Unix and Bioinformatics Version 3

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Abstract

This protocol details the use of various unix commands commonly used in bioinformatics.

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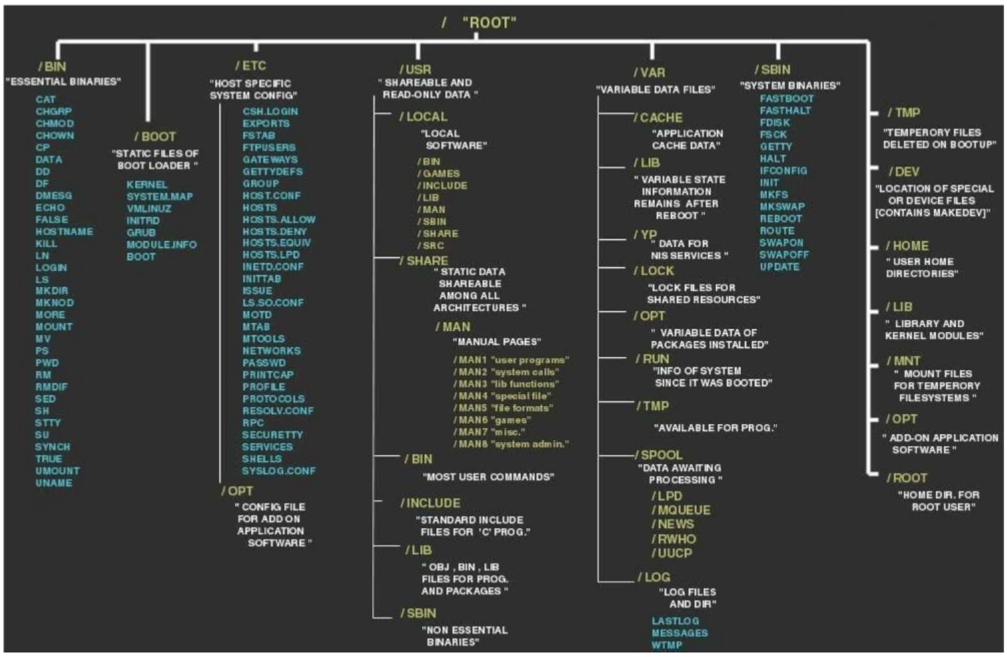
Guidelines

Unix Commands

pwd	rm	grep	tail	install
ls	'>'	sed	cut	
cd	cat	nano	top	
mkdir	'<'	history	screen	
touch	'|'	$PATH	ssh	
cp	sort	less	df	
mv	uniq	head	rsync/scp	

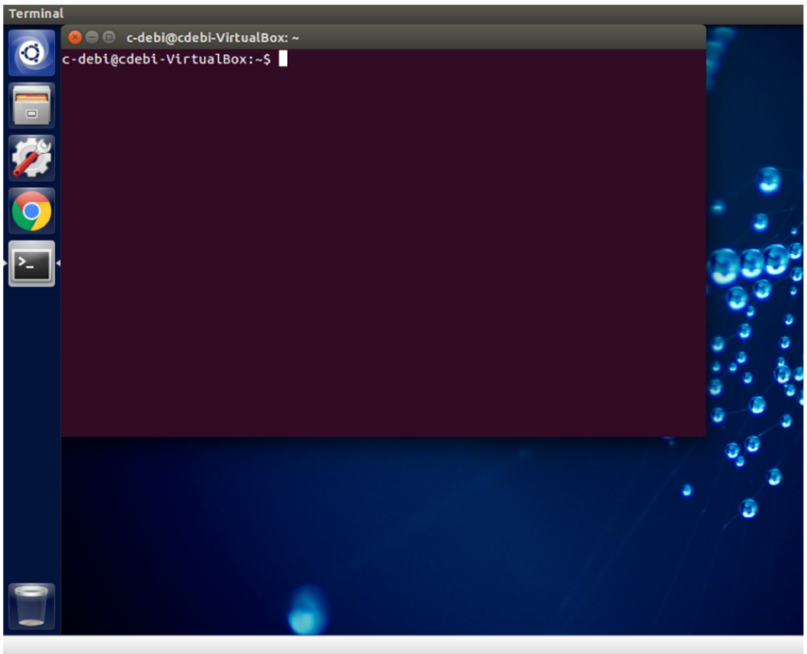


Protocol

The Start

Step 1.

Open terminal window



```
c-debi@cdebi-VirtualBox:~$
```

The Start

Step 2.

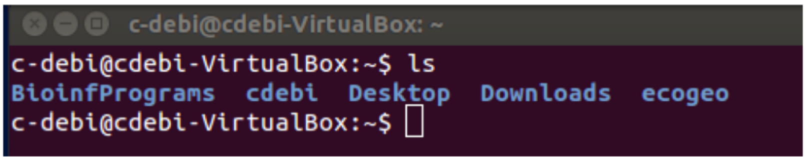
Use ls to list items in the current directory.

cmd COMMAND

```
ls
```

lists items in the current directory

EXPECTED RESULTS



```
c-debi@cdebi-VirtualBox:~$ ls
BioinfPrograms  cdebi  Desktop  Downloads  ecogeo
c-debi@cdebi-VirtualBox:~$
```

The Start

Step 3.

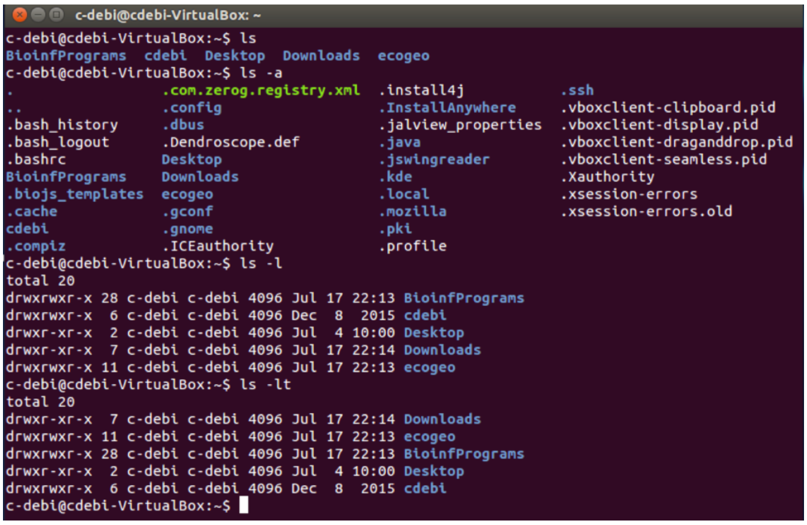
Many commands have additional options that can be set by a '-'

cmd COMMAND

```
ls -a
ls -l
ls -lt
```

lists all files/directories, including hidden files '.' lists the long format lists the long format, but ordered by date last modified

EXPECTED RESULTS



```
c-debi@cdebi-VirtualBox:~$ ls
BioinfPrograms  cdebi  Desktop  Downloads  ecogeo
c-debi@cdebi-VirtualBox:~$ ls -a
.                 .com.zerog.registry.xml  .install4j           .ssh
..                .config                  .InstallAnywhere     .vboxclient-clipboard.pid
.bash_history     .dbus                    .jalview_properties  .vboxclient-display.pid
.bash_logout      .Dendroscope.def         .java                .vboxclient-draganddrop.pid
.bashrc           Desktop                  .jswingreader        .vboxclient-seamless.pid
BioinfPrograms    Downloads                .kde                 .Xauthority
.biojs_templates  ecogeo                   .local               .xsession-errors
.cache            .gconf                   .mozilla             .xsession-errors.old
cdebi             .gnome                   .pki
.compiz           .ICEauthority            .profile
c-debi@cdebi-VirtualBox:~$ ls -l
total 20
drwxrwxr-x 28 c-debi c-debi 4096 Jul 17 22:13 BioinfPrograms
drwxrwxr-x  6 c-debi c-debi 4096 Dec  8  2015 cdebi
drwxr-xr-x  2 c-debi c-debi 4096 Jul  4 10:00 Desktop
drwxr-xr-x  7 c-debi c-debi 4096 Jul 17 22:14 Downloads
drwxrwxr-x 11 c-debi c-debi 4096 Jul 17 22:13 ecogeo
c-debi@cdebi-VirtualBox:~$ ls -lt
total 20
drwxr-xr-x  7 c-debi c-debi 4096 Jul 17 22:14 Downloads
drwxrwxr-x 11 c-debi c-debi 4096 Jul 17 22:13 ecogeo
drwxrwxr-x 28 c-debi c-debi 4096 Jul 17 22:13 BioinfPrograms
drwxr-xr-x  2 c-debi c-debi 4096 Jul  4 10:00 Desktop
drwxrwxr-x  6 c-debi c-debi 4096 Dec  8  2015 cdebi
c-debi@cdebi-VirtualBox:~$
```

Directory System

Step 4.

cd - change directory

cmd COMMAND

```
cd ecogeo/
```

Directory System

Step 5.

List the contents of the current directory.

Directory System

Step 6.

Move into the directory called **unix**

Directory System

Step 7.

pwd (present working directory) can be used to show the current directory.

cmd COMMAND

```
pwd
```

prints the path to the current directory

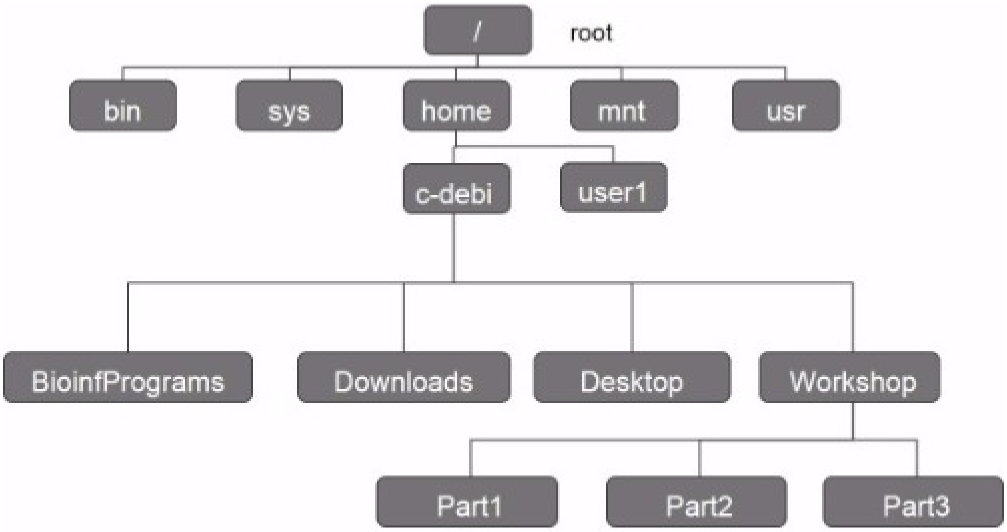
EXPECTED RESULTS

cd /home/c-debi/ecogeo/unix

Directory System

Step 8.

Move to the root directory.



cmd COMMAND

```
cd /
```

NOTES

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This is where everything is stored in the computer. All the commands we are running live in /bin.

Directory System

Step 9.

Change directory to **home**

Change directory to **c-debi**

Change directory to **ecogeo**

Change directory to **unix**

List contents

Change directory to **data**

Change directory to **root**

NOTES

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Tabs can be used to auto complete names.

Directory System

Step 10.

Change directory to **unix/data** in one step

cmd COMMAND

```
$ cd /home/c-debi/ecogeo/unix/data
```

Directory System

Step 11.

cd '..' allows you to step back up through the path directory. Display present working directory path.

cmd COMMAND

```
cd ..
pwd
```

moves back in the path directory

EXPECTED RESULTS

/home/c-debi/ecogeo/unix

Directory System

Step 12.

Step back up to the c-debi directory.

Directory System

Step 13.

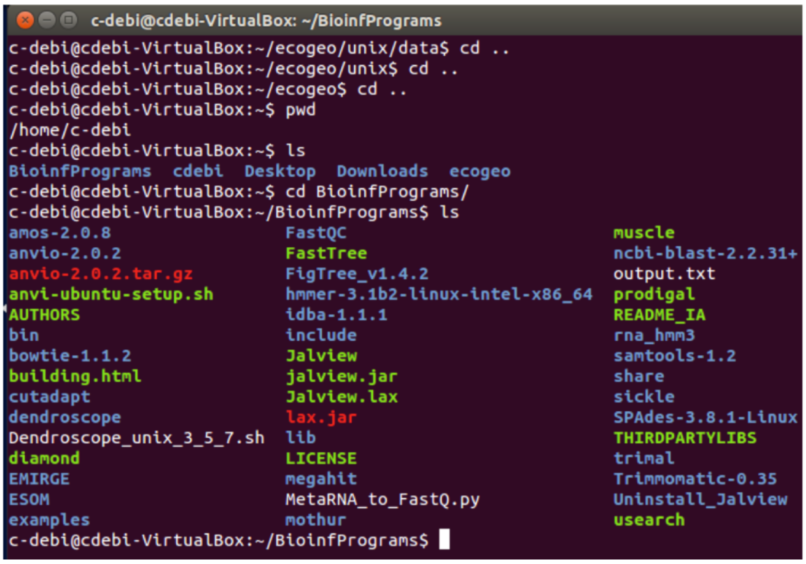
Change directory to BioinfPrograms

Directory System

Step 14.

List contents

EXPECTED RESULTS



```
c-debi@cdebi-VirtualBox:~/ecogeo/unix/data$ cd ..
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ cd ..
c-debi@cdebi-VirtualBox:~/ecogeo$ cd ..
c-debi@cdebi-VirtualBox:~$ pwd
/home/c-debi
c-debi@cdebi-VirtualBox:~$ ls
BioinfPrograms  cdebi  Desktop  Downloads  ecogeo
c-debi@cdebi-VirtualBox:~$ cd BioinfPrograms/
c-debi@cdebi-VirtualBox:~/BioinfPrograms$ ls
amos-2.0.8                  FastQC                          muscle
anvio-2.0.2                 FastTree                        ncbi-blast-2.2.31+
anvio-2.0.2.tar.gz          FigTree_v1.4.2                  output.txt
anvi-ubuntu-setup.sh        hmmer-3.1b2-linux-intel-x86_64  prodigal
AUTHORS                     idba-1.1.1                      README_IA
bin                         include                         rna_hmm3
bowtie-1.1.2                Jalview                         samtools-1.2
building.html               jalview.jar                     share
cutadapt                    Jalview.lax                     sickle
dendroscope                 lax.jar                         SPAdes-3.8.1-Linux
Dendroscope_unix_3_5_7.sh   lib                             THIRDPARTYLIBS
diamond                     LICENSE                         trimal
EMIRGE                      megahit                         Trimmomatic-0.35
ESOM                        MetaRNA_to_FastQ.py             Uninstall_Jalview
examples                    mothur                          usearch
c-debi@cdebi-VirtualBox:~/BioinfPrograms$ 
```

Directory System

Step 15.

Change directory to unix/

Directory System

Step 16.

Make a directory named "storage".

cmd COMMAND

```
mkdir storage
```

Directory System

Step 17.

List contents of directory.

Directory System

Step 18.

Move into the storage directory.

Manipulating files

Step 19.

The 'touch' command allows you to create a blank file of the input name.

cmd COMMAND

```
touch temp.txt
```

creates a blank file of the input name

Manipulating files

Step 20.

The 'cp' command allows you to copy a file and can be used to move a copy of a file to a directory.

cmd COMMAND

```
$ cp
```

Manipulating files

Step 21.

The 'mv' or move command "destroys" the original and places the content elsewhere.

cmd COMMAND

```
$ mv
```

Manipulating files

Step 22.

Using copy:

cmd COMMAND

```
$ cp temp.txt newtemp.txt
$ cp temp.txt ../
```

Manipulating files

Step 23.

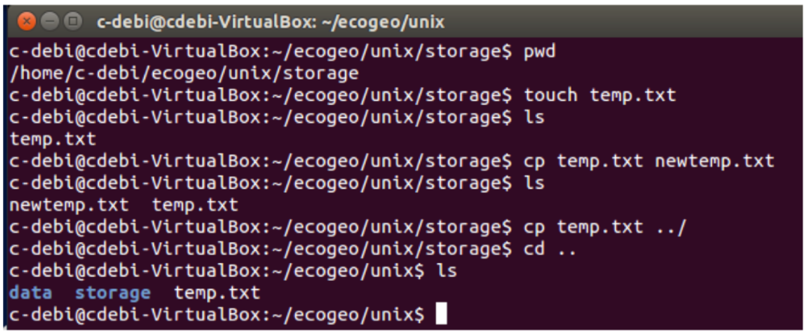
Change directory up a level.

Manipulating files

Step 24.

List contents.

EXPECTED RESULTS



```
c-debi@cdebi-VirtualBox:~/ecogeo/unix/storage$ pwd
/home/c-debi/ecogeo/unix/storage
c-debi@cdebi-VirtualBox:~/ecogeo/unix/storage$ touch temp.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/storage$ ls
temp.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/storage$ cp temp.txt newtemp.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/storage$ ls
newtemp.txt  temp.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/storage$ cp temp.txt ../
c-debi@cdebi-VirtualBox:~/ecogeo/unix/storage$ cd ..
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ ls
data  storage  temp.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ 
```

Manipulating files

Step 25.

Change directory to storage.

Manipulating files

Step 26.

Utilize move command:

cmd COMMAND

```
$ mv newtemp.txt oldtemp.txt
$ mv oldtemp.txt /home/c-debi/ecogeo/unix/data
```

Manipulating files

Step 27.

Change directory to data, list content.

Manipulating files

Step 28.

List current working directory.

cmd COMMAND

```
/home/c-debi/ecogeo/unix/data
```

Manipulating files

Step 29.

The 'rm' remove command deleted a file PERMANENTLY

cmd COMMAND

```
rm oldtemp.txt
```

Manipulating files

Step 30.

Change directory to **storage**.

Manipulating files

Step 31.

Remove **temp.txt**

Manipulating files

Step 32.

Change directory to **unix**

Manipulating files

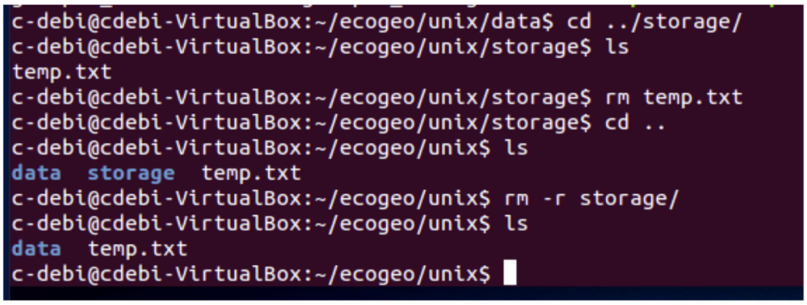
Step 33.

Remove storage directory:

cmd COMMAND

```
$ rm -r storage
```

EXPECTED RESULTS



```
c-debi@cdebi-VirtualBox:~/ecogeo/unix/data$ cd ../storage/
c-debi@cdebi-VirtualBox:~/ecogeo/unix/storage$ ls
temp.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/storage$ rm temp.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/storage$ cd ..
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ ls
data  storage  temp.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ rm -r storage/
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ ls
data  temp.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ 
```

Manipulating files

Step 34.

Create a directory called **bestdirectoryever**

Change directory to **bestdirectoryever**

Create a file called **glam.txt**

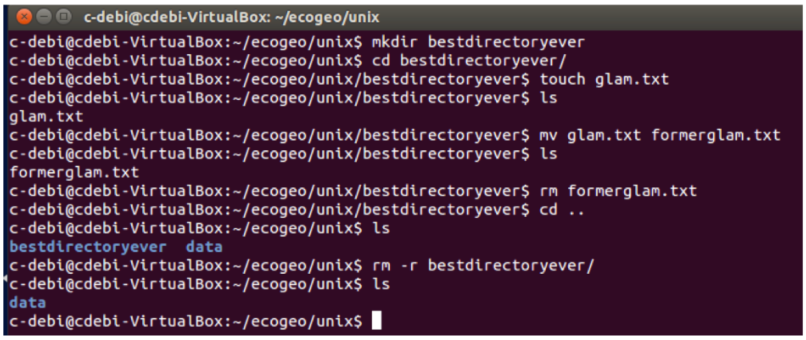
Change **glam.txt** to **formerglam.txt**

Remove **formerglam.txt**

Change directory to **unix**

Remove **bestdirectoryever**

EXPECTED RESULTS



```
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ mkdir bestdirectoryever
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ cd bestdirectoryever/
c-debi@cdebi-VirtualBox:~/ecogeo/unix/bestdirectoryever$ touch glam.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/bestdirectoryever$ ls
glam.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/bestdirectoryever$ mv glam.txt formerglam.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/bestdirectoryever$ ls
formerglam.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/bestdirectoryever$ rm formerglam.txt
c-debi@cdebi-VirtualBox:~/ecogeo/unix/bestdirectoryever$ cd ..
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ ls
bestdirectoryever  data
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ rm -r bestdirectoryever/
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ ls
data
c-debi@cdebi-VirtualBox:~/ecogeo/unix$ 
```

Manipulating files

Step 35.

Change directory to data.

Manipulating files

Step 36.

List contents.

Manipulating files

Step 37.

Remove oldtemp.txt

Manipulating files

Step 38.

group12_contigs.fasta

group20_contigs.fasta

group24_contigs.fasta

FASTA files - specific format

> Header line, contains ID and information about...

ATGATAGCTAGCAGCAGCTA[...] 80bp and then a newline.

Looking at the contents of a file

Step 39.

'head' will allow you to view the first 10 lines of a file.

cmd COMMAND

```
$ head [filename]
```

default displays the first 10 lines

Looking at the contents of a file

Step 40.

'tail' allows you to view the last 10 lines of a file.

cmd COMMAND

```
$ tail [filename]
```

default displays last 10 lines

Looking at the contents of a file

Step 41.

'less' allows you to scroll through a file using arrow keys or spacebar = advanced page | b = reverse page | q = quit

cmd COMMAND

```
$ less [filename]
```

Looking at the contents of a file

Step 42.

Use head to display the first 10 lines of **group12_contigs.fasta**

Display the first 5 lines of **group12_contigs.fasta**

Display the last 10 lines of **group12_contigs.fasta**

Display the last 5 lines of **group12_contigs.fasta**

Looking at the contents of a file

Step 43.

grep - file pattern searcher

cmd COMMAND

```
$ grep
```

Looking at the contents of a file

Step 44.

wc - count the number of words, lines, characters

Looking at the contents of a file

Step 45.

Use grep on group12_contigs.fasta

cmd COMMAND

```
$ grep “>” group12_contigs.fasta
```

stdout prints all matches of “>” in the file

Looking at the contents of a file

Step 46.

How many? Combine grep and wc?

Use the "|" (pipe) symbol

cmd COMMAND

```
$ grep “>” group12_contigs.fasta | wc
```

Looking at the contents of a file

Step 47.

Repeat but add the option -l to wc

Looking at the contents of a file

Step 48.

Use the same technique to determine the number of sequences in **group20_contigs.fasta**

Looking at the contents of a file

Step 49.

What about the number of matches to “47” in **group12_contigs.fasta**?

Or “_47”?

cmd COMMAND

```
$ grep '>' group12_contigs.fasta | grep 47
```

NOTES

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grep '>' group12_contigs.fasta | grep 47

Looking at the contents of a file

Step 50.

Redirecting output to file:

cmd COMMAND

```
$ grep “>” group12_contigs.fasta > group12_ids
```

‘>’ - redirects the output of STDOUT to a file

Looking at the contents of a file

Step 51.

Look at the contents of **group12_ids**

cmd COMMAND

```
$ grep “47” group12_contigs.fasta > group12_ids_with_47
```

Looking at the contents of a file

Step 52.

cat - has multiple functions:

cmd COMMAND

```
$ cat group12_ids_with_47
```

With a single input - prints file contents

Looking at the contents of a file

Step 53.

With ‘>’ cat has the same function as cp

cmd COMMAND

```
$ cat group12_ids_with_47 > temp1_ids
$ cp group12_ids_with_47 temp2_ids
```

Looking at the contents of a file

Step 54.

Double check to make sure **temp1_ids** = **temp2_ids**

Looking at the contents of a file

Step 55.

Concatenate files with cat - most important function:

cmd COMMAND

```
$ cat temp1_ids temp2_ids > duplicate_ids
```

Looking at the contents of a file

Step 56.

Check contents of duplicate_ids using less or cat

Looking at the contents of a file

Step 57.

Grab all of the contigs IDs from **group20_contigs.fasta** that contain the number “51”

cmd COMMAND

```
$ grep 51 group20_contigs.fasta
```

Looking at the contents of a file

Step 58.

Concatenate the new IDs to the duplicate_ids file in a file called **multiple_ids**

Looking at the contents of a file

Step 59.

uniq - can be used to remove duplicates or identify lines with 1 occurrence or multiple occurrences

cmd COMMAND

```
$ uniq
```

Looking at the contents of a file

Step 60.

sort - sort lines in a file alphanumerically

cmd COMMAND

```
$ sort
```

Looking at the contents of a file

Step 61.

Compare **multiple_ids** before and after uniq

cmd COMMAND

```
$ uniq multiple_ids
```

Looking at the contents of a file

Step 62.

Why was there no change?

uniq has a weakness, can only identify duplicates in adjacent lines cmd COMMAND

```
$ sort multiple_ids | uniq > clean_ids
```

**note the version of sorting used by Unix

Looking at the contents of a file

Step 63.

Clear all present files with temp in title

cmd COMMAND

```
$ rm temp*
```

'*' - acts as a wildcard, so any file that starts with temp would be identified and removed, no matter the suffix

Looking at the contents of a file

Step 64.

How do **temp1_ids** & **temp2_ids** compare?

cmd COMMAND

```
$ sort multiple_ids | uniq -d > temp1_ids
$ sort multiple_ids | uniq -u > temp2_ids
```

Looking at the contents of a file

Step 65.

Identify duplicates:

cmd COMMAND

```
$ sort multiple_ids | uniq -d > temp1_ids
```

Uniq -d identifies only duplicates

Looking at the contents of a file

Step 66.

Identify unique entries:

cmd COMMAND

```
$ sort multiple_ids | uniq -u > temp2_ids
```

Uniq -u identifies only unique entries

Looking at the contents of a file

Step 67.

temp1_ids = **group12_ids_with_47** &

temp2_ids = **group20_ids_with_51**

Looking at the contents of a file

Step 68.

Remove all present files with temp in title

Looking at the contents of a file

Step 69.

sed - modify files a file based on the issued commands

cmd COMMAND

```
$ sed
```

Looking at the contents of a file

Step 70.

Want a list of sequence IDs without the '>'?

cmd COMMAND

```
$ sed 's/C/c/' clean_ids
$ sed 's/_/./' clean_ids
$ sed 's/>//' clean_ids > newclean_ids
```

NOTES

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sed 's/C/c/'

between the single quotes, **s**ubstitute the occurrence of upper case C to lower case c

Looking at the contents of a file

Step 71.

seqmagick

Wrapper designed to utilize built in Biopython modules to manipulate and change FASTA files

Requires Biopython

http://fhcrc.github.io/seqmagick/

Looking at the contents of a file

Step 72.

Discuss:

convert - produce a modified new file

mogrify - change the input file

info - present information of files in a directory

Additionally: backtrans-align, extract-ids, quality-filter, and primer-trim

cmd COMMAND

```
$ seqmagick
```

Looking at the contents of a file

Step 73.

Execute seqmagick convert:

cmd COMMAND

```
$ seqmagick convert --include-from-
file newclean_ids group12_contigs.fasta newgroup12_contigs.fasta
```

Looking at the contents of a file

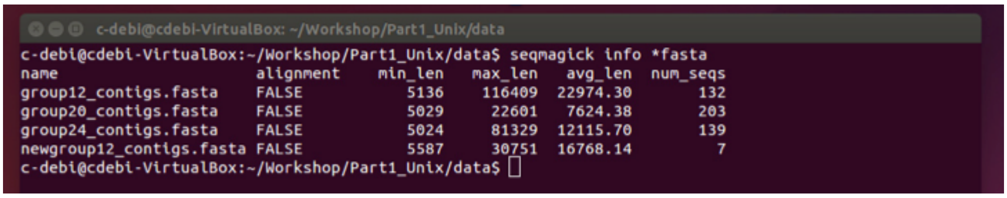
Step 74.

How many sequences are in **newgroup12_contigs.fasta**? Using grep '>':

cmd COMMAND

```
$ seqmagick extract-ids newgroup12_contigs.fasta | wc
$ seqmagick info *fasta
```

EXPECTED RESULTS



```
c-debi@cdebi-VirtualBox:~/Workshop/Part1_Unix/data$ seqmagick info *fasta
name                     alignment    min_len   max_len    avg_len  num_seqs
group12_contigs.fasta    FALSE           5136    116409   22974.30       132
group20_contigs.fasta    FALSE           5029     22601    7624.38       203
group24_contigs.fasta    FALSE           5024     81329   12115.70       139
newgroup12_contigs.fasta FALSE           5587     30751   16768.14         7
c-debi@cdebi-VirtualBox:~/Workshop/Part1_Unix/data$ 
```

Looking at the contents of a file

Step 75.

Store the information generated by ‘seqmagick info’ in a new file

fasta_info

cmd COMMAND

```
$ cut
$ cut -f 2 fasta_info
$ cut -f 2,4 fasta_info
$ cut -f 2-4 fasta_info
```

cut - pulling out columns from a table file -d allows for the assignment of the type of delimiter between fields, if not TAB -f delineates which fields to preserve, starting at 1

Some additional tools

Step 76.

history - prints a sequential list of all commands in the current session

echo $PATH - lists the directories for which the OS is checking for commands and data

Some additional tools

Step 77.

nano - in window text editor

cmd COMMAND

```
$ nano fasta_info
```

Additional text can be entered like any text editor To close out - Ctrl+X, hit ‘Y’, then ENTER Create a new file - nano and then enter file name after Ctrl+X

Some additional tools

Step 78.

Simple bash scripts: Text file with a list of commands that can be executed as a batch. Look at the contents of **simplebashscript**

Some additional tools

Step 79.

chmod - change file modes

cmd COMMAND

```
$ chmod 775 simplebashscript
```

NOTES

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chmod 755 simplebashscript

Some additional tools

Step 80.

Plain text file -> executable text file.

cmd COMMAND

```
$ ./simplebashscript
```