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Loops



Teaching: 40 min Exercises: 10 min

Questions

How can I perform the same actions on many different files?

Objectives

- · Write a loop that applies one or more commands separately to each file in a set of files.
- Trace the values taken on by a loop variable during execution of the loop.
- Explain the difference between a variable's name and its value.
- Explain why spaces and some punctuation characters shouldn't be used in file names.
- Demonstrate how to see what commands have recently been executed.
- · Re-run recently executed commands without retyping them.

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 <code>basilisk.dat</code>, <code>unicorn.dat</code>, and so on. For this example, we'll use the creatures directory which only has two example files, but the principles can be applied to many many more files at once. We would like to print out the classification for each species, which is given on the second line of the file. For each file, we would need to execute the command <code>head -n 2</code> and pipe this to <code>tail -n 1</code>. 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 unicorn.dat
> do
> head -n 2 $filename | tail -n 1
> done
```

CLASSIFICATION: basiliscus vulgaris 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 two filenames: basilisk.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 unicorn.dat. This time, the shell runs head on unicorn.dat and pipes the first two lines to the tail command, which then prints the second line of unicorn.dat. Since the list was only two 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 \$filename. 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 unicorn.dat
> do
> head -n 2 $x | tail -n 1
> done
```

or:

```
$ for temperature in basilisk.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?

Why do these two loops give different outputs?

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 1s . The expanded loop would look like this:

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

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 1s.

```
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

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.

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

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

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.

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 <code>cubane.pdb</code> , <code>ethane.pdb</code> , <code>methane.pdb</code> , <code>octane.pdb</code> , <code>pentane.pdb</code> and <code>propane.pdb</code> would be concatenated and saved to a file called <code>all.pdb</code> .
- 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

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, echo, just 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 just 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 just 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 unicorn.dat original-*.dat
```

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

```
$ for filename in *.dat
> do
> cp $filename original-$filename
> done
```

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

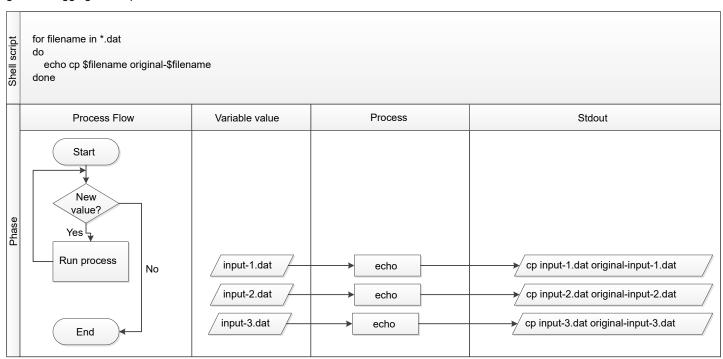
```
cp basilisk.dat original-basilisk.dat
```

The second time, the command is:

```
cp 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.



Nelle's Pipeline: Processing Files

Nelle is now ready to process her data files using <code>goostats</code> — 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
```

```
NENE01729A.txt stats-NENE01729A.txt
NENE01729B.txt stats-NENE01729B.txt
NENE01736A.txt stats-NENE01736A.txt
...
NENE02043A.txt stats-NENE02043A.txt
NENE02043B.txt stats-NENE02043B.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 reentering her loop, she presses the up arrow. 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 Ctr1-C, uses up-arrow 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:

```
NENE01729A.txt
NENE01729B.txt
NENE01736A.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 NENE0*.txt
457 rm stats-NENE01729B.txt.txt
458 bash goostats NENE01729B.txt stats-NENE01729B.txt
459 ls -l NENE0*.txt
460 history

then she can re-run goostats on NENE01729B.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.
- !! retrieves the immediately preceding command (you may or may not find this more convenient than using the up-arrow)
- !\$ 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 up-arrow 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 file in *.pdb
> do
> analyze $file > analyzed-$file
> done
```

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

```
# Version 1
$ for file in *.pdb
> do
> echo analyze $file > analyzed-$file
> done

# Version 2
$ for file in *.pdb
> do
> echo "analyze $file > analyzed-$file"
> done
```


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 redirects the output from the command echo analyze \$file to a file, analyzed-\$file . A series of files is generated: analyzed-cubane.pdb , analyzed-ethane.pdb etc.

Try both versions for yourself to see the output! Be sure to open the analyzed-*.pdb files to view their contents.

Nested Loops

Suppose we want to set up 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
```


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!

The Unix Shell: Loops

Key Points

- · A for loop repeats commands once for every thing in a list.
- Every for loop needs a variable to refer to the thing it is currently operating on.
- Use \$name to expand a variable (i.e., get its value). \${name} can also be used.
- Do not use spaces, quotes, or wildcard characters such as '*' or '?' in filenames, as it complicates variable expansion.
- Give files consistent names that are easy to match with wildcard patterns to make it easy to select them for looping.
- · Use the up-arrow key to scroll up through previous commands to edit and repeat them.
- Use Ctrl-R to search through the previously entered commands.
- Use history to display recent commands, and !number to repeat a command by number.



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