

Lecture 05 - Unix shell scripts

why write a shell script?

why write a shell script?

- ▶ repeat tasks easily
- ▶ reproducible and documented (comments!!!!)
- ▶ modularize your analysis processes

arguments to a shell script

- ▶ \$1, \$2, \$3, etc.
- ▶ \$@ - useful with loops in a shell script!

shell scripts in an 'orthogonal' manner

- ▶ remember the power of Unix is it's modularity
- ▶ BUILD SCRIPTS TO READ FROM `stdin` AND WRITE TO `stdout`

convert a SWC shell script to use stdin and stdout

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

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

convert a SWC shell script to use stdin and stdout

```
# Select lines from the middle of a file.  
# Usage: middle2.sh end_line num_lines  
head -n "$1" | tail -n "$2"
```

```
cat pentane.pdb | bash middle2.sh 15 5
```

making scripts behave even more like a function

To behave like other basic functions a shell script needs:

- ▶ a 'shebang' as the first line
 - ▶ `#!/path/to/interpreter`
 - ▶ this tells the shell what to use to run the text in the script
- ▶ the script file must be executable by the user

file permissions

if we use `ls -l *.sh` to look at our shell scripts, we can see read, write, and execute permissions

- ▶ usually the first character indicates files vs. directories
- ▶ the next nine characters indicate the presence or absence of read (r), write (w), and execute (x) permissions for the “owner”, “group”, and “other” users

changing file permissions

- ▶ the function `chmod` can be used to change permissions
- ▶ to add executable permission for the owner try: `chmod u+x filename`
 - ▶ *who* comes first: user (u), group (g), other (o), or all (a)
 - ▶ “op” comes next: this indicates if we are adding (+) or removing (-) permissions
 - ▶ “permission” is last: read (r), write (w), and execute (x) are the most common

convert a SWC shell script to use stdin and stdout

```
#!/usr/bin/env bash
```

```
# Select lines from the middle of a file.
```

```
# Usage: middle3.sh end_line num_lines
```

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

```
chmod u+x middle3.sh
```

```
cat pentane.pdb | ./middle3.sh 15 5
```

convert a SWC shell script to use stdin and stdout

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

```
cat pentane.pdb | bash middle2.sh 15 5
```

```
cat pentane.pdb | ./middle3.sh 15 5
```

version control and Git

A computational best practice that solves this problem, among others...



version control and Git

- ▶ A set of functions that allow tracking of progress in a project and facilitate collaboration.
- ▶ Becoming the gold standard in biocomputation-focused research.
- ▶ Sets up a hidden directory that stores information about changes in a working directory.

```
git init
```

```
git add file_names
```

```
git commit -m "custom commit message"
```

- ▶ Consult documentation ('Git_Setup.pdf') available on Sakai for installation instructions.

function review

`chmod`

`#!/path/to/interpreter`