Session 4: Shell scripts (Part II) (Andrew Weisman)

Notes:

- The notes below are based on the "bottom" part of this webpage
- The page you are reading can be found here: https://github.com/CBIIT/p2p-datasci/blob/master/workshop_materials/2021-09-21-introduction_to_linux/instructors_notes/shell_scripts_part_2-andrew.md
- Copy that link into the chat, including the link for the course website: https://cbiit.github.io/p2p-datasci/2021-09-09-introduction_to_linux

Review of Part I

A shell script is a single file that contains a bunch of shell (e.g., Bash) commands.

For example, create a file ~/Desktop/shell-lesson-data/molecules/middle.sh that contains:

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

Run the script using:

```
bash middle.sh
```

Modify the script to use arguments:

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

Run the script using:

```
bash middle.sh octane.pdb 15 5
```

Increase clarity using comments:

```
# Select lines from the middle of a file.
# Usage: bash middle.sh <FILENAME> <END-LINE> <NUM-LINES>
head -n "$2" "$1" | tail -n "$3"
```

Increase clarity in the code itself:

```
# Select lines from the middle of a file.
# Usage: bash middle.sh <FILENAME> <END-LINE> <NUM-LINES>

filename="$1"
end_line="$2"
num_lines="$3"

head -n "$end_line" "$filename" | tail -n "$num_lines"
```

New material

Arbitrary numbers of arguments

What if you want to write a script to process an arbitrary number of arguments? For example, in order to sort by length all the .pdb files in the ~/Desktop/shell-lesson-data/molecules directory, you would run from the command line:

```
# From the command line:
wc -l *.pdb | sort -n
```

You could put this into a script called sorted.sh and run it using

```
# From the command line:
bash sorted.sh
```

and it would indeed sort all the .pdb files by length.

What if you wanted to sort an arbitrary set of files given on the command line? E.g.,

```
# From the command line:
bash sorted.sh *.pdb ../creatures/*.dat
```

The answer is to use the special variable \$@ to refer to "all command-line arguments to the shell script":

```
# Contents of sorted.sh:
wc -1 "$@" | sort -n
```

Note: "\$@" is special syntax and is equivalent to "\$1" "\$2" "\$3"

Homework: List unique species

Saving commands from history into a script

If you have done something useful in the shell that you would like to be able to repeat in the future, you can save these commands from history, e.g.:

```
# From the command line:
history | tail -n 5 > redo_steps.sh
```

Then clean up the file and you will be able to simply run the script in the future to repeat your work, such as creating a plot for a presentation.

Note that the shell always adds the last call to the history stack prior to calling the last line in case the last line crashes the shell; this would allow you to see which command caused the crash.

Nelle's pipeline: creating a script

Nelle's supervisor wants to create a script of her analysis so that it is repeatable.

```
# From the command line:
cd ../north-pacific-gyre/2012-07-03/
nano do-stats.sh
```

```
# Contents of do-stats.sh:

for datafile in "$@"; do
    echo $datafile
    bash goostats.sh $datafile stats-$datafile
done
```

Note that goostats.sh runs some analysis on the first argument (a file) and writes the results to the second argument (another file).

Nelle can then run her analysis on her datafiles using:

Exercise: Variables in shell scripts

Exercise: Find the longest file with a given extension

Exercise: Script reading comprehension

Exercise: Debugging scripts

Key Points