Advanced Shell Scripting for Bioinformatics

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Outline

Topic

Motivation: why write a bash script?

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1. Reusable

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   - Do something once; do it a thousand times

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4. Computer Programming is JUST DARN FUN!!!

Basic Bash Scripting

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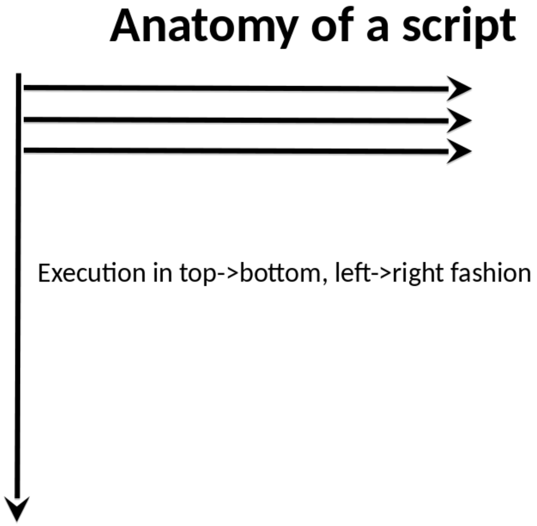
    - comment, comment, comment!!!
    - worst enemy in 6 months?
    - YOU ARE!!!!

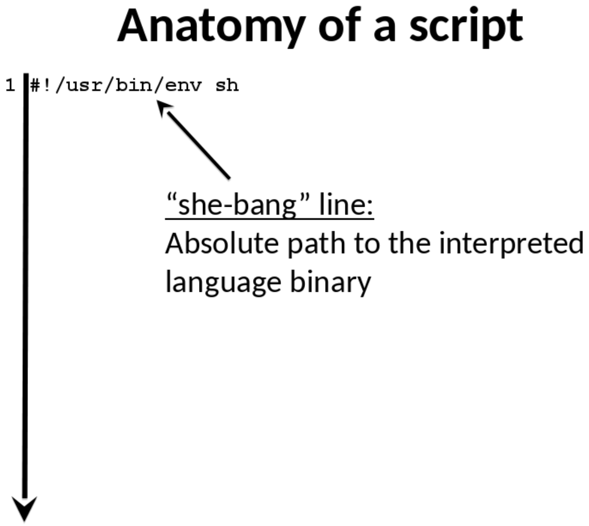
Anatomy of a script

Anatomy of a script


Anatomy of a script

Execution in top->bottom, left->right fashion

Anatomy of a script

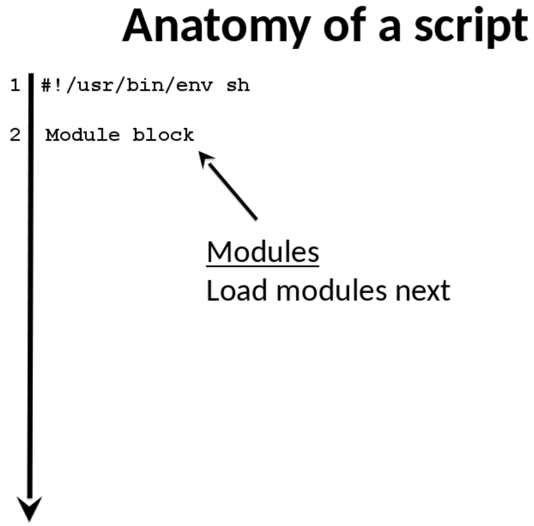


Anatomy of a script

```
#!/usr/bin/env sh
```

"she-bang" line:
Absolute path to the interpreted language binary

Anatomy of a script



Anatomy of a script

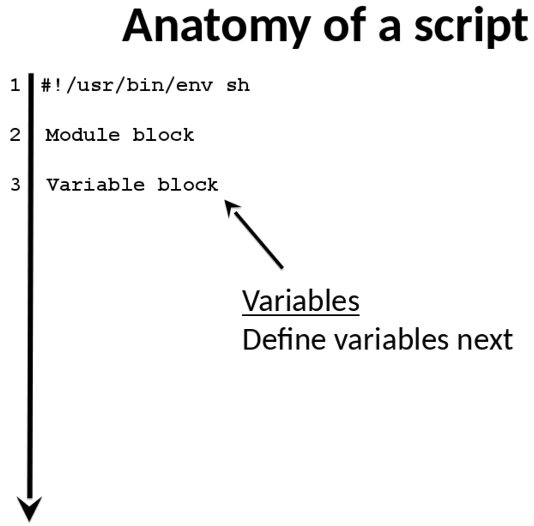
```
1 #!/usr/bin/env sh

2 Module block
```

Modules

Load modules next

Anatomy of a script



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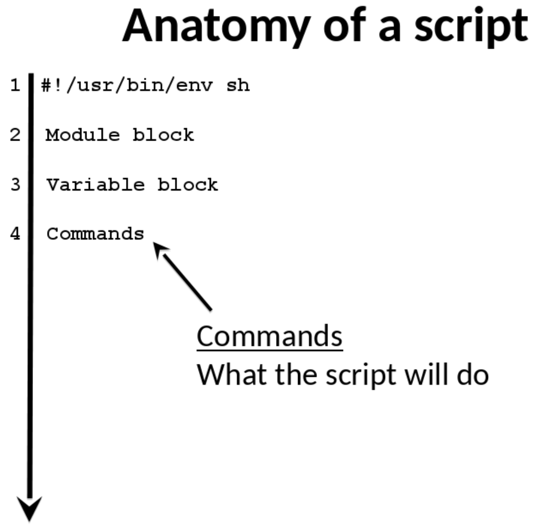

Anatomy of a script

```
1 #!/usr/bin/env sh
2  Module block
3  Variable block
4  Commands
```

<ins>Commands</ins>
What the script will do

What are variables?

1. Environmental variables

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     - contains no special characters (i.e., $)
     - separated by underscores raw_counts

Why are variables important?

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2. easily readable

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3. less mistakes

Why are variables important?

1. tidy code
2. easily readable
3. less mistakes
    - type once use multiple times

Variable creation

1. directly

```
wd=${HOME}/analysis_directory
echo ${wd}
```

```
/home/ssefick/analysis_directory
```

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```
wd=${HOME}/analysis_directory
echo ${wd}
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```
/home/ssefick/analysis_directory
```

1. dynamically

```
##direct
input_dir=input
##dynamic
files=(‘ls ${input_dir} | grep sh$‘)
echo ${files[@]}
```

```
awesome_script1.sh awesome_script2.sh awesome_script3.sh
```

Topic

An example: work smarter not harder

1. I accidentally named files with .sh and not .pl

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An example: work smarter not harder

1. I accidentally named files with .sh and not .pl
2. What we know about the problem
   - more than 1 mislabeled file
   - Contained in a folder called input
3. What is a sensible way to go about this?
4. Let's write a little script to fix it

Let's build a script interactively

Parts of a script

1. Shebang -language specific

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Let's build a script interactively

Parts of a script

1. Shebang -language specific
2. Module block
   - all HPC modules (e.g., module load)
3. Variable block
   - all variables
4. Commands
   - instruction set

input

1. I think the files are in "input"

Let's check

```
########################
wd=`ls input | grep sh$`
echo ${wd}
```

```
awesome_script1.sh awesome_script2.sh awesome_script3.sh
```

Shebang and module block

shebang

1. top of file

```
#########################
#!/usr/bin/env sh
#########################
```

Shebang and module block

shebang

1. top of file

```
#########################
#!/usr/bin/env sh
#########################
```

module block

1. Load all modules here
2. Easily find/remember what modules loaded
3. No modules to load because I built this presentation on a PC

```
######################
##Modules
##module load something
######################
```

Variable Block

1. Easily find input/output directories
2. Tidy programming

variable block

```
#######################
##Variables
input_dir=input
out_dir=output
##input/output files arrays
files=(‘ls ${input_dir} | grep sh$‘)
out_files=(‘echo ${files[@]} | sed s/sh/pl/g‘)

##parameter expansion
##parameter/patten/string
input_with_path=( "${files[@]/#/${input_dir}/}" )
output_with_path=( "${out_files[@]/#/${out_dir}/}" )
#######################
```

Commands

For loop

```
########################
##commands
##make the output dir
mkdir -p ${out_dir}

##for loop
##use length to iterate in order to index input output arrays
for ((i=0; i<${#input_with_path[@]}; i++)); do

    echo ${i}

    echo cp ${input_with_path[${i}]} ${output_with_path[${i}]}

done
######################
```

Understanding the script

```
files=(`ls ${input_dir} | grep sh$`)
```

awesome_script1.sh
awesome_script2.sh
awesome_script3.sh

```
input_with_path=( "${files[@]/#/${
    input_dir}/}" )
```

input/awesome_script1.sh
input/awesome_script2.sh
input/awesome_script3.sh

```
out_files=(`echo ${files[@]} | sed s/
    sh/pl/g`)
```

awesome_script1.pl
awesome_script2.pl
awesome_script3.pl

```
output_with_path=( "${out_files[@]/#/$
    {out_dir}/}" )
```

output/awesome_script1.pl
output/awesome_script2.pl
output/awesome_script3.pl

Understanding the for loop

```
for ((i=0; i<${#input_with_path[@]}; i++)); do
    ${i}
    cp ${input_with_path[${i}]} ${output_with_path[${i}]}
done
echo ${i}
```

```
0
1
2
```

```
cp ${input_with_path[${i}]} ${output_with_path[${i}]}
```

```
cp    input/awesome_script1.sh    output/awesome_script1.pl
cp    input/awesome_script2.sh    output/awesome_script2.pl
cp    input/awesome_script3.sh    output/awesome_script3.pl
```

Topic

History to script

1. blast history to script from last class

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2. Use some information from today

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3. Why in the world would we want to redo an analysis?

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4. ~20 min

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3. Why in the world would we want to redo an analysis?
    - reproducible research artifact
4. ~20 min
    - HW5

Topic

Gold standard: literate programming

"Let us change our traditional attitude to the construction of programs: Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to human beings what we want a computer to do."
-Knuth

Some Tools

LaTeX

10 suggestions from the paper

1. For every result, keep track of how it was produced
2. Avoid manual data manipulation steps
3. Archive the exact versions of all external programs used
4. Version control all custom scripts
5. Record all intermediate results, when possible in standardized formats
6. For analyses that include randomness, note underlying random seeds
7. Always store raw data behind plots
8. Generate hierarchical analysis output, allowing layers of increasing detail to be inspected
9. Connect textual statements to underlying results
10. Provide public access to scripts, runs, and results