top -u
kill -9	Terminate a process emphatically, using its process ID. Retrieve PID from the ps or top command	kill -9 5567
killall	Terminate processes by name	killall Firefox
nohup	Run command in background and don't terminate it when logging out or closing the shell window Use in this odd format shown, to prevent program output to cause the command to quit	nohup command 2> /dev/ null < /dev/null &
ctrl Z	Suspend the operation to move it into the background or perform other operations	
jobs	Show backgrounded or suspended jobs, won't show normal active processes	
bg	Move a suspended process into the background. Optional number after it in the format \$1 will specify the job number	
apt-get yum rpm port	Package installers for various Unix distributions. Search for and install remote software packages. Typically used with sudo	sudo apt-get install agrep yum search imagemagick

Appendix 4

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PYTHON QUICK REFERENCE

Conventions for this appendix

In the examples below, italicized terms are not real variable or function names, but are stand-ins for an actual name. If a function name is shown as .function() then the dot means it is used as a method, coming after the variable name, as in MyString.upper().

Format, syntax, and punctuation in Python

- Indented lines define blocks of statements that are executed in loops, decisions, and functions.
- Comments are marked by # and extend from that symbol to the end of the line. Multi-line comments can be bracketed on both sides by three quote marks.
- To continue a statement on the next line, use the \ character at the end of a line.
- Parentheses () pass parameters to functions.¹
- Square brackets [] define lists and retrieve subsets of values from strings, lists, dictionaries, and other types.
- Curly brackets {} define dictionary entries.

Python scripts begin with the shebang line, and can include an optional line to enable support of Unicode characters:

```
#! /usr/bin/env python
# coding: utf-8
```

 $^{^1\}mathrm{They}$ also are used to define tuples, non-changeable list-like variables that we don't address in this book.

The command-line interpreter

Start by typing python at the command line. Cycle up through history of previous Python commands using ①. Use quit() or ctrl D to exit (ctrl Z in Windows).

You should be able to paste entire programs into the interpreter, but sometimes the indented block of a loop or conditional statement might not be carried over properly. Pasting commands at the Python prompt also does not work well for things involving user input or reading and writing files. In addition, the buffer of your terminal program may not keep up with large pasted blocks, resulting in errors on the text pasted.

Command summary

Variable types and statistics

Changing variable types and getting information	
Convert numbers and other types to strings This conversion is required for the .write() function used with a file or the sys.stderr.write() function	str()
Convert integers or strings to floating point	float()
Can specify the base in alternate base systems. To specify the number in hex, use int(MyString, 16)	<pre>int(3.14) int("3") int("4F",16)</pre>
Give the length of a string, list, or dictionary	<pre>len("ABCD") len([1,2,4,8]) len(Diction)</pre>

Strings

Defining and formatting strings	
Strings are defined by pairs of single (') or double (") quotation marks, not curly quotes ("")	Location = "Hawai'i" Region = "3'-polyA" Genus = 'Gymnopraia'
Multi-line strings are defined by three quote marks in a row	MultiString = """ Triple-quoted strings can span several lines. They also act like comments """
Convert from number to string	str(100.5)
Find the ASCII code for a string character with ord()	ord('A')

Manipulating strings	
Change case with .upper() and .lower()	<pre>MyString.upper() MyString.lower()</pre>
Join two strings with +	MyString + YourString 'Value' + str(MyValue) + '\n'
Repeat a string with *	print '='*30 =========
Literal substitution (not using wildcards or regular expressions) with .replace()	<pre>MyString.replace('jellyfish','medusa')</pre>
Count occurrences of 'A' in MyString with .count()	MyString.count('A')
Remove all white space from rightmost end of string with .rstrip()	MyString.rstrip()
Remove only linefeeds, not tabs	MyString.rstrip('\n')
Strip all white space from both sides of string with .strip()	MyString.strip()

See *Working with lists* in this appendix for converting strings or characters to lists and *Searching with regular expressions*, also in this appendix, for advanced search and replace techniques.

Gathering user input

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Get user input during execution of program	<pre>raw_input("Enter a value:")</pre>
Get space-separated parameters given when program is run at the command line. You can pass parameters with wildcards, like dive*.csv	import sys sys.argv
The script or program name, using the zeroth parameter	sys.argv[0]
All subsequent command-line arguments	sys.argv[1:]
Determine how many command-line parameters were provided, via the len() function	if len(sys.argv) > 1:

Building strings

Printing strings	
Print variables separated by a space	print MyString, MyNumber
Print variables not separated by space	<pre>print MyString + str(MyNumber)</pre>

Generating strings with the formatting operator, %:

```
MyString = '%s %.2f %d' % ("Value",4.1666,256)
              → Substitution points → Values to insert
```

This creates the string: 'Value 4.17 256'

Given the string $s = {}^{1} x^{1} + (4.13)$ where x is a placeholder listed below:		
Placeholder	Туре	Result
%s	String variable	'four'
%d	Integer digits	'4'
%5d	Integer padded to at least five spaces	' 4'
%f	Floating point	'4.130000'
%.2f	Float with precision of two decimal points	'4.13'
%5.1f	Float with one decimal, padded to at least five total spaces (includes decimal point)	' 4.1'

Comparisons and logical operators

Comparison operators ^a	
Comparison	Is True if
х == у	x is equal to y
x != y	x is not equal y
x > y	x is greater than y
х < у	x is less than y
х >= у	x is greater than or equal to y
х <= у	${f x}$ is less than or equal to ${f y}$

^aThese operators return True (1) or False (0) based on the result of the comparison.

Logical operators ^a		
Logical operator	Is True if	
A and B	Both A and B are True	
A or B	Either A or B is True	
not B	B is False (inverts the value of B)	
(not A) or B	A is False or B is True	
not (A or B)	A and B are both False	

^aIn this table, A and B represent a True/False comparison like those listed in the previous table.

Note that in Python, when an expression involving logical operators is found to be true, the value returned is that of the first true item being tested, not True itself.

```
>>> 1 and 2
>>> 3 or 4
```

Math operators

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Normal order of precedence applies. Operations involving only integers produce only integers, even at the expense of accuracy.

Addition	+
Subtraction	-
Multiplication	*
Division	/
Modulo (remainder after division)	% 7 % 2 → 1
Power	** 2**8=256
Truncated division (result without remainder)	// 7//2.0 = 3.0
Increment a variable by a value	+= X += 2

Decisions

The if, elif, and else commands control the flow of a program according to logical tests. Statements built on these commands end with a colon. Below is a description of each, with example code on the right.

```
if logical1:
    # do indented lines
    # if logical1 is True

elif logical2:
    # if logical1 is False
    # and logical2 is True

else:
    # do if all tests
    # above are False
A=5
if A < 0:
prin
elif A >
prin
else:
prin
else:
```

```
A=5
if A < 0:
    print "Negative number"

elif A > 0:
    print "Zero or positive number"

else:
    print "Zero"
```

Loops

For and while loop definitions end with a colon. Use for loops to step through ranges and lists. Below are a series of loop examples, with code shown on the right.

```
for loop using range()

for Num in range(10):
    print Num * 10

for loop with a list

for Item in MyList:
    print Item

for loop with a string

for Letter in "FEDCBA":
    print Letter

while loop

X=0
    while X < 11:
        print X
        X = X + 2</pre>
```

Searching with regular expressions

Regexp to find matching subsets in a string

Use regexp within your program to extract and substitute portions of a string. The basic format is:

```
Results = re.search(query,string)
```

The query is a text string containing the regular expressions pattern that you would enter into a Find dialog box.

Regexp to substitute into a string

The basic format is:

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```
re.sub(query, replacement, string)
```

When used in a program, this is the same as a Replace All command for that string.

```
Import the module import re

Define a search query, using a raw string MyRe = r"(\w)(\w+) (.*)"

Define the replacement term, using \( \)1, \2, etc., to represent entities captured with parentheses

String to search MyString = "Agalma elegans"

Search and save matches NewString = re.sub(MyRe, MySub, MyString)

The result saved in NewString "A. elegans"
```

print list(set(Mylist))
['a','b','c','d']

NewList=MyList.sorted()

Keys=Diction.keys()
Keys.sort()

MyList.sort()

Working with lists

Lists are ordered collections of objects. Items in a list can be of any type, including other lists and heterogeneous mixes of variable types. The first element has an index of 0; so, for example, a list with five members does not have an item at index 5.

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Sort lists

Return a sorted list, leaving original list unaltered

Sort in place, modifying original list

Creating lists	
Create a list from string or other variable type If the variable is a string, the list elements will be each character of the string	list(MyString)
Define with square brackets	MyList = [1,2,3] OtherList = [[2,4,6],[3,5,7]]
Define an empty list; required before the list can be appended to	MyList=[]
Define numerical lists with the range () function The left element is included in the retrieval, the right index is not Given one parameter, range (N) creates N elements, from 0 to N-1. A third parameter optionally sets the step size between elements, positive or negative	Function Result range(5) [0, 1, 2, 3, 4] range(1,8,2) [1, 3, 5, 7] range(5,0,-1) [5, 4, 3, 2, 1]
Parse strings into lists with .split() Default delimiter is any amount of white space, or specify delimiter character in the ()	<pre>MyList = MyString.split()</pre>
Add elements with .append()	MyList.append(10)
Insert elements with a single index repeated on both sides of the colon	MyList=range(5) MyList[3:3]=[9,8,7] >>> MyList [0, 1, 2, 9, 8, 7, 3, 4]
Delete elements from list with del Assign =[] to delete indexed elements	<pre>del MyList[2:5] MyList[2:5]=[]</pre>

	,
Accessing list elements	
Extract elements with [] Index range: Start element is retrieved, finish element is not Indices can count from either the beginning, or, using negative numbers, the end of the list	<pre>MyList[Start:Finish] MyList[begin:end+1:step]</pre>
Skip first element of a list	MyList[1:]
All but last element	MyList[:-1]
Return list elements in reverse order, leaving the original list unchanged Sort list in place, modify original	<pre>MyList[::-1] MyList.reverse()</pre>
Extract even or odd elements	MyList=range(8) MyList [1::2] [1, 3, 5, 7] MyList[0::2] [0, 2, 4, 6]
Unpacking two or more values at once	a,b=MyList[0,1]
List information and conversions	
Convert lists of strings to strings with .join() The .join() method works a bit backwards, acting on the character used to join, with the list as a parameter	<pre>''.join(MyList) MyList = ['A', 'B', 'C', 'D'] print '-'.join(MyList) A-B-C-D</pre>
Test if an item is in a list with the in operator	print 'A' in MyList True
Create a list of unique elements of a list with set ()	MyList=list('aabbbcdaa')

Retrieve elements and their indices together, using enumerate() Ind, Elem = enumerate(MyList)

List comprehension

Performs an operation on each item in a list, and returns a list of the results. List comprehensions are very useful for manipulating lists in Python.

```
Squares = [Val**2 for Val in MyList]
Strings = [str(Val) for Val in MyList]
```

Dictionaries

Dictionaries are somewhat like lists, except that instead of values being accessed by sequential numerical keys (indexes), they are accessed by non-sequential keys defined as you wish. Keys and values can be of many types, including numbers, strings, or lists, and they can occur together in one dictionary. Only one instance of a key is allowed in a dictionary, but values can occur repeatedly; that is, it is keys that are required to be unique, not values. Dictionaries have no intrinsic order to their contents, and values are returned only by key, not by position or order of entry.

```
Defining dictionaries
Define entries within curly brackets with the format
                                                   Diction = {1:'a', 2:'b'}
 {key: value}
                                                   Diction={
Key-value pairs are separated by commas
                                                   'Lilyopsis' :3, 'Resomia'
Between the brackets, the definition can span several
                                                   'Rhizophysa':1, 'Gymnopraia':3 }
 lines and indentation is not important
A list of keys and a list of values having the same
                                                   SiphKeys = ['Lilyopsis', 'Rhizophysa',
 number of elements can be zipped together to
                                                     'Resomia', 'Gymnopraia']
 form a dictionary
                                                   SiphVals = [3,1,2,3]
                                                   Diction = dict(zip(SiphKeys,SiphVals))
Add entries using indexed values with square brackets Diction={}
Requires a pre-existing dictionary, which can have no
                                                   Diction['Marrus'] = 2
 entries
Delete dictionary entries with del
                                                   del Diction['Marrus']
The method used to clear list elements by assigning
 to [] does not work with dictionaries. The key will
 still exist
```

```
Extracting values from a dictionary

Index with square brackets [] and the key print Diction['Resomia']

2

If the key is not present, results in an error print Diction ['Erenna']

...KeyError: 'Erenna'

Retrieve with .get() print Diction.get('Resomia')

Optionally, provide a value to return if the key is not present print Diction.get('Erenna', -99)

-99
```

```
Information about a dictionary

Get a list of keys or values with .keys() and .values(), but not in any predictable order

The order, however, will be internally consistent between the two lists

Diction.keys()
['Resomia', 'Lilyopsis', 'Gymnopraia', 'Rhizophysa']
Diction.values()
[2, 3, 3, 1]

Number of entries in a dictionary

len(Diction)
```

Creating functions

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Define the function in the program before it is used, or in an external file which is imported. Functions can be generated with or without additional parameters, and parameters can be assigned default values.

```
def function_name(Parameter = Defaultvalue):
    # insert statements that calculate values
    return Result # send back the result
```

Call the function from within the program, passing values in parentheses:

```
MyValue = function_name(200)
```

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Working with files

Reading from a file	
Open the connection to the file	<pre>InFile = open(FileName, 'rU')</pre>
Read lines in succession	for Line in InFile: # perform operation on Lines
Alternatively, read all lines into a list at once. (This can't be used after the command above since InFile is already at the end of the file)	AllLines = InFile.readlines()
Close the file connection	InFile.close()

An example of a short file-reading program in action:

```
FileName="/Users/lucy/pcfb/examples/FPexcerpt.fta"
InFile = open(FileName, 'rU')
for Line in InFile:
   MyLine = Line.strip()
    if MyLine[0]==">":
        print MyLine[1:]
InFile.close()
```

Getting information about files	
Use the os module	import os
Check if string is path to a file; fails if it is not found or if it is a folder rather than a file	os.path.isfile('/Users/lucy/pcfb/')
Check if a folder or file exists Fails with ~/ as part of path	<pre>os.path.exists('/Users/lucy/pcfb/') True os.path.exists('~/pcfb/') False</pre>
Get a list of files matching the parameter, using * as a wildcard	<pre>import glob FileList = glob.glob('pcfb/*.txt')</pre>

Using modules and functions

Writing to a file

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file if it already exists

Line endings are not automatically

First import the module, then call the function, usually followed by parentheses.

Ways to import functions from a module	
Import all the functions and use them thereafter by appending the function name to the module	<pre>import themodule themodule.thefunction()</pre>
Import a module, but use a different name for it within the program	<pre>import longmodulename as shortname shortname.thefunction()</pre>
Import all the functions from a module, and use them with only the function name	<pre>from themodule import * thefunction()</pre>
Import a particular function, and use it with just its name	from themodule import thefunction thefunction()
To see a list of commands in the module, after importing in the Python interactive environment	<pre>dir(modulename) help(modulename)</pre>

To create your own modules, use def to define functions as indicated above, place them in their own file, and save with a filename ending in .py somewhere in your PATH. Import them into your script using the filename without the .py extension.

Some built-in modules		
random	Random sampling and random number generation	
urllib	Downloading and interacting with Web resources	
time	Information related to the current time and elapsed time	
math	Some basic trigonometric functions and constants	
os	Items related to the file system	
sys	System-level commands, such as command-line arguments	
re	The regular expressions library for search and replace	
datetime	Date conversion and calculation functions	
xml	Reading and writing XML files	
csv	Read in a comma-delimited file using the function ${\tt csv.reader}$ ()	

Other installable modules	
MySQLdb	Interact with a mysql database
PySerial	Connect through the serial port to external devices. Use with import serial
matplotlib	MATLAB-like plotting functionality
numpy, Scipy	Large package of numerical and statistical capabilities
Biopython	Functions for dealing with molecular sequence files and searches. Use with import Bio or from Bio import Seq

Miscellaneous Python operations

Presenting warnings and feedback

sys.stderr.write()

Sends output to screen (but does not send output to a file when a redirect such as >> is used).

Catching errors

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Statements indented under a try: function will be executed until an error occurs. If there is an error, then the block of code indented under a subsequent except: statement will be executed.

Shell operations within Python

os.popen("rmdir sandbox")

The shell command specified in parentheses is executed. If you want to read the results the command would usually print to the screen, append .read():

Contents = os.popen("ls -l").read()

For example, os.popen(pwd) will try to operate whether or not there is printed feedback.

Reference and getting help

- From the python command line, use dir(item) to see functions within a variable or imported module. Use type(item) to get a simple statement of the variable type.
- Depending on the variable, help(item) may give you the information pages related to a function or a variable, showing you information pertinent to its type.
- Consult Web sites such as diveintopython.org when stuck.

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SQL COMMANDS

SQL, short for Structured Query Language, is the language used to interact with relational databases, as discussed in Chapter 15. Although our specific examples are drawn from MySQL, learning the basics of SQL can help you work with nearly any database system. MySQL has excellent online references, tutorials, and examples. Many are at the site: dev.mysql.com/doc/refman/5.1/en/.

Installing MySQL is described in Chapter 15. The commands listed in the tables below would be entered at the mysql> prompt, launched using the command:

mysql -u root

If you have assigned a password to the root account, the command above should end with -p. You can also log in as a user other than root if you have configured other users.

Databases are organized into tables containing fields (corresponding to columns), which in turn contain values of related information organized into rows.

Working at the MySQL prompt	
Purpose	Example
Entering commands Commands can span several lines. They are only executed when the line is terminated with a semicolon. Indentation and capitalization are just for readability and are not interpreted	SELECT genus FROM specimens WHERE vehicle LIKE 'Tib%' AND depth > 100
Interrupt a command or cancel a partially typed command. Do not type ctrl C, which will end your entire mysql session	\c return
Quit MySQL	EXIT;
Get general help, or help on a command or topic	HELP HELP SELECT

HELP LOAD DATA



See Appendix 1 for installation and launching instructions.

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K		

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Selected MySQL data types			
Data type	Description		
INTEGER	An integer. Also abbreviated	An integer. Also abbreviated as INT	
FLOAT	A floating point number, incl	uding scientific notation	
DATE	A date in 'YYYY-MM-DD' fo	rmat	
DATETIME	A date and time in 'YYYY-M	M-DD HH:MM:SS' format	
TEXT	A string containing up to 65,	535 characters	
TINYTEXT	A string containing up to 25	5 characters	
BLOB	A binary object, including im	nages or other non-text data	
Creating da	tabases and tables		
-		DATABASE databasename;	
Select a database as the target USE databasename; of subsequent commands			
Make a new table containing field type definitions CREATE TABLE tablename (fieldname1 TYPE, fieldname2 TYPE2);			
Make a new table with an autoincrementing primary key, then other column definitions CREATE TABLE tablename (primarykeyname INTEGER NOT NULL AUTO_INCREMENT PRIMARY KEY, nextfield TYPE, anotherfield TYPE);			
Adding data into table fields			
Import formatted text data whose columns correspond exactly to predefined table fields		LOAD DATA LOCAL INFILE 'path/to/infile';	
	f values to a table in the order nes the predefined fields	INSERT INTO tablename VALUES (1, "Beroe", 5.2, "1865-12-18");	
Redefine val criterion	ues based on another	UPDATE tablename SET values = x WHERE othervalues = y;	
Database and table information			
List the name	es of the databases or tables	SHOW DATABASES; SHOW TABLES;	
	type, and other information fields of a table	DESCRIBE tablename;	
Show the nu	mber of entries in the table	SELECT COUNT(*) FROM tablename;	

Extracting data from tab	les with SELECT			
List all the rows in all colu The rows retrieved can WHERE statements at th	be refined with	SELECT	* FROM tablenam	e;
Show the values of the lis from the table	ted columns		vehicle,date OM specimens;	
Show the unique values o column	f a named		DISTINCT vehicl OM specimens;	е
Show a count of the value table	es in a named		COUNT(*) OM specimens;	
Show a count of the value field, clustered by the u that field. Like SELECT with counts	inique values of	FR	vehicle,COUNT(* OM specimens OUP BY vehicle;)
Qualifying which rows to	retrieve using W	HERE		
WHERE refines the records (rows) retrieved from a SELECT command. Criteria include comparisons like greater than and less than, or comparisons of equality, which can apply to numbers or strings. Use != for not equal			500	
Find approximate matche wildcard of any charact			WHERE vehicle	LIKE "Tib%"
Find matches using regular expressions. Wild- cards are not all supported, but beginning and end of line, . [] + are supported			WHERE field RE WHERE vehicle WHERE species	
Combine criteria with log Use parentheses to group		SELE	CT vehicle from WHERE (vehicle OR (vehicle LI	LIKE "Ven%")
Mathematical and statist	ical operators			
Basic math operators	+, -, *, ,/			
Basic comparisons	<,>,=,!=			
Average of the values	AVG()			
Count of the values	COUNT()			
Maximum value	MAX()			
Minimum value	MIN()			
Standard deviation	STD()			
Sum of the values	SUM()			

Deleting entries and tables

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Clear all entries from a table	DELETE FROM tablename;
Clear entries matching WHERE criteria	DELETE FROM tablename WHERE vehicle LIKE "Tib%";
Delete an entire table. Use with caution. Can't undo it	DROP tablename;
Saving to a file	
Save the results from a query into a tab-delimited file	<pre>SELECT * FROM midwater INTO OUTFILE '/export.txt' FIELDS TERMINATED BY '\t' LINES TERMINATED BY '\n' ;</pre>
Export the entire database to an archive. This command is run at the shell prompt, not the mysql prompt. The resulting file has all the commands necessary to recreate the original database tables	<pre>mysqldump -u root databasename > datafile.sql</pre>
Read back in a database created via dun Read in a file of SQL commands This command is also run at the bash prompt, and the target database must already exist	np mysql -u root <i>targetdb</i> < mw.sql
User management ^a	
Set the password for the current user (from the mysql prompt). Remember the equal sign	<pre>SET PASSWORD = PASSWORD('mypass'); SET PASSWORD FOR 'python_user'@'localhost' = PASSWORD('newpass') OLD_PASSWORD('oldpass');</pre>
Add a new user with defined addresses that they can connect from and a preset password	CREATE USER 'newuser'@'localhost' IDENTIFIED BY 'newpassword';
Give a user privileges. The capabilities, database and tables, and user and host are specified. Host IP ranges use % as the wildcard character	GRANT SELECT, INSERT, UPDATE, CREATE, DELETE ON midwater.* TO 'newuser'@'localhost';
Log in with password (from the shell prompt)	mysql -u newuser -p

^aThese commands can also be accomplished from within the Dashboard or SQuirrelSQL GUIs.