$Bash-UNIX_CarpentriesBootcamp$

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Working With Files and Directories

Before we start, make sure to clone or update the github folder MarineGenomics in the user directory

```
$ cd /home/margeno/
$ git clone https://github.com/BayLab/MarineGenomics
```

Creating directories

We now know how to explore files and directories, but how do we create them in the first place?

Step one: see where we are and what we already have

Let's open the folder Week2 inside of /home/margeno/MarineGenomics/data/Week2 and see where what it contains with $\verb"ls -F"$:

Bash

- \$ cd /home/margeno/MarineGenomics/data/Week2/data-shell
- \$ pwd

Output

/home/margeno/MarineGenomics/data/Week2/data-shell

Bash

\$ ls -F

Output

creatures/ data/ molecules/ north-pacific-gyre/ notes.txt pizza.cfg solar.pdf writing/

Create a directory

Let's create a new directory called thesis using the command mkdir thesis (which has no output):

Bash

\$ mkdir thesis

As you might guess from its name, mkdir means 'make directory'. Since thesis is a relative path (i.e., does not have a leading slash, like /what/ever/thesis), the new directory is created in the current working directory:

Bash

\$ ls -F

Output

creatures/ data/ molecules/ north-pacific-gyre/ notes.txt pizza.cfg solar.pdf thesis/ writing/

Since we've just created the thesis directory, there's nothing in it yet:

Bash

```
$ ls -F thesis
```

Note that mkdir is not limited to creating single directories one at a time. The -p option allows mkdir to create a directory with any number of nested subdirectories in a single operation:

Bash

```
$ mkdir -p thesis/chapter_1/section_1/subsection_1
```

The -R option to the ls command will list all nested subdirectories within a directory. Let's use ls -FR to recursively list the new directory hierarchy we just created beneath the thesis directory:

Bash

```
$ ls -FR thesis
chapter_1/
thesis/chapter_1:
section_1/
thesis/chapter_1/section_1:
subsection_1/
thesis/chapter_1/section_1/subsection_1:
```

Two ways of doing the same thing

Using the shell to create a directory is no different than using a file explorer. If you open the current directory using your operating system's graphical file explorer, the thesis directory will appear there too. While the shell and the file explorer are two different ways of interacting with the files, the files and directories themselves are the same.

Good names for files and directories

Complicated names of files and directories can make your life painful when working on the command line. Here we provide a few useful tips for the names of your files.

- 1. Don't use spaces.
 - Spaces can make a name more meaningful, but since spaces are used to separate arguments on the command line it is better to avoid them in names of files and directories. You can use or _ instead (e.g. north-pacific-gyre/ rather than north pacific gyre/).
- Don't begin the name with (dash).
 Commands treat names starting with as options.
- 3. Stick with letters, numbers, . (period or 'full stop'), (dash) and _ (underscore). Many other characters have special meanings on the command line. We will learn about some of these during this lesson. There are special characters that can cause your command to not work as expected and can even result in data loss.

If you need to refer to names of files or directories that have spaces or other special characters, you should surround the name in quotes ("").

Create a text file

Let's change our working directory to thesis using cd, then run a text editor called Nano to create a file called draft.txt:

Bash

\$ cd thesis
\$ nano draft.txt

Which Editor?

When we say, 'nano is a text editor' we really do mean 'text': it can only work with plain character data, not tables, images, or any other human-friendly media. We use it in examples because it is one of the least complex text editors. However, because of this trait, it may not be powerful enough or flexible enough for the work you need to do after this workshop. On Unix systems (such as Linux and macOS), many programmers use Emacs or Vim (both of which require more time to learn), or a graphical editor such as Gedit. On Windows, you may wish to use Notepad++. Windows also has a built-in editor called notepad that can be run from the command line in the same way as nano for the purposes of this lesson.

No matter what editor you use, you will need to know where it searches for and saves files. If you start it from the shell, it will (probably) use your current working directory as its default location. If you use your computer's start menu, it may want to save files in your desktop or documents directory instead. You can change this by navigating to another directory the first time you 'Save As...'

Let's type in a few lines of text. Once we're happy with our text, we can press Ctrl+O (press the Ctrl or Control key and, while holding it down, press the O key) to write our data to disk (we'll be asked what file we want to save this to: press Return to accept the suggested default of draft.txt).

GNU nano 2.0.6 File: draft.txt Modified

It's not "publish or perish" any more,
it's "share and thrive".



Once our file is saved, we can use Ctrl+X to quit the editor and return to the shell.

Control, Ctrl, or ^ Key

The Control key is also called the 'Ctrl' key. There are various ways in which using the Control key may be described. For example, you may see an instruction to press the Control key and, while holding it down, press the X key, described as any of:

- Control-X
- Control+X
- Ctrl-X
- Ctrl+X
- ^X
- C-x

In nano, along the bottom of the screen you'll see ^G Get Help ^O WriteOut. This means that you can use Control-G to get help and Control-O to save your file.

nano doesn't leave any output on the screen after it exits, but ls now shows that we have created a file called draft.txt:

Bash

\$ ls

Output

draft.txt

Creating Files a Different Way

We have seen how to create text files using the nano editor. Now, try the following command: Bash

\$ touch my_file.txt

- 1. What did the touch command do? When you look at your current directory using the GUI file explorer, does the file show up?
- 2. Use ls -1 to inspect the files. How large is my_file.txt?
- 3. When might you want to create a file this way?

- 1. The touch command generates a new file called my_file.txt in your current directory. You can observe this newly generated file by typing ls at the command line prompt. my_file.txt can also be viewed in your GUI file explorer.
- 2. When you inspect the file with ls -1, note that the size of my_file.txt is 0 bytes. In other words, it contains no data. If you open my_file.txt using your text editor it is blank.
- 3. Some programs do not generate output files themselves, but instead require that empty files have already been generated. When the program is run, it searches for an existing file to populate with its output. The touch command allows you to efficiently generate a blank text file to be used by such programs.

What's In A Name?

You may have noticed that all of Nelle's files are named 'something dot something', and in this part of the lesson, we always used the extension .txt. This is just a convention: we can call a file mythesis or almost anything else we want. However, most people use two-part names most of the time to help them (and their programs) tell different kinds of files apart. The second part of such a name is called the filename extension, and indicates what type of data the file holds: .txt signals a plain text file, .pdf indicates a PDF document, .cfg is a configuration file full of parameters for some program or other, .png is a PNG image, and so on.

This is just a convention, albeit an important one. Files contain bytes: it's up to us and our programs to interpret those bytes according to the rules for plain text files, PDF documents, configuration files, images, and so on.

Naming a PNG image of a whale as $\mathtt{whale.mp3}$ doesn't somehow magically turn it into a recording of whalesong, though it might cause the operating system to try to open it with a music player when someone double-clicks it.

Moving files and directories

Returning to the data-shell directory,

Bash

cd /home/margeno/MarineGenomics/data/Week2/data-shell

In our thesis directory we have a file draft.txt which isn't a particularly informative name, so let's change the file's name using mv, which is short for 'move':

Bash

\$ mv thesis/draft.txt thesis/quotes.txt

The first argument tells mv what we're 'moving', while the second is where it's to go. In this case, we're moving thesis/draft.txt to thesis/quotes.txt, which has the same effect as renaming the file. Sure enough, ls shows us that thesis now contains one file called quotes.txt:

Bash

\$ ls thesis

Output

quotes.txt

One has to be careful when specifying the target file name, since mv will silently overwrite any existing file with the same name, which could lead to data loss. An additional option, mv -i (or mv --interactive), can be used to make mv ask you for confirmation before overwriting.

Note that mv also works on directories.

Let's move quotes.txt into the current working directory. We use mv once again, but this time we'll use just the name of a directory as the second argument to tell mv that we want to keep the filename, but put the file somewhere new. (This is why the command is called 'move'.) In this case, the directory name we use is the special directory name . that we mentioned earlier.

Bash

\$ mv thesis/quotes.txt .

The effect is to move the file from the directory it was in to the current working directory. 1s now shows us that thesis is empty:

Bash

\$ ls thesis

Further, 1s with a filename or directory name as an argument only lists that file or directory. We can use this to see that quotes.txt is still in our current directory:

Bash

\$ ls quotes.txt

Output

quotes.txt

Moving Files to a new folder

After running the following commands, Jamie realizes that she put the files sucrose.dat and maltose.dat into the wrong folder. The files should have been placed in the raw folder.

```
$ ls -F
analyzed/ raw/
$ ls -F analyzed
fructose.dat glucose.dat maltose.dat sucrose.dat
$ cd analyzed
```

Fill in the blanks to move these files to the raw/ folder (i.e. the one she forgot to put them in) Bash

\$ mv sucrose.dat maltose.dat ____/___

Bash

```
$ mv sucrose.dat maltose.dat ../raw
```

Recall that .. refers to the parent directory (i.e. one above the current directory) and that . refers to the current directory.

Copying files and directories

The cp command works very much like mv, except it copies a file instead of moving it. We can check that it did the right thing using 1s with two paths as arguments — like most Unix commands, 1s can be given multiple paths at once:

Bash

```
$ cp quotes.txt thesis/quotations.txt
$ ls quotes.txt thesis/quotations.txt
Output
```

```
quotes.txt thesis/quotations.txt
```

We can also copy a directory and all its contents by using the recursive option $-\mathbf{r}$, e.g. to back up a directory: Bash

```
$ cp -r thesis thesis_backup
```

We can check the result by listing the contents of both the thesis and thesis_backup directory:

 Bash

```
$ ls thesis thesis_backup
```

Output

```
thesis:
quotations.txt
```

thesis_backup:
quotations.txt

Renaming Files

Suppose that you created a plain-text file in your current directory to contain a list of the statistical tests you will need to do to analyze your data, and named it: statstics.txt

After creating and saving this file you realize you misspelled the filename! You want to correct the mistake, which of the following commands could you use to do so?

```
    cp statstics.txt statistics.txt
    mv statstics.txt statistics.txt
    mv statstics.txt .
    cp statstics.txt .
```

Solution

Solution

- 1. No. While this would create a file with the correct name, the incorrectly named file still exists in the directory and would need to be deleted.
- 2. Yes, this would work to rename the file.
- 3. No, the period(.) indicates where to move the file, but does not provide a new file name; identical file names cannot be created.
- 4. No, the period(.) indicates where to copy the file, but does not provide a new file name; identical file names cannot be created.

Moving and Copying

What is the output of the closing 1s command in the sequence shown below? Bash

\$ pwd

Output

/Users/jamie/data

Bash

\$ ls

OUtput

proteins.dat

Bash

```
$ mkdir recombined
$ mv proteins.dat recombined/
$ cp recombined/proteins.dat ../proteins-saved.dat
$ ls
```

- 1. proteins-saved.dat recombined
- 2. recombined
- 3. proteins.dat recombined
- 4. proteins-saved.dat

We start in the /Users/jamie/data directory, and create a new folder called recombined. The second line moves (mv) the file proteins.dat to the new folder (recombined). The third line makes a copy of the file we just moved. The tricky part here is where the file was copied to. Recall that .. means 'go up a level', so the copied file is now in /Users/jamie. Notice that .. is interpreted with respect to the current working directory, not with respect to the location of the file being copied. So, the only thing that will show using ls (in /Users/jamie/data) is the recombined folder.

- 1. No, see explanation above. proteins-saved.dat is located at /Users/jamie
- 2. Yes
- 3. No, see explanation above. proteins.dat is located at /Users/jamie/data/recombined
- 4. No, see explanation above. proteins-saved.dat is located at /Users/jamie

Removing files and directories

Returning to the MarineGenomics directory, let's tidy up this directory by removing the quotes.txt file we created. The Unix command we'll use for this is rm (short for 'remove'):

```
$ rm quotes.txt
```

We can confirm the file has gone using 1s:

```
$ ls quotes.txt
```

ls: cannot access 'quotes.txt': No such file or directory

Deleting Is Forever

The Unix shell doesn't have a trash bin that we can recover deleted files from (though most graphical interfaces to Unix do). Instead, when we delete files, they are unlinked from the file system so that their storage space on disk can be recycled. Tools for finding and recovering deleted files do exist, but there's no guarantee they'll work in any particular situation, since the computer may recycle the file's disk space right away.

Using rm Safely

What happens when we execute rm -i thesis_backup/quotations.txt? Why would we want this protection when using rm?

Solution

Solution

```
$ rm: remove regular file 'thesis backup/quotations.txt'? y
```

The -i option will prompt before (every) removal (use Y to confirm deletion or N to keep the file). The Unix shell doesn't have a trash bin, so all the files removed will disappear forever. By using the -i option, we have the chance to check that we are deleting only the files that we want to remove.

If we try to remove the thesis directory using rm thesis, we get an error message:

\$ rm thesis

Error

```
rm: cannot remove 'thesis': Is a directory
```

This happens because rm by default only works on files, not directories.

rm can remove a directory and all its contents if we use the recursive option -r, and it will do so without any confirmation prompts:

```
$ rm -r thesis
```

Given that there is no way to retrieve files deleted using the shell, rm -r should be used with great caution (you might consider adding the interactive option rm -r -i).

Operations with multiple files and directories

Oftentimes one needs to copy or move several files at once. This can be done by providing a list of individual filenames, or specifying a naming pattern using wildcards.

Copy with Multiple Filenames

For this exercise, you can test the commands in the data-shell/data directory.

In the example below, what does cp do when given several filenames and a directory name?

```
$ mkdir backup
$ cp amino-acids.txt animals.txt backup/
```

In the example below, what does cp do when given three or more file names?

```
$ ls -F
```

amino-acids.txt animals.txt backup/ elements/ morse.txt pdb/ planets.txt salmon.txt sunspot
\$ cp amino-acids.txt animals.txt morse.txt

Solution

Solution

If given more than one file name followed by a directory name (i.e. the destination directory must be the last argument), cp copies the files to the named directory. If given three file names, cp throws an error such as the one below, because it is expecting a directory name as the last argument.

Output

```
cp: target 'morse.txt' is not a directory
```

Wildcards

- * is a wildcard, which matches zero or more characters. Let's consider the data-shell/molecules directory: *.pdb matches ethane.pdb, propane.pdb, and every file that ends with '.pdb'. On the other hand, p*.pdb only matches pentane.pdb and propane.pdb, because the 'p' at the front only matches filenames that begin with the letter 'p'.
- ? is also a wildcard, but it matches exactly one character. So ?ethane.pdb would match methane.pdb whereas *ethane.pdb matches both ethane.pdb, and methane.pdb.

Wildcards can be used in combination with each other e.g. ???ane.pdb matches three characters followed by ane.pdb, giving cubane.pdb ethane.pdb octane.pdb.

When the shell sees a wildcard, it expands the wildcard to create a list of matching filenames before running the command that was asked for. As an exception, if a wildcard expression does not match any file, Bash will pass the expression as an argument to the command as it is. For example typing ls *.pdf in the molecules directory (which contains only files with names ending with .pdb) results in an error message that there is no file called *.pdf. However, generally commands like wc and ls see the lists of file names matching these expressions, but not the wildcards themselves. It is the shell, not the other programs, that deals with expanding wildcards, and this is another example of orthogonal design.

List filenames matching a pattern

When run in the molecules directory, which ls command(s) will produce this output? ethane.pdb methane.pdb

- 1. ls *t*ane.pdb
- 2. ls *t?ne.*
- 3. ls *t??ne.pdb
- 4. ls ethane.*

Solution

Solution

The solution is 3.

- 1. shows all files whose names contain zero or more characters (*) followed by the letter t, then zero or more characters (*) followed by ane.pdb. This gives ethane.pdb methane.pdb octane.pdb pentane.pdb.
- 2. shows all files whose names start with zero or more characters (*) followed by the letter t, then a single character (?), then ne. followed by zero or more characters (*). This will give us octane.pdb and pentane.pdb but doesn't match anything which ends in thane.pdb.
- 3. fixes the problems of option 2 by matching two characters (??) between t and ne. This is the solution.
- 4. only shows files starting with ethane..

Solution

More on Wildcards

Sam has a directory containing calibration data, datasets, and descriptions of the datasets:

```
| -- 2015-10-23-calibration.txt
-- 2015-10-23-dataset1.txt
| -- 2015-10-23-dataset2.txt
| -- 2015-10-23-dataset overview.txt
| -- 2015-10-26-calibration.txt
| -- 2015-10-26-dataset1.txt
| -- 2015-10-26-dataset2.txt
| -- 2015-10-26-dataset_overview.txt
| -- 2015-11-23-calibration.txt
| -- 2015-11-23-dataset1.txt
| -- 2015-11-23-dataset2.txt
| -- 2015-11-23-dataset_overview.txt
| -- backup
1 | -- calibration
  l-- datasets
1-- send_to_bob
    | -- all_datasets_created_on_a_23rd
    l-- all_november_files
```

Before heading off to another field trip, she wants to back up her data and send some datasets to her colleague Bob. Sam uses the following commands to get the job done:

```
$ cp *dataset* backup/datasets
$ cp ____calibration____ backup/calibration
$ cp 2015-____send_to_bob/all_november_files/
$ cp ____ send_to_bob/all_datasets_created_on_a_23rd/
```

Help Sam by filling in the blanks.

The resulting directory structure should look like this

```
| -- 2015-10-23-calibration.txt
| -- 2015-10-23-dataset1.txt
| -- 2015-10-23-dataset2.txt
| -- 2015-10-23-dataset overview.txt
| -- 2015-10-26-calibration.txt
| -- 2015-10-26-dataset1.txt
| -- 2015-10-26-dataset2.txt
| -- 2015-10-26-dataset overview.txt
| -- 2015-11-23-calibration.txt
| -- 2015-11-23-dataset1.txt
| -- 2015-11-23-dataset2.txt
| -- 2015-11-23-dataset_overview.txt
| -- backup
  | -- calibration
   l | -- 2015-10-23-calibration.txt
1
   1 | -- 2015-10-26-calibration.txt
   1 1-- 2015-11-23-calibration.txt
1
1
   1-- datasets
1
       | -- 2015-10-23-dataset1.txt
       | -- 2015-10-23-dataset2.txt
1
       | -- 2015-10-23-dataset overview.txt
```

```
-- 2015-10-26-dataset1.txt
        | -- 2015-10-26-dataset2.txt
1
        | -- 2015-10-26-dataset overview.txt
1
        | -- 2015-11-23-dataset1.txt
1
        | -- 2015-11-23-dataset2.txt
1
        1-- 2015-11-23-dataset overview.txt
1-- send to bob
    | -- all_datasets_created_on_a_23rd
        | -- 2015-10-23-dataset1.txt
        | -- 2015-10-23-dataset2.txt
        | -- 2015-10-23-dataset_overview.txt
        | -- 2015-11-23-dataset1.txt
        | -- 2015-11-23-dataset2.txt
        1-- 2015-11-23-dataset_overview.txt
    l-- all_november_files
        | -- 2015-11-23-calibration.txt
        | -- 2015-11-23-dataset1.txt
        -- 2015-11-23-dataset2.txt
        1-- 2015-11-23-dataset_overview.txt
```

Solution

Bash

```
$ cp *calibration.txt backup/calibration
$ cp 2015-11-* send_to_bob/all_november_files/
$ cp *-23-dataset* send_to_bob/all_datasets_created_on_a_23rd/
```

Solution

Organizing Directories and Files

Jamie is working on a project and she sees that her files aren't very well organized:

```
$ ls -F
analyzed/ fructose.dat raw/ sucrose.dat
```

The fructose.dat and sucrose.dat files contain output from her data analysis. What command(s) covered in this lesson does she need to run so that the commands below will produce the output shown?

```
$ ls -F
analyzed/ raw/
$ ls analyzed
fructose.dat sucrose.dat
```

```
mv *.dat analyzed
```

Jamie needs to move her files fructose.dat and sucrose.dat to the analyzed directory. The shell will expand *.dat to match all .dat files in the current directory. The mv command then moves the list of .dat files to the 'analyzed' directory.

Solution

Reproduce a folder structure

You're starting a new experiment, and would like to duplicate the directory structure from your previous experiment so you can add new data.

Assume that the previous experiment is in a folder called '2016-05-18', which contains a data folder that in turn contains folders named raw and processed that contain data files. The goal is to copy the folder structure of the 2016-05-18-data folder into a folder called 2016-05-20 so that your final directory structure looks like this:

```
2016-05-20 l- data l- processed l- raw
```

Which of the following set of commands would achieve this objective? What would the other commands do?

```
$ mkdir 2016-05-20
$ mkdir 2016-05-20/data
$ mkdir 2016-05-20/data/processed
$ mkdir 2016-05-20/data/raw
$ mkdir 2016-05-20
$ cd 2016-05-20
$ mkdir data
$ cd data
$ mkdir raw processed
$ mkdir 2016-05-20/data/raw
$ mkdir 2016-05-20/data/processed
$ mkdir -p 2016-05-20/data/raw
$ mkdir -p 2016-05-20/data/processed
$ mkdir 2016-05-20
$ cd 2016-05-20
$ mkdir data
$ mkdir raw processed
```

Solution

Solution

The first two sets of commands achieve this objective. The first set uses relative paths to create the top level directory before the subdirectories.

The third set of commands will give an error because the default behavior of mkdir won't create a subdirectory of a non-existant directory: the intermediate level folders must be created first.

The fourth set of commands achieve this objective. Remember, the -p option, followed by a path of one or more directories, will cause mkdir to create any intermediate subdirectories as required.

The final set of commands generates the 'raw' and 'processed' directories at the same level as the 'data' directory.

Solution

Pipes and Filters

Now that we know a few basic commands, we can finally look at the shell's most powerful feature: the ease with which it lets us combine existing programs in new ways. We'll start with the directory called data-shell/molecules that contains six files describing some simple organic molecules. The .pdb extension indicates that these files are in Protein Data Bank format, a simple text format that specifies the type and position of each atom in the molecule.

\$ ls molecules

```
cubane.pdb ethane.pdb methane.pdb
octane.pdb pentane.pdb propane.pdb
```

Let's go into that directory with cd and run an example command wc cubane.pdb:

```
$ cd molecules
$ wc cubane.pdb
20 156 1158 cubane.pdb
```

wc is the 'word count' command: it counts the number of lines, words, and characters in files (from left to right, in that order).

If we run the command wc *.pdb, the * in *.pdb matches zero or more characters, so the shell turns *.pdb into a list of all .pdb files in the current directory:

\$ wc *.pdb

```
cubane.pdb
20 156 1158
12 84
         622
               ethane.pdb
               methane.pdb
 9
    57
         422
30
    246 1828
               octane.pdb
21
    165
         1226
               pentane.pdb
15
    111
         825
               propane.pdb
107
    819
         6081
               total
```

Note that wc *.pdb also shows the total number of all lines in the last line of the output.

If we run wc -1 instead of just wc, the output shows only the number of lines per file:

```
$ wc -1 *.pdb
```

```
20 cubane.pdb
```

- 12 ethane.pdb
- 9 methane.pdb
- 30 octane.pdb
- 21 pentane.pdb
- 15 propane.pdb
- 107 total

The -m and -w options can also be used with the wc command, to show only the number of characters or the number of words in the files.

Why Isn't It Doing Anything?

What happens if a command is supposed to process a file, but we don't give it a filename? For example, what if we type:

\$ wc -1

but don't type *.pdb (or anything else) after the command? Since it doesn't have any filenames, wc assumes it is supposed to process input given at the command prompt, so it just sits there and waits for us to give it some data interactively. From the outside, though, all we see is it sitting there: the command doesn't appear to do anything.

If you make this kind of mistake, you can escape out of this state by holding down the control key (Ctrl) and typing the letter C once and letting go of the Ctrl key. Ctrl+C

Which of these files contains the fewest lines? It's an easy question to answer when there are only six files, but what if there were 6000? Our first step toward a solution is to run the command:

```
$ wc -l *.pdb > lengths.txt
```

The greater than symbol, >, tells the shell to **redirect** the command's output to a file instead of printing it to the screen. (This is why there is no screen output: everything that wc would have printed has gone into the file lengths.txt instead.) The shell will create the file if it doesn't exist. If the file exists, it will be silently overwritten, which may lead to data loss and thus requires some caution. ls lengths.txt confirms that the file exists:

\$ ls lengths.txt

lengths.txt

We can now send the content of lengths.txt to the screen using cat lengths.txt. The cat command gets its name from 'concatenate' i.e. join together, and it prints the contents of files one after another. There's only one file in this case, so cat just shows us what it contains:

\$ cat lengths.txt

- 20 cubane.pdb
- 12 ethane.pdb
- 9 methane.pdb
- 30 octane.pdb
- 21 pentane.pdb
- 15 propane.pdb
- 107 total

Output Page by Page

We'll continue to use cat in this lesson, for convenience and consistency, but it has the disadvantage that it always dumps the whole file onto your screen. More useful in practice is the command less, which you use with less lengths.txt. This displays a screenful of the file, and then stops. You can go forward one screenful by pressing the spacebar, or back one by pressing b. Press q to quit.

Now let's use the sort command to sort its contents.

What Does sort -n Do?

If we run **sort** on a file containing the following lines:

If we run sort -n on the same input, we get this instead:

19 22

Explain why -n has this effect.

Solution

Solution

The -n option specifies a numerical rather than an alphanumerical sort.

Solution

We will also use the -n option to specify that the sort is numerical instead of alphanumerical. This does *not* change the file; instead, it sends the sorted result to the screen:

```
$ sort -n lengths.txt
```

```
9 methane.pdb
```

- 12 ethane.pdb
- 15 propane.pdb
- 20 cubane.pdb
- 21 pentane.pdb
- 30 octane.pdb
- 107 total

We can put the sorted list of lines in another temporary file called sorted-lengths.txt by putting > sorted-lengths.txt after the command, just as we used > lengths.txt to put the output of wc into lengths.txt. Once we've done that, we can run another command called head to get the first few lines in sorted-lengths.txt:

```
$ sort -n lengths.txt > sorted-lengths.txt
$ head -n 1 sorted-lengths.txt
```

9 methane.pdb

Using -n 1 with head tells it that we only want the first line of the file; -n 20 would get the first 20, and so on. Since sorted-lengths.txt contains the lengths of our files ordered from least to greatest, the output of head must be the file with the fewest lines.

Redirecting to the same file

It's a very bad idea to try redirecting the output of a command that operates on a file to the same file. For example:

```
$ sort -n lengths.txt > lengths.txt
```

Doing something like this may give you incorrect results and/or delete the contents of lengths.txt.

What Does >> Mean?

We have seen the use of >, but there is a similar operator >> which works slightly differently. We'll learn about the differences between these two operators by printing some strings. We can use the echo command to print strings e.g.

```
$ echo The echo command prints text
```

The echo command prints text

Now test the commands below to reveal the difference between the two operators:

```
$ echo hello > testfile01.txt
```

and:

```
$ echo hello >> testfile02.txt
```

Hint: Try executing each command twice in a row and then examining the output files.

In the first example with >, the string 'hello' is written to testfile01.txt, but the file gets overwritten each time we run the command.

We see from the second example that the >> operator also writes 'hello' to a file (in this casetestfile02.txt), but appends the string to the file if it already exists (i.e. when we run it for the second time).

Solution

Appending Data

We have already met the head command, which prints lines from the start of a file. tail is similar, but prints lines from the end of a file instead.

Consider the file data-shell/data/animals.txt. After these commands, select the answer that corresponds to the file animals-subset.txt:

```
$ head -n 3 animals.txt > animals-subset.txt
$ tail -n 2 animals.txt >> animals-subset.txt
```

- 1. The first three lines of animals.txt
- 2. The last two lines of animals.txt
- 3. The first three lines and the last two lines of animals.txt
- 4. The second and third lines of animals.txt

Solution

Solution

Option 3 is correct. For option 1 to be correct we would only run the head command. For option 2 to be correct we would only run the tail command. For option 4 to be correct we would have to pipe the output of head into tail -n 2 by doing head -n 3 animals.txt | tail -n 2 > animals-subset.txt

Solution

If you think this is confusing, you're in good company: even once you understand what wc, sort, and head do, all those intermediate files make it hard to follow what's going on. We can make it easier to understand by running sort and head together:

```
$ sort -n lengths.txt | head -n 1
9 methane.pdb
```

The vertical bar, I, between the two commands is called a **pipe**. It tells the shell that we want to use the output of the command on the left as the input to the command on the right.

Nothing prevents us from chaining pipes consecutively. That is, we can for example send the output of wc directly to sort, and then the resulting output to head. Thus we first use a pipe to send the output of wc to sort:

```
$ wc -l *.pdb | sort -n
```

```
9 methane.pdb
```

- 12 ethane.pdb
- 15 propane.pdb
- 20 cubane.pdb
- 21 pentane.pdb
- 30 octane.pdb
- 107 total

And now we send the output of this pipe, through another pipe, to head, so that the full pipeline becomes:

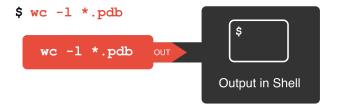
```
$ wc -l *.pdb | sort -n | head -n 1
```

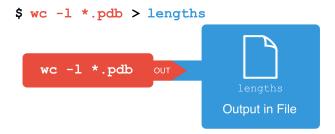
9 methane.pdb

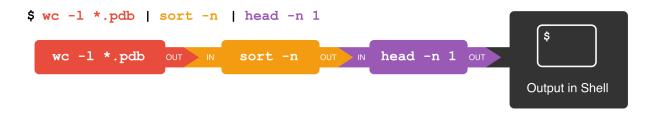
This is exactly like a mathematician nesting functions like log(3x) and saying 'the log of three times x'. In our case, the calculation is 'head of sort of line count of *.pdb'.

The redirection and pipes used in the last few commands are illustrated below:

Redirects and Pipes of different commands: "wc -l .pdb" will direct the output to the shell. "wc -l .pdb > lengths" will direct output to the file "lengths". "wc -l *.pdb | sort -n | head -n 1" will build a pipeline where the output of the "wc" command is the input to the "sort" command, the output of the "sort" command is the input to the "head" command is directed to the shell







Piping Commands Together

In our current directory, we want to find the 3 files which have the least number of lines. Which command listed below would work?

```
1. wc -1 * > sort -n > head -n 3
2. wc -1 * | sort -n | head -n 1-3
3. wc -1 * | head -n 3 | sort -n
4. wc -1 * | sort -n | head -n 3
```

Solution

Solution

Option 4 is the solution. The pipe character | is used to connect the output from one command to the input of another. > is used to redirect standard output to a file. Try it in the data-shell/molecules directory!

Solution

This idea of linking programs together is why Unix has been so successful. Instead of creating enormous programs that try to do many different things, Unix programmers focus on creating lots of simple tools that each do one job well, and that work well with each other. This programming model is called 'pipes and filters'. We've already seen pipes; a **filter** is a program like wc or sort that transforms a stream of input into a stream of output. Almost all of the standard Unix tools can work this way: unless told to do otherwise, they read from standard input, do something with what they've read, and write to standard output.

The key is that any program that reads lines of text from standard input and writes lines of text to standard output can be combined with every other program that behaves this way as well. You can *and should* write your programs this way so that you and other people can put those programs into pipes to multiply their power.

Pipe Reading Comprehension

A file called animals.txt (in the data-shell/data folder) contains the following data:

```
2012-11-05,deer
2012-11-05,rabbit
2012-11-05,raccoon
2012-11-06,rabbit
2012-11-06,deer
2012-11-06,fox
2012-11-07,rabbit
2012-11-07,bear
```

What text passes through each of the pipes and the final redirect in the pipeline below?

```
$ cat animals.txt | head -n 5 | tail -n 3 | sort -r > final.txt
```

Hint: build the pipeline up one command at a time to test your understanding

The head command extracts the first 5 lines from animals.txt. Then, the last 3 lines are extracted from the previous 5 by using the tail command. With the sort -r command those 3 lines are sorted in reverse order and finally, the output is redirected to a file final.txt. The content of this file can be checked by executing cat final.txt. The file should contain the following lines:

```
2012-11-06, rabbit
2012-11-06, deer
2012-11-05, raccoon
```

Solution

Pipe Construction

For the file animals.txt from the previous exercise, consider the following command:

```
$ cut -d , -f 2 animals.txt
```

The cut command is used to remove or 'cut out' certain sections of each line in the file, and cut expects the lines to be separated into columns by a Tab character. A character used in this way is a called a **delimiter**. In the example above we use the -d option to specify the comma as our delimiter character. We have also used the -f option to specify that we want to extract the second field (column). This gives the following output:

```
deer
rabbit
raccoon
rabbit
deer
fox
rabbit
bear
```

The uniq command filters out adjacent matching lines in a file. How could you extend this pipeline (using uniq and another command) to find out what animals the file contains (without any duplicates in their names)?

Solution

Solution

```
$ cut -d , -f 2 animals.txt | sort | uniq
```

Solution

Which Pipe?

The file animals.txt contains 8 lines of data formatted as follows:

```
2012-11-05,deer
2012-11-05,rabbit
2012-11-05,raccoon
2012-11-06,rabbit
```

The uniq command has a -c option which gives a count of the number of times a line occurs in its input. Assuming your current directory is data-shell/data/, what command would you use to produce a table that shows the total count of each type of animal in the file?

```
1. sort animals.txt | uniq -c
2. sort -t, -k2,2 animals.txt | uniq -c
3. cut -d, -f 2 animals.txt | uniq -c
4. cut -d, -f 2 animals.txt | sort | uniq -c
5. cut -d, -f 2 animals.txt | sort | uniq -c | wc -l
```

Solution

Solution

Option 4. is the correct answer. If you have difficulty understanding why, try running the commands, or sub-sections of the pipelines (make sure you are in the data-shell/data directory).

Solution

Nelle's Pipeline: Checking Files

Nelle has run her samples through the assay machines and created 17 files in the north-pacific-gyre/2012-07-03 directory described earlier. As a quick check, starting from her home directory, Nelle types:

```
$ cd north-pacific-gyre/2012-07-03
$ wc -1 *.txt
The output is 18 lines that look like this:
300 NENE01729A.txt
300 NENE01729B.txt
300 NENEO1736A.txt
300 NENEO1751A.txt
300 NENEO1751B.txt
300 NENE01812A.txt
. . . . . .
Now she types this:
$ wc -1 *.txt | sort -n | head -n 5
240 NENEO2018B.txt
 300 NENE01729A.txt
300 NENE01729B.txt
300 NENE01736A.txt
 300 NENE01751A.txt
```

Whoops: one of the files is 60 lines shorter than the others. When she goes back and checks it, she sees that she did that assay at 8:00 on a Monday morning — someone was probably in using the machine on the weekend, and she forgot to reset it. Before re-running that sample, she checks to see if any files have too much data:

```
$ wc -l *.txt | sort -n | tail -n 5
300 NENE02040B.txt
300 NENE02040Z.txt
300 NENE02043A.txt
300 NENE02043B.txt
5040 total
```

Those numbers look good — but what's that 'Z' doing there in the third-to-last line? All of her samples should be marked 'A' or 'B'; by convention, her lab uses 'Z' to indicate samples with missing information. To find others like it, she does this:

```
NENE01971Z.txt NENE02040Z.txt
```

\$ ls *Z.txt

Sure enough, when she checks the log on her laptop, there's no depth recorded for either of those samples. Since it's too late to get the information any other way, she must exclude those two files from her analysis. She could delete them using rm, but there are actually some analyses she might do later where depth doesn't matter, so instead, she'll have to be careful later on to select files using the wildcard expression *[AB].txt. As always, the * matches any number of characters; the expression [AB] matches either an 'A' or a 'B', so this matches all the valid data files she has.

Wildcard Expressions

Wildcard expressions can be very complex, but you can sometimes write them in ways that only use simple syntax, at the expense of being a bit more verbose. Consider the directory data-shell/north-pacific-gyre/2012-07-03: the wildcard expression *[AB].txt matches all files ending in A.txt or B.txt. Imagine you forgot about this.

- 1. Can you match the same set of files with basic wildcard expressions that do not use the [] syntax? *Hint*: You may need more than one command, or two arguments to the ls command.
- 2. If you used two commands, the files in your output will match the same set of files in this example. What is the small difference between the outputs?
- 3. If you used two commands, under what circumstances would your new expression produce an error message where the original one would not?

Solution

Solution

- 1. A solution using two wildcard commands: ~~~ \$ ls A.txt \$ ls B.txt ~~~ A solution using one command but with two arguments: ~~~ \$ ls A.txt B.txt ~~~
- The output from the two new commands is separated because there are two commands.
- 3. When there are no files ending in A.txt, or there are no files ending in B.txt, then one of the two commands will fail.

Removing Unneeded Files

Suppose you want to delete your processed data files, and only keep your raw files and processing script to save storage. The raw files end in .dat and the processed files end in .txt. Which of the following would remove all the processed data files, and *only* the processed data files?

```
1. rm ?.txt
2. rm *.txt
3. rm * .txt
4. rm *.*
```

Solution

Solution

- 1. This would remove .txt files with one-character names
- 2. This is correct answer
- 3. The shell would expand * to match everything in the current directory, so the command would try to remove all matched files and an additional file called .txt
- 4. The shell would expand *.* to match all files with any extension, so this command would delete all files

Solution

Loops

Loops are a programming construct which allow us to repeat a command or set of commands for each item in a list. As such they are key to productivity improvements through automation. Similar to wildcards and tab completion, using loops also reduces the amount of typing required (and hence reduces the number of typing mistakes).

Suppose we have several hundred genome data files named basilisk.dat, minotaur.dat, and unicorn.dat. For this example, we'll use the creatures directory which only has three example files, but the principles can be applied to many many more files at once.

The structure of these files is the same: the common name, classification, and updated date are presented on the first three lines, with DNA sequences on the following lines. Let's look at the files:

```
$ head -n 5 basilisk.dat minotaur.dat unicorn.dat
```

We would like to print out the classification for each species, which is given on the second line of each file. For each file, we would need to execute the command head -n 2 and pipe this to tail -n 1. We'll use a loop to solve this problem, but first let's look at the general form of a loop:

```
for thing in list_of_things
do
    operation_using $thing  # Indentation within the loop is not required, but aids legibility
done
```

and we can apply this to our example like this:

```
$ for filename in basilisk.dat minotaur.dat unicorn.dat
> do
> head -n 2 $filename | tail -n 1
> done

CLASSIFICATION: basiliscus vulgaris
CLASSIFICATION: bos hominus
CLASSIFICATION: equus monoceros
```

Follow the Prompt

The shell prompt changes from \$ to > and back again as we were typing in our loop. The second prompt, >, is different to remind us that we haven't finished typing a complete command yet. A semicolon, ;, can be used to separate two commands written on a single line.

When the shell sees the keyword for, it knows to repeat a command (or group of commands) once for each item in a list. Each time the loop runs (called an iteration), an item in the list is assigned in sequence to the **variable**, and the commands inside the loop are executed, before moving on to the next item in the list. Inside the loop, we call for the variable's value by putting \$ in front of it. The \$ tells the shell interpreter to treat the variable as a variable name and substitute its value in its place, rather than treat it as text or an external command.

In this example, the list is three filenames: basilisk.dat, minotaur.dat, and unicorn.dat. Each time the loop iterates, it will assign a file name to the variable filename and run the head command. The first time through the loop, \$filename is basilisk.dat. The interpreter runs the command head on basilisk.dat and pipes the first two lines to the tail command, which then prints the second line of basilisk.dat. For the second iteration, \$filename becomes minotaur.dat. This time, the shell runs head on minotaur.dat and pipes the first two lines to the tail command, which then prints the second line of minotaur.dat. For the third iteration, \$filename becomes unicorn.dat, so the shell runs the head command on that file, and tail on the output of that. Since the list was only three items, the shell exits the for loop.

Same Symbols, Different Meanings

Here we see > being used a shell prompt, whereas > is also used to redirect output. Similarly, \$ is used as a shell prompt, but, as we saw earlier, it is also used to ask the shell to get the value of a variable.

If the shell prints > or \$ then it expects you to type something, and the symbol is a prompt.

If you type > or \$ yourself, it is an instruction from you that the shell should redirect output or get the value of a variable.

When using variables it is also possible to put the names into curly braces to clearly delimit the variable name: **\$filename** is equivalent to **\${filename}**, but is different from **\${file}name**. You may find this notation in other people's programs.

We have called the variable in this loop filename in order to make its purpose clearer to human readers. The shell itself doesn't care what the variable is called; if we wrote this loop as:

```
$ for x in basilisk.dat minotaur.dat unicorn.dat
> do
>         head -n 2 $x | tail -n 1
> done
```

or:

```
$ for temperature in basilisk.dat minotaur.dat unicorn.dat
> do
>          head -n 2 $temperature | tail -n 1
> done
```

it would work exactly the same way. Don't do this. Programs are only useful if people can understand them, so meaningless names (like x) or misleading names (like temperature) increase the odds that the program won't do what its readers think it does.

Variables in Loops

This exercise refers to the data-shell/molecules directory. 1s gives the following output:

```
cubane.pdb ethane.pdb methane.pdb octane.pdb pentane.pdb propane.pdb
```

What is the output of the following code?

```
$ for datafile in *.pdb
> do
> ls *.pdb
> done
```

Now, what is the output of the following code?

```
$ for datafile in *.pdb
> do
> ls $datafile
> done
```

Why do these two loops give different outputs?

Solution

Solution

The first code block gives the same output on each iteration through the loop. Bash expands the wildcard *.pdb within the loop body (as well as before the loop starts) to match all files ending in .pdb and then lists them using ls. The expanded loop would look like this:

```
$ for datafile in cubane.pdb ethane.pdb methane.pdb octane.pdb pentane.pdb propane.pdb
     ls cubane.pdb ethane.pdb methane.pdb octane.pdb pentane.pdb propane.pdb
> done
cubane.pdb
           ethane.pdb
                       methane.pdb
                                     octane.pdb
                                                 pentane.pdb
                                                              propane.pdb
cubane.pdb
           ethane.pdb
                       methane.pdb
                                     octane.pdb
                                                 pentane.pdb
                                                              propane.pdb
cubane.pdb
           ethane.pdb
                       methane.pdb
                                     octane.pdb
                                                 pentane.pdb
                                                              propane.pdb
           ethane.pdb
                       methane.pdb
cubane.pdb
                                     octane.pdb
                                                 pentane.pdb
                                                              propane.pdb
cubane.pdb
           ethane.pdb
                       methane.pdb
                                     octane.pdb
                                                 pentane.pdb
                                                             propane.pdb
cubane.pdb
           ethane.pdb
                       methane.pdb
                                    octane.pdb
                                                pentane.pdb
                                                             propane.pdb
```

The second code block lists a different file on each loop iteration. The value of the datafile variable is evaluated using \$datafile, and then listed using ls.

```
cubane.pdb
ethane.pdb
methane.pdb
octane.pdb
pentane.pdb
propane.pdb
```

Limiting Sets of Files

What would be the output of running the following loop in the data-shell/molecules directory?

```
$ for filename in c*
> do
> ls $filename
> done
```

- 1. No files are listed.
- 2. All files are listed.
- 3. Only cubane.pdb, octane.pdb and pentane.pdb are listed.
- 4. Only cubane.pdb is listed.

Solution

Solution

4 is the correct answer. * matches zero or more characters, so any file name starting with the letter c, followed by zero or more other characters will be matched.

Solution

How would the output differ from using this command instead?

```
$ for filename in *c*
> do
> ls $filename
> done
```

- 1. The same files would be listed.
- 2. All the files are listed this time.
- 3. No files are listed this time.
- 4. The files cubane.pdb and octane.pdb will be listed.
- 5. Only the file octane.pdb will be listed.

Solution

Solution

4 is the correct answer. * matches zero or more characters, so a file name with zero or more characters before a letter c and zero or more characters after the letter c will be matched.

Saving to a File in a Loop - Part One

In the data-shell/molecules directory, what is the effect of this loop?

```
for alkanes in *.pdb
do
    echo $alkanes
    cat $alkanes > alkanes.pdb
done
```

- 1. Prints cubane.pdb, ethane.pdb, methane.pdb, octane.pdb, pentane.pdb and propane.pdb, and the text from propane.pdb will be saved to a file called alkanes.pdb.
- 2. Prints cubane.pdb, ethane.pdb, and methane.pdb, and the text from all three files would be concatenated and saved to a file called alkanes.pdb.
- 3. Prints cubane.pdb, ethane.pdb, methane.pdb, octane.pdb, and pentane.pdb, and the text from propane.pdb will be saved to a file called alkanes.pdb.
- 4. None of the above.

Solution

Solution

1. The text from each file in turn gets written to the alkanes.pdb file. However, the file gets overwritten on each loop interation, so the final content of alkanes.pdb is the text from the propane.pdb file.

Solution

Saving to a File in a Loop - Part Two

Also in the data-shell/molecules directory, what would be the output of the following loop?

```
for datafile in *.pdb
do
    cat $datafile >> all.pdb
done
```

- 1. All of the text from cubane.pdb, ethane.pdb, methane.pdb, octane.pdb, and pentane.pdb would be concatenated and saved to a file called all.pdb.
- 2. The text from ethane.pdb will be saved to a file called all.pdb.
- 3. All of the text from cubane.pdb, ethane.pdb, methane.pdb, octane.pdb, pentane.pdb and propane.pdb would be concatenated and saved to a file called all.pdb.
- 4. All of the text from cubane.pdb, ethane.pdb, methane.pdb, octane.pdb, pentane.pdb and propane.pdb would be printed to the screen and saved to a file called all.pdb.

Solution

Solution

3 is the correct answer. >> appends to a file, rather than overwriting it with the redirected output from a command. Given the output from the cat command has been redirected, nothing is printed to the screen.

Let's continue with our example in the data-shell/creatures directory. Here's a slightly more complicated loop:

```
$ for filename in *.dat
> do
> echo $filename
> head -n 100 $filename | tail -n 20
> done
```

The shell starts by expanding *.dat to create the list of files it will process. The **loop body** then executes two commands for each of those files. The first command, echo, prints its command-line arguments to standard output. For example:

```
$ echo hello there
```

prints:

hello there

In this case, since the shell expands \$filename to be the name of a file, echo \$filename prints the name of the file. Note that we can't write this as:

because then the first time through the loop, when **\$filename** expanded to **basilisk.dat**, the shell would try to run **basilisk.dat** as a program. Finally, the **head** and **tail** combination selects lines 81-100 from whatever file is being processed (assuming the file has at least 100 lines).

Spaces in Names

Spaces are used to separate the elements of the list that we are going to loop over. If one of those elements contains a space character, we need to surround it with quotes, and do the same thing to our loop variable. Suppose our data files are named:

```
red dragon.dat
purple unicorn.dat
```

To loop over these files, we would need to add double quotes like so:

```
$ for filename in "red dragon.dat" "purple unicorn.dat"
> do
> head -n 100 "$filename" | tail -n 20
> done
```

It is simpler to avoid using spaces (or other special characters) in filenames.

The files above don't exist, so if we run the above code, the head command will be unable to find them, however the error message returned will show the name of the files it is expecting:

head: cannot open 'red dragon.dat' for reading: No such file or directory head: cannot open 'purple unicorn.dat' for reading: No such file or directory

Try removing the quotes around **\$filename** in the loop above to see the effect of the quote marks on spaces. Note that we get a result from the loop command for unicorn.dat when we run this code in the **creatures** directory:

head: cannot open 'red' for reading: No such file or directory head: cannot open 'dragon.dat' for reading: No such file or directory head: cannot open 'purple' for reading: No such file or directory CGGTACCGAA AAGGGTCGCG CAAGTGTTCC

We would like to modify each of the files in data-shell/creatures, but also save a version of the original files, naming the copies original-basilisk.dat and original-unicorn.dat. We can't use:

```
$ cp *.dat original-*.dat
```

because that would expand to:

\$ cp basilisk.dat minotaur.dat unicorn.dat original-*.dat

This wouldn't back up our files, instead we get an error:

Error

```
cp: target 'original-*.dat' is not a directory
```

This problem arises when cp receives more than two inputs. When this happens, it expects the last input to be a directory where it can copy all the files it was passed. Since there is no directory named original-*.dat in the creatures directory we get an error.

Instead, we can use a loop: $\sim\sim$ \$ for filename in *.dat > do > cp filenameoriginal-filename > done $\sim\sim$

This loop runs the cp command once for each filename. The first time, when \$filename expands to basilisk.dat, the shell executes:

cp basilisk.dat original-basilisk.dat

The second time, the command is:

cp minotaur.dat original-minotaur.dat

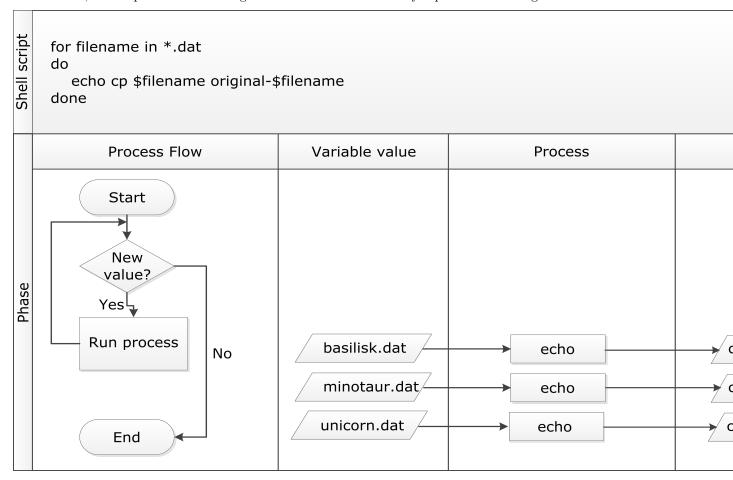
The third and last time, the command is:

cp unicorn.dat original-unicorn.dat

Since the cp command does not normally produce any output, it's hard to check that the loop is doing the correct thing. However, we learned earlier how to print strings using echo, and we can modify the loop to use echo to print our commands without actually executing them. As such we can check what commands would be run in the unmodified loop.

The following diagram shows what happens when the modified loop is executed, and demonstrates how the judicious use of echo is a good debugging technique.

The for loop "for filename in .dat; do echo cp filenameoriginal—filename; done" will successively assign the names of all ".dat" files in your current directory to the variable "\$filename" and then execute the command. With the files "basilisk.dat", "minotaur.dat" and "unicorn.dat" in the current directory the loop will successively call the echo command three times and print three lines: "cp basislisk.dat original-basilisk.dat", then "cp minotaur.dat original-minotaur.dat" and finally "cp unicorn.dat original-unicorn.dat"



Nelle's Pipeline: Processing Files

Nelle is now ready to process her data files using goostats — a shell script written by her supervisor. This calculates some statistics from a protein sample file, and takes two arguments:

- 1. an input file (containing the raw data)
- 2. an output file (to store the calculated statistics)

Since she's still learning how to use the shell, she decides to build up the required commands in stages. Her first step is to make sure that she can select the right input files — remember, these are ones whose names end in 'A' or 'B', rather than 'Z'. Starting from her home directory, Nelle types:

```
$ cd north-pacific-gyre/2012-07-03
$ for datafile in NENE*[AB].txt
> do
> echo $datafile
> done

NENE01729A.txt
NENE01729B.txt
NENE01736A.txt
...
NENE02043A.txt
NENE02043B.txt
```

Her next step is to decide what to call the files that the goostats analysis program will create. Prefixing each input file's name with 'stats' seems simple, so she modifies her loop to do that:

```
$ for datafile in NENE*[AB].txt
> do
> echo $datafile stats-$datafile
> done

NENEO1729A.txt stats-NENEO1729A.txt
NENEO1729B.txt stats-NENEO1729B.txt
NENEO1736A.txt stats-NENEO1736A.txt
...
NENEO2043A.txt stats-NENEO2043A.txt
NENEO2043B.txt stats-NENEO2043B.txt
```

She hasn't actually run goostats yet, but now she's sure she can select the right files and generate the right output filenames.

Typing in commands over and over again is becoming tedious, though, and Nelle is worried about making mistakes, so instead of re-entering her loop, she presses \uparrow . In response, the shell redisplays the whole loop on one line (using semi-colons to separate the pieces):

```
$ for datafile in NENE*[AB].txt; do echo $datafile stats-$datafile; done
```

Using the left arrow key, Nelle backs up and changes the command echo to bash goostats:

```
$ for datafile in NENE*[AB].txt; do bash goostats $datafile stats-$datafile; done
```

When she presses Enter, the shell runs the modified command. However, nothing appears to happen — there is no output. After a moment, Nelle realizes that since her script doesn't print anything to the screen any longer, she has no idea whether it is running, much less how quickly. She kills the running command by typing Ctrl+C, uses ↑ to repeat the command, and edits it to read:

\$ for datafile in NENE*[AB].txt; do echo \$datafile; bash goostats \$datafile stats-\$datafile; done

Beginning and End

We can move to the beginning of a line in the shell by typing Ctrl+A and to the end using Ctrl+E.

When she runs her program now, it produces one line of output every five seconds or so:

```
NENEO1729A.txt
NENEO1729B.txt
NENEO1736A.txt
```

1518 times 5 seconds, divided by 60, tells her that her script will take about two hours to run. As a final check, she opens another terminal window, goes into north-pacific-gyre/2012-07-03, and uses cat stats-NENE01729B.txt to examine one of the output files. It looks good, so she decides to get some coffee and catch up on her reading.

Those Who Know History Can Choose to Repeat It

Another way to repeat previous work is to use the history command to get a list of the last few hundred commands that have been executed, and then to use !123 (where '123' is replaced by the command number) to repeat one of those commands. For example, if Nelle types this:

```
$ history | tail -n 5

456  ls -l NENEO*.txt
457  rm stats-NENE01729B.txt.txt
458  bash goostats NENE01729B.txt stats-NENE01729B.txt
459  ls -l NENEO*.txt
460  history
```

then she can re-run goostats on NENEO1729B.txt simply by typing !458.

Other History Commands

There are a number of other shortcut commands for getting at the history.

- Ctrl+R enters a history search mode 'reverse-i-search' and finds the most recent command in your history that matches the text you enter next. Press Ctrl+R one or more additional times to search for earlier matches. You can then use the left and right arrow keys to choose that line and edit it then hit Return to run the command.
- !! retrieves the immediately preceding command (you may or may not find this more convenient than using \uparrow)
- !\$ retrieves the last word of the last command. That's useful more often than you might expect: after bash goostats NENE01729B.txt stats-NENE01729B.txt, you can type less !\$ to look at the file stats-NENE01729B.txt, which is quicker than doing ↑ and editing the command-line.

Doing a Dry Run

A loop is a way to do many things at once — or to make many mistakes at once if it does the wrong thing. One way to check what a loop *would* do is to **echo** the commands it would run instead of actually running them.

Suppose we want to preview the commands the following loop will execute without actually running those commands:

```
$ for datafile in *.pdb
> do
> cat $datafile >> all.pdb
> done
```

What is the difference between the two loops below, and which one would we want to run?

```
# Version 1
$ for datafile in *.pdb
> do
>          echo cat $datafile >> all.pdb
> done
# Version 2
$ for datafile in *.pdb
> do
>          echo "cat $datafile >> all.pdb"
> done
```

Solution

Solution

The second version is the one we want to run. This prints to screen everything enclosed in the quote marks, expanding the loop variable name because we have prefixed it with a dollar sign.

The first version appends the output from the command echo cat \$datafile to the file, all.pdb. This file will just contain the list; cat cubane.pdb, cat ethane.pdb, cat methane.pdb etc.

Try both versions for yourself to see the output! Be sure to open the all.pdb file to view its contents.

Solution

Nested Loops

Suppose we want to set up a directory structure to organize some experiments measuring reaction rate constants with different compounds and different temperatures. What would be the result of the following code:

```
$ for species in cubane ethane methane
> do
> for temperature in 25 30 37 40
> do
> mkdir $species-$temperature
> done
> done
```

Solution

We have a nested loop, i.e. contained within another loop, so for each species in the outer loop, the inner loop (the nested loop) iterates over the list of temperatures, and creates a new directory for each combination.

Try running the code for yourself to see which directories are created!

Solution

Shell Scripts

We are finally ready to see what makes the shell such a powerful programming environment. We are going to take the commands we repeat frequently and save them in files so that we can re-run all those operations again later by typing a single command. For historical reasons, a bunch of commands saved in a file is usually called a **shell script**, but make no mistake: these are actually small programs.

Let's start by going back to molecules/ and creating a new file, middle.sh which will become our shell script:

```
$ cd molecules
$ nano middle.sh
```

The command nano middle.sh opens the file middle.sh within the text editor 'nano' (which runs within the shell). If the file does not exist, it will be created. We can use the text editor to directly edit the file – we'll simply insert the following line:

```
head -n 15 octane.pdb | tail -n 5
```

This is a variation on the pipe we constructed earlier: it selects lines 11-15 of the file octane.pdb. Remember, we are *not* running it as a command just yet: we are putting the commands in a file.

Then we save the file (Ctrl-O in nano), and exit the text editor (Ctrl-X in nano). Check that the directory molecules now contains a file called middle.sh.

Once we have saved the file, we can ask the shell to execute the commands it contains. Our shell is called bash, so we run the following command:

\$ bash middle.sh

ATOM	9	Н	1	-4.502	0.681	0.785	1.00	0.00
MOTA	10	Н	1	-5.254	-0.243	-0.537	1.00	0.00
MOTA	11	Н	1	-4.357	1.252	-0.895	1.00	0.00
MOTA	12	Н	1	-3.009	-0.741	-1.467	1.00	0.00
MOTA	13	Н	1	-3.172	-1.337	0.206	1.00	0.00

Sure enough, our script's output is exactly what we would get if we ran that pipeline directly.

Text vs. Whatever

We usually call programs like Microsoft Word or LibreOffice Writer "text editors", but we need to be a bit more careful when it comes to programming. By default, Microsoft Word uses .docx files to store not only text, but also formatting information about fonts, headings, and so on. This extra information isn't stored as characters, and doesn't mean anything to tools like head: they expect input files to contain nothing but the letters, digits, and punctuation on a standard computer keyboard. When editing programs, therefore, you must either use a plain text editor, or be careful to save files as plain text.

What if we want to select lines from an arbitrary file? We could edit middle.sh each time to change the filename, but that would probably take longer than typing the command out again in the shell and executing it with a new file name. Instead, let's edit middle.sh and make it more versatile:

\$ nano middle.sh

Now, within "nano", replace the text octane.pdb with the special variable called \$1:

```
head -n 15 "$1" | tail -n 5
```

Inside a shell script, \$1 means 'the first filename (or other argument) on the command line'. We can now run our script like this:

\$ bash middle.sh octane.pdb

MOTA	9	Η	1	-4.502	0.681	0.785	1.00	0.00
MOTA	10	Н	1	-5.254	-0.243	-0.537	1.00	0.00
MOTA	11	Н	1	-4.357	1.252	-0.895	1.00	0.00
MOTA	12	Н	1	-3.009	-0.741	-1.467	1.00	0.00
ATOM	13	Н	1	-3.172	-1.337	0.206	1.00	0.00

or on a different file like this:

\$ bash middle.sh pentane.pdb

MOTA	9	Н	1	1.324	0.350	-1.332	1.00	0.00
MOTA	10	Н	1	1.271	1.378	0.122	1.00	0.00
MOTA	11	Н	1	-0.074	-0.384	1.288	1.00	0.00
MOTA	12	Н	1	-0.048	-1.362	-0.205	1.00	0.00
MOTA	13	Η	1	-1.183	0.500	-1.412	1.00	0.00

Double-Quotes Around Arguments

For the same reason that we put the loop variable inside double-quotes, in case the filename happens to contain any spaces, we surround \$1 with double-quotes.

Currently, we need to edit middle.sh each time we want to adjust the range of lines that is returned. Let's fix that by configuring our script to instead use three command-line arguments. After the first command-line argument (\$1), each additional argument that we provide will be accessible via the special variables \$1, \$2, \$3, which refer to the first, second, third command-line arguments, respectively.

Knowing this, we can use additional arguments to define the range of lines to be passed to head and tail respectively:

\$ nano middle.sh

```
head -n "$2" "$1" | tail -n "$3"
```

We can now run:

\$ bash middle.sh pentane.pdb 15 5

MOTA	9	Н	1	1.324	0.350	-1.332	1.00	0.00
MOTA	10	Η	1	1.271	1.378	0.122	1.00	0.00
MOTA	11	Η	1	-0.074	-0.384	1.288	1.00	0.00
MOTA	12	Н	1	-0.048	-1.362	-0.205	1.00	0.00
ATOM	13	Н	1	-1.183	0.500	-1.412	1.00	0.00

By changing the arguments to our command we can change our script's behaviour:

\$ bash middle.sh pentane.pdb 20 5

ATOM	14	Н	1	-1.259	1.420	0.112	1.00	0.00
ATOM	15	Н	1	-2.608	-0.407	1.130	1.00	0.00
ATOM	16	Н	1	-2.540	-1.303	-0.404	1.00	0.00
ATOM	17	Н	1	-3.393	0.254	-0.321	1.00	0.00
TER	18		1					

This works, but it may take the next person who reads middle.sh a moment to figure out what it does. We can improve our script by adding some **comments** at the top:

```
$ nano middle.sh
```

```
# Select lines from the middle of a file.
# Usage: bash middle.sh filename end_line num_lines
head -n "$2" "$1" | tail -n "$3"
```

A comment starts with a # character and runs to the end of the line. The computer ignores comments, but they're invaluable for helping people (including your future self) understand and use scripts. The only caveat is that each time you modify the script, you should check that the comment is still accurate: an explanation that sends the reader in the wrong direction is worse than none at all.

What if we want to process many files in a single pipeline? For example, if we want to sort our .pdb files by length, we would type:

```
$ wc -l *.pdb | sort -n
```

because wc -1 lists the number of lines in the files (recall that wc stands for 'word count', adding the -1 option means 'count lines' instead) and sort -n sorts things numerically. We could put this in a file, but then it would only ever sort a list of .pdb files in the current directory. If we want to be able to get a sorted list of other kinds of files, we need a way to get all those names into the script. We can't use \$1, \$2, and so on because we don't know how many files there are. Instead, we use the special variable \$0, which means, 'All of the command-line arguments to the shell script'. We also should put \$0 inside double-quotes to handle the case of arguments containing spaces ("\$0" is special syntax and is equivalent to "\$1" "\$2" ...).

Here's an example:

```
$ nano sorted.sh

# Sort files by their length.

# Usage: bash sorted.sh one_or_more_filenames
wc -l "$@" | sort -n

$ bash sorted.sh *.pdb ../creatures/*.dat

9 methane.pdb
12 ethane.pdb
15 propane.pdb
20 cubane.pdb
21 pentane.pdb
21 pentane.pdb
30 octane.pdb
30 octane.pdb
163 ../creatures/basilisk.dat
163 ../creatures/minotaur.dat
163 ../creatures/unicorn.dat
596 total
```

List Unique Species

Leah has several hundred data files, each of which is formatted like this:

```
2013-11-05,deer,5

2013-11-05,rabbit,22

2013-11-05,raccoon,7

2013-11-06,rabbit,19

2013-11-06,deer,2

2013-11-06,fox,1

2013-11-07,rabbit,18

2013-11-07,bear,1
```

An example of this type of file is given in data-shell/data/animal-counts/animals.txt.

We can use the command cut -d , -f 2 animals.txt | sort | uniq to produce the unique species in animals.txt. In order to avoid having to type out this series of commands every time, a scientist may choose to write a shell script instead.

Write a shell script called **species.sh** that takes any number of filenames as command-line arguments, and uses a variation of the above command to print a list of the unique species appearing in each of those files separately.

Solution

Solution

done

```
# Script to find unique species in csv files where species is the second data field
# This script accepts any number of file names as command line arguments
# Loop over all files
for file in $0
do
    echo "Unique species in $file:"
    # Extract species names
    cut -d , -f 2 $file | sort | uniq
```

Solution

Suppose we have just run a series of commands that did something useful — for example, that created a graph we'd like to use in a paper. We'd like to be able to re-create the graph later if we need to, so we want to save the commands in a file. Instead of typing them in again (and potentially getting them wrong) we can do this:

```
$ history | tail -n 5 > redo-figure-3.sh
```

The file redo-figure-3.sh now contains:

```
297 bash goostats NENEO1729B.txt stats-NENEO1729B.txt
298 bash goodiff stats-NENEO1729B.txt /data/validated/01729.txt > 01729-differences.txt
299 cut -d ',' -f 2-3 01729-differences.txt > 01729-time-series.txt
300 ygraph --format scatter --color bw --borders none 01729-time-series.txt figure-3.png
301 history | tail -n 5 > redo-figure-3.sh
```

After a moment's work in an editor to remove the serial numbers on the commands, and to remove the final line where we called the history command, we have a completely accurate record of how we created that figure.

Why Record Commands in the History Before Running Them?

If you run the command:

```
$ history | tail -n 5 > recent.sh
```

the last command in the file is the history command itself, i.e., the shell has added history to the command log before actually running it. In fact, the shell *always* adds commands to the log before running them. Why do you think it does this?

Solution

Solution

If a command causes something to crash or hang, it might be useful to know what that command was, in order to investigate the problem. Were the command only be recorded after running it, we would not have a record of the last command run in the event of a crash.

Solution

In practice, most people develop shell scripts by running commands at the shell prompt a few times to make sure they're doing the right thing, then saving them in a file for re-use. This style of work allows people to recycle what they discover about their data and their workflow with one call to history and a bit of editing to clean up the output and save it as a shell script.

Nelle's Pipeline: Creating a Script

Nelle's supervisor insisted that all her analytics must be reproducible. The easiest way to capture all the steps is in a script.

First we return to Nelle's data directory:

```
$ cd ../north-pacific-gyre/2012-07-03/
```

She runs the editor and writes the following:

```
# Calculate stats for data files.
for datafile in "$0"
do
    echo $datafile
    bash goostats $datafile stats-$datafile
done
```

She saves this in a file called do-stats.sh so that she can now re-do the first stage of her analysis by typing:

```
$ bash do-stats.sh NENE*[AB].txt
```

She can also do this:

```
$ bash do-stats.sh NENE*[AB].txt | wc -1
```

so that the output is just the number of files processed rather than the names of the files that were processed.

One thing to note about Nelle's script is that it lets the person running it decide what files to process. She could have written it as:

```
# Calculate stats for Site A and Site B data files.
for datafile in NENE*[AB].txt
do
    echo $datafile
    bash goostats $datafile stats-$datafile
done
```

The advantage is that this always selects the right files: she doesn't have to remember to exclude the 'Z' files. The disadvantage is that it *always* selects just those files — she can't run it on all files (including the 'Z' files), or on the 'G' or 'H' files her colleagues in Antarctica are producing, without editing the script. If she wanted to be more adventurous, she could modify her script to check for command-line arguments, and use NENE*[AB].txt if none were provided. Of course, this introduces another tradeoff between flexibility and complexity.

Variables in Shell Scripts

In the molecules directory, imagine you have a shell script called script.sh containing the following commands:

```
head -n $2 $1 tail -n $3 $1
```

While you are in the molecules directory, you type the following command:

```
bash script.sh '*.pdb' 1 1
```

Which of the following outputs would you expect to see?

- 1. All of the lines between the first and the last lines of each file ending in .pdb in the molecules directory
- 2. The first and the last line of each file ending in .pdb in the molecules directory
- 3. The first and the last line of each file in the molecules directory
- 4. An error because of the quotes around *.pdb

Solution

Solution

The correct answer is 2.

The special variables \$1, \$2 and \$3 represent the command line arguments given to the script, such that the commands run are:

```
$ head -n 1 cubane.pdb ethane.pdb octane.pdb pentane.pdb propane.pdb
$ tail -n 1 cubane.pdb ethane.pdb octane.pdb pentane.pdb propane.pdb
```

The shell does not expand '*.pdb' because it is enclosed by quote marks. As such, the first argument to the script is '*.pdb' which gets expanded within the script by head and tail.

Solution

Find the Longest File With a Given Extension

Write a shell script called longest.sh that takes the name of a directory and a filename extension as its arguments, and prints out the name of the file with the most lines in that directory with that extension. For example:

```
$ bash longest.sh /tmp/data pdb
```

would print the name of the .pdb file in /tmp/data that has the most lines.

Solution

```
# Shell script which takes two arguments:
# 1. a directory name
# 2. a file extension
# and prints the name of the file in that directory
# with the most lines which matches the file extension.
wc -l $1/*.$2 | sort -n | tail -n 2 | head -n 1
```

The first part of the pipeline, wc -l \$1/*.\$2 | sort -n, counts the lines in each file and sorts them numerically (largest last). When there's more than one file, wc also outputs a final summary line, giving the total number of lines across *all* files. We use tail -n 2 | head -n 1 to throw away this last line.

With wc -l \$1/*.\$2 | sort -n | tail -n 1 we'll see the final summary line: we can build our pipeline up in pieces to be sure we understand the output.

Solution

Script Reading Comprehension

For this question, consider the data-shell/molecules directory once again. This contains a number of .pdb files in addition to any other files you may have created. Explain what each of the following three scripts would do when run as bash script1.sh *.pdb, bash script2.sh *.pdb, and bash script3.sh *.pdb respectively.

```
# Script 1
echo *.*

# Script 2
for filename in $1 $2 $3
do
     cat $filename
done

# Script 3
echo $0.pdb
```

Solutions

In each case, the shell expands the wildcard in *.pdb before passing the resulting list of file names as arguments to the script.

Script 1 would print out a list of all files containing a dot in their name. The arguments passed to the script are not actually used anywhere in the script.

Script 2 would print the contents of the first 3 files with a .pdb file extension. \$1, \$2, and \$3 refer to the first, second, and third argument respectively.

Script 3 would print all the arguments to the script (i.e. all the .pdb files), followed by .pdb. \$0 refers to all the arguments given to a shell script.

cubane.pdb ethane.pdb methane.pdb octane.pdb pentane.pdb propane.pdb.pdb

Solution

Debugging Scripts

Suppose you have saved the following script in a file called do-errors.sh in Nelle's north-pacific-gyre/2012-07-03 directory:

```
# Calculate stats for data files.
for datafile in "$0"
do
    echo $datfile
    bash goostats $datafile stats-$datafile
done
```

When you run it:

\$ bash do-errors.sh NENE*[AB].txt

the output is blank. To figure out why, re-run the script using the -x option:

bash -x do-errors.sh NENE*[AB].txt

What is the output showing you? Which line is responsible for the error?

Solution

Solution

The -x option causes bash to run in debug mode. This prints out each command as it is run, which will help you to locate errors. In this example, we can see that echo isn't printing anything. We have made a typo in the loop variable name, and the variable datfile doesn't exist, hence returning an empty string.

Solution

Finding Things

In the same way that many of us now use 'Google' as a verb meaning 'to find', Unix programmers often use the word 'grep'. 'grep' is a contraction of 'global/regular expression/print', a common sequence of operations in early Unix text editors. It is also the name of a very useful command-line program.

grep finds and prints lines in files that match a pattern. For our examples, we will use a file that contains three haikus taken from a 1998 competition in *Salon* magazine. For this set of examples, we're going to be working in the writing subdirectory:

- \$ cd
- \$ cd Desktop/data-shell/writing
- \$ cat haiku.txt

The Tao that is seen Is not the true Tao, until You bring fresh toner.

With searching comes loss and the presence of absence: "My Thesis" not found.

Yesterday it worked Today it is not working Software is like that.

Forever, or Five Years

We haven't linked to the original haikus because they don't appear to be on *Salon*'s site any longer. As Jeff Rothenberg said, 'Digital information lasts forever — or five years, whichever comes first.' Luckily, popular content often has backups.

Let's find lines that contain the word 'not':

\$ grep not haiku.txt

Is not the true Tao, until "My Thesis" not found Today it is not working

Here, not is the pattern we're searching for. The grep command searches through the file, looking for matches to the pattern specified. To use it type grep, then the pattern we're searching for and finally the name of the file (or files) we're searching in.

The output is the three lines in the file that contain the letters 'not'.

By default, grep searches for a pattern in a case-sensitive way. In addition, the search pattern we have selected does not have to form a complete word, as we will see in the next example.

Let's search for the pattern: 'The'.

\$ grep The haiku.txt

The Tao that is seen "My Thesis" not found.

This time, two lines that include the letters 'The' are outputted, one of which contained our search pattern within a larger word, 'Thesis'.

To restrict matches to lines containing the word 'The' on its own, we can give grep with the -w option. This will limit matches to word boundaries.

Later in this lesson, we will also see how we can change the search behavior of grep with respect to its case sensitivity.

\$ grep -w The haiku.txt

The Tao that is seen

Note that a 'word boundary' includes the start and end of a line, so not just letters surrounded by spaces. Sometimes we don't want to search for a single word, but a phrase. This is also easy to do with grep by putting the phrase in quotes.

\$ grep -w "is not" haiku.txt

Today it is not working

We've now seen that you don't have to have quotes around single words, but it is useful to use quotes when searching for multiple words. It also helps to make it easier to distinguish between the search term or phrase and the file being searched. We will use quotes in the remaining examples.

Another useful option is -n, which numbers the lines that match:

```
$ grep -n "it" haiku.txt
5:With searching comes loss
```

9:Yesterday it worked 10:Today it is not working

Here, we can see that lines 5, 9, and 10 contain the letters 'it'.

We can combine options (i.e. flags) as we do with other Unix commands. For example, let's find the lines that contain the word 'the'. We can combine the option -w to find the lines that contain the word 'the' and -n to number the lines that match:

```
$ grep -n -w "the" haiku.txt
```

2:Is not the true Tao, until 6:and the presence of absence:

Now we want to use the option -i to make our search case-insensitive:

```
$ grep -n -w -i "the" haiku.txt
```

1:The Tao that is seen 2:Is not the true Tao, until 6:and the presence of absence:

Now, we want to use the option -v to invert our search, i.e., we want to output the lines that do not contain the word 'the'.

```
$ grep -n -w -v "the" haiku.txt
```

```
1:The Tao that is seen
3:You bring fresh toner.
4:
5:With searching comes loss
7:"My Thesis" not found.
8:
9:Yesterday it worked
10:Today it is not working
11:Software is like that.
```

If we use the -r (recursive) option, grep can search for a pattern recursively through a set of files in subdirectories.

Let's search recursively for Yesterday in the data-shell/writing directory:

```
$ grep -r Yesterday .
```

data/LittleWomen.txt:"Yesterday, when Aunt was asleep and I was trying to be as still as a data/LittleWomen.txt:Yesterday at dinner, when an Austrian officer stared at us and then data/LittleWomen.txt:Yesterday was a quiet day spent in teaching, sewing, and writing in my haiku.txt:Yesterday it worked

grep has lots of other options. To find out what they are, we can type:

```
$ grep --help
Usage: grep [OPTION]... PATTERN [FILE]...
Search for PATTERN in each FILE or standard input.
PATTERN is, by default, a basic regular expression (BRE).
Example: grep -i 'hello world' menu.h main.c
Regexp selection and interpretation:
  -E, --extended-regexp
                            PATTERN is an extended regular expression (ERE)
  -F, --fixed-strings
                            PATTERN is a set of newline-separated fixed strings
  -G, --basic-regexp
                            PATTERN is a basic regular expression (BRE)
  -P, --perl-regexp
                            PATTERN is a Perl regular expression
  -e, --regexp=PATTERN
                            use PATTERN for matching
  -f, --file=FILE
                            obtain PATTERN from FILE
                            ignore case distinctions
  -i, --ignore-case
  -w, --word-regexp
                            force PATTERN to match only whole words
                            force PATTERN to match only whole lines
  -x, --line-regexp
  -z, --null-data
                            a data line ends in 0 byte, not newline
Miscellaneous:
```

Using grep

Which command would result in the following output:

and the presence of absence:

```
    grep "of" haiku.txt
    grep -E "of" haiku.txt
    grep -w "of" haiku.txt
    grep -i "of" haiku.txt
```

Solution

Solution

The correct answer is 3, because the -w option looks only for whole-word matches. The other options will also match 'of' when part of another word.

Solution

Wildcards

grep's real power doesn't come from its options, though; it comes from the fact that patterns can include wildcards. (The technical name for these is **regular expressions**, which is what the 're' in 'grep' stands for.) Regular expressions are both complex and powerful; if you want to do complex searches, please look at the lesson on our website. As a taster, we can find lines that have an 'o' in the second position like this:

```
$ grep -E "^.o" haiku.txt
You bring fresh toner.
Today it is not working
Software is like that.
```

We use the -E option and put the pattern in quotes to prevent the shell from trying to interpret it. (If the pattern contained a *, for example, the shell would try to expand it before running grep.) The ^ in the pattern anchors the match to the start of the line. The . matches a single character (just like? in the shell), while the o matches an actual 'o'.

Tracking a Species

Leah has several hundred data files saved in one directory, each of which is formatted like this:

```
2013-11-05,deer,5
2013-11-05,rabbit,22
2013-11-05,raccoon,7
2013-11-06,rabbit,19
2013-11-06,deer,2
```

She wants to write a shell script that takes a species as the first command-line argument and a directory as the second argument. The script should return one file called **species.txt** containing a list of dates and the number of that species seen on each date. For example using the data shown above, **rabbit.txt** would contain:

```
2013-11-05,22
2013-11-06,19
```

Put these commands and pipes in the right order to achieve this:

```
cut -d : -f 2
>
|
grep -w $1 -r $2
|
$1.txt
cut -d , -f 1,3
```

Hint: use man grep to look for how to grep text recursively in a directory and man cut to select more than one field in a line.

An example of such a file is provided in data-shell/data/animal-counts/animals.txt

Solution

Solution

```
grep -w 1 - r 2 \mid cut - d : -f 2 \mid cut - d , -f 1,3 > 1.txt
You would call the script above like this: bash count-species.sh bear .
```

Little Women

You and your friend, having just finished reading *Little Women* by Louisa May Alcott, are in an argument. Of the four sisters in the book, Jo, Meg, Beth, and Amy, your friend thinks that Jo was the most mentioned. You, however, are certain it was Amy. Luckily, you have a file LittleWomen.txt containing the full text of the novel (data-shell/writing/data/LittleWomen.txt). Using a for loop, how would you tabulate the number of times each of the four sisters is mentioned?

Hint: one solution might employ the commands grep and wc and a |, while another might utilize grep options. There is often more than one way to solve a programming task, so a particular solution is usually chosen based on a combination of yielding the correct result, elegance, readability, and speed.

Solution

Solutions

```
for sis in Jo Meg Beth Amy
do
        echo $sis:
grep -ow $sis LittleWomen.txt | wc -l
done

Alternative, slightly inferior solution:
for sis in Jo Meg Beth Amy
do
        echo $sis:
grep -ocw $sis LittleWomen.txt
done
```

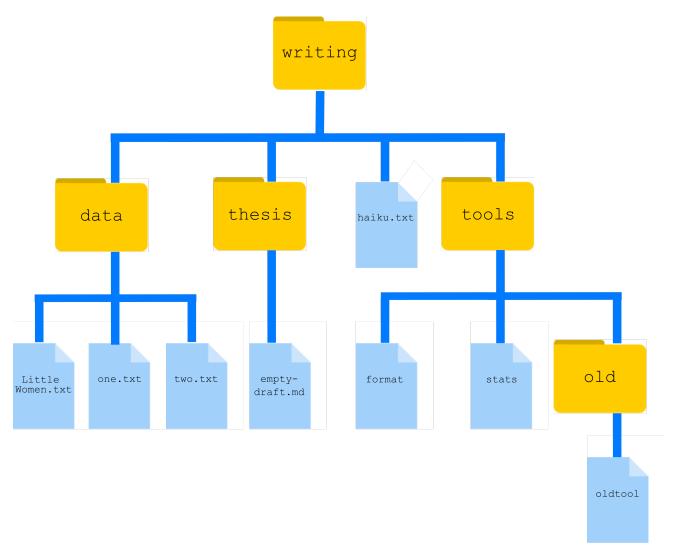
This solution is inferior because grep -c only reports the number of lines matched. The total number of matches reported by this method will be lower if there is more than one match per line.

Perceptive observers may have noticed that character names sometimes appear in all-uppercase in chapter titles (e.g. 'MEG GOES TO VANITY FAIR'). If you wanted to count these as well, you could add the -i option for case-insensitivity (though in this case, it doesn't affect the answer to which sister is mentioned most frequently).

Solution

While grep finds lines in files, the find command finds files themselves. Again, it has a lot of options; to show how the simplest ones work, we'll use the directory tree shown below.

A file tree under the directory "writing" contians several sub-directories and files such that "writing" contains directories "data", "thesis", "tools" and a file "haiku.txt"; "writing/data" contains the files "Little Women.txt", "one.txt" and "two.txt"; "writing/thesis" contains the file "empty-draft.md"; "writing/tools" contains the directory "old" and the files "format" and "stats"; and "writing/tools/old" contains a file "old-tool"



Nelle's writing directory contains one file called haiku.txt and three subdirectories: thesis (which contains a sadly empty file, empty-draft.md); data (which contains three files LittleWomen.txt, one.txt and two.txt); and a tools directory that contains the programs format and stats, and a subdirectory called old, with a file oldtool.

For our first command, let's run find . (remember to run this command from the data-shell/writing folder).

\$ find .

- ./data
- ./data/one.txt
- ./data/LittleWomen.txt
- ./data/two.txt
- ./tools
- ./tools/format
- ./tools/old
- ./tools/old/oldtool
- ./tools/stats
- ./haiku.txt

```
./thesis
./thesis/empty-draft.md
```

As always, the . on its own means the current working directory, which is where we want our search to start. find's output is the names of every file and directory under the current working directory. This can seem useless at first but find has many options to filter the output and in this lesson we will discover some of them.

The first option in our list is -type d that means 'things that are directories'. Sure enough, find's output is the names of the five directories in our little tree (including .):

```
$ find . -type d
./
./data
./thesis
./tools
./tools/old
```

Notice that the objects find finds are not listed in any particular order. If we change -type d to -type f, we get a listing of all the files instead:

```
$ find . -type f

./haiku.txt
./tools/stats
./tools/old/oldtool
./tools/format
./thesis/empty-draft.md
./data/one.txt
./data/LittleWomen.txt
./data/two.txt
```

Now let's try matching by name:

```
$ find . -name *.txt
./haiku.txt
```

We expected it to find all the text files, but it only prints out ./haiku.txt. The problem is that the shell expands wildcard characters like * before commands run. Since *.txt in the current directory expands to haiku.txt, the command we actually ran was:

```
$ find . -name haiku.txt
```

find did what we asked; we just asked for the wrong thing.

To get what we want, let's do what we did with grep: put *.txt in quotes to prevent the shell from expanding the * wildcard. This way, find actually gets the pattern *.txt, not the expanded filename haiku.txt:

```
$ find . -name "*.txt"
./data/one.txt
./data/LittleWomen.txt
./data/two.txt
./haiku.txt
```

Listing vs. Finding

ls and find can be made to do similar things given the right options, but under normal circumstances, ls lists everything it can, while find searches for things with certain properties and shows them.

As we said earlier, the command line's power lies in combining tools. We've seen how to do that with pipes; let's look at another technique. As we just saw, find . -name "*.txt" gives us a list of all text files in or below the current directory. How can we combine that with wc -1 to count the lines in all those files?

The simplest way is to put the find command inside \$():

```
$ wc -l $(find . -name "*.txt")

11 ./haiku.txt
300 ./data/two.txt
21022 ./data/LittleWomen.txt
70 ./data/one.txt
21403 total
```

When the shell executes this command, the first thing it does is run whatever is inside the \$(). It then replaces the \$() expression with that command's output. Since the output of find is the four filenames ./data/one.txt, ./data/LittleWomen.txt, ./data/two.txt, and ./haiku.txt, the shell constructs the command:

```
$ wc -l ./data/one.txt ./data/LittleWomen.txt ./data/two.txt ./haiku.txt
```

which is what we wanted. This expansion is exactly what the shell does when it expands wildcards like * and ?, but lets us use any command we want as our own 'wildcard'.

It's very common to use find and grep together. The first finds files that match a pattern; the second looks for lines inside those files that match another pattern. Here, for example, we can find PDB files that contain iron atoms by looking for the string 'FE' in all the .pdb files above the current directory:

Matching and Subtracting

The -v option to grep inverts pattern matching, so that only lines which do not match the pattern are printed. Given that, which of the following commands will find all files in /data whose names end in s.txt but whose names also do not contain the string net? (For example, animals.txt or amino-acids.txt but not planets.txt.) Once you have thought about your answer, you can test the commands in the data-shell directory.

```
1. find data -name "*s.txt" | grep -v net
2. find data -name *s.txt | grep -v net
3. grep -v "net" $(find data -name "*s.txt")
```

4. None of the above.

Solution

The correct answer is 1. Putting the match expression in quotes prevents the shell expanding it, so it gets passed to the find command.

Option 2 is incorrect because the shell expands *s.txt instead of passing the wildcard expression to find.

Option 3 is incorrect because it searches the contents of the files for lines which do not match 'net', rather than searching the file names.

Solution

Binary Files

We have focused exclusively on finding patterns in text files. What if your data is stored as images, in databases, or in some other format?

A handful of tools extend grep to handle a few non text formats. But a more generalizable approach is to convert the data to text, or extract the text-like elements from the data. On the one hand, it makes simple things easy to do. On the other hand, complex things are usually impossible. For example, it's easy enough to write a program that will extract X and Y dimensions from image files for grep to play with, but how would you write something to find values in a spreadsheet whose cells contained formulas?

A last option is to recognize that the shell and text processing have their limits, and to use another programming language. When the time comes to do this, don't be too hard on the shell: many modern programming languages have borrowed a lot of ideas from it, and imitation is also the sincerest form of praise.

The Unix shell is older than most of the people who use it. It has survived so long because it is one of the most productive programming environments ever created — maybe even the most productive. Its syntax may be cryptic, but people who have mastered it can experiment with different commands interactively, then use what they have learned to automate their work. Graphical user interfaces may be better at the first, but the shell is still unbeaten at the second. And as Alfred North Whitehead wrote in 1911, 'Civilization advances by extending the number of important operations which we can perform without thinking about them.'

find Pipeline Reading Comprehension

Write a short explanatory comment for the following shell script:

```
wc -1 $(find . -name "*.dat") | sort -n
```

Solution

Solution

- 1. Find all files with a .dat extension recursively from the current directory
- 2. Count the number of lines each of these files contains
- 3. Sort the output from step 2. numerically