Microbiome Bioinformatics

Microbiome Analysis Metagenomics Metatranscriptomics **Genome Assembly & Annotation SNP & Variant Detection** Microbiome & Metagenomic analysis

# Genomics

**Genome Sequencing Next Gen Genetic Mapping** RNA-Seq **Bisulfite Sequencing** 



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# **Proteomics**

**Mass Determination Protein Identification** Post-translational modification

# **CSB1021HF LEC0131** FUNDAMENTALS OF GENOMIC DATA SCIENCE

# 0.0.0 Module 4: Introduction to the command line

# 0.1.0 About Fundamentals of Genomic Data Science

Fundamentals of Genomic Data Science is brought to you by the Centre for the Analysis of Genome Evolution & Function (CAGEF) bioinformatics training initiative. This course was developed based on feedback on the needs and interests of the Department of Cell & Systems Biology and the Department of Ecology and Evolutionary Biology.

The structure of this course is a "code-along", hands-on style! A few hours prior to each lecture, materials will be made available for download at QUERCUS (https://g.utoronto.ca/). The teaching materials will consist of a weekly PDF that you can use to follow along with the instructor along with any datasets that you'll need to complete the module. This learning approach will allow you to spend the time coding and not taking notes!

As we go along, there will be some in-class challenge questions for you to solve. Post lecture assessments will also be available for each module, building upon the concepts learned in class (see syllabus for grading scheme and percentages of the final mark).

#### 0.1.1 Where is this course going?

We'll take a blank slate approach here to learning genomic data science and assume you know nothing about programming or working directly with next generation sequencing data. From the beginning of this course to the end we want to guide you from potential scenarios like:

You don't know what to do with a set of raw sequencing files fresh from a facility like CAGEF.

- You've been handed a legacy pipeline to analyse your data or maintain for the lab, but you don't know what it runs or how.
- You plan on generating high-throughput data but there are no bioinformaticians around to help you out.

and get you to the point where you can:

- Recognize the basic tools in sequence analysis.
- Plan and write your own data analysis pipelines.
- Explain your data analysis methods to labmates, supervisors, and other colleagues.

#### 0.1.2 How do we get there?

In the first half of this course, we'll focus on how to generate analysis pipelines using the Galaxy platform – a user-friendly graphical interface that provides access to common sequence analysis tools. After we are comfortable with these tools, we'll look at life through the lens of a command-line interface. It is here that we will learn the basics of file manipulation and how to program scripts that can carry out multiple tasks for us. From there we'll revisit tools from the first half and learn skills to make your data analysis life easier.

## 0.2.0 Goals of the module

- 1. Learn how to move around your file system at the command line.
- 2. Learn how to manipulate file contents using basic commands.
- 3. Learn how to combine a series of commands in an executable bash script.
- 4. Learn how to regulate access and set permissions for files.
- 5. Learn how to run operations on a remote server through the command line.

## 0.3.0 Pre-class modules with Coursera

Each week we strongly encourage you to complete the assigned Coursera modules and/or readings **before** class. These are meant to provide you with sufficient background material on each week's module so that we can focus on the act of "doing" something with that data rather than spend a lot of time on the origins of it. You'll find a section outlining the next set of Coursera modules and readings at the end of each module.

- **0.3.1** Go to <u>www.coursera.org</u> and sign up for an account with your e-mail.
- **0.3.2** Search the following courses and enroll to audit each course (audit):
- Genomic Data Science with Galaxy, Johns Hopkins University.
- Command Line Tools for Genomic Data Science, Johns Hopkins University.

# 0.4.0 Setting up your working directory

We suggest that you create a new directory (folder) for this course directly off your root directory called "**FGDS**". Working from your root directory is not necessary, but it will make some of the aspects of the course a little easier to manage. For Mac OS users, we suggest you create this as a subfolder in your <u>user</u> directory.

- 0.4.1 Within this directory, create another directory called "**Module4**". This is where we will store the data used in this week's module.
- 0.4.2 Create a subdirectory called "**downloads**" to store the initial files as we download them before decompressing and working with them in later steps.

# 1.0.0 Navigating command-line files

This module is designed as an introduction to some of the most commonly-used commands in the bash shell for genomic data science. Depending on your application, however, there are many shell commands/options that you may find useful. You can find a more detailed summary of some of the most common shell commands in the **section 6.0.0 Appendix**.

Don't be scared to come back to this module to review commands or search new commands online in the future. I've been working at the command line on and off for years and still search and review command options all the time. Most users will not memorize all this stuff! You can also use the man command to print the manual for any given command (e.g. man cd).

## 1.0.1 Important command-line wild cards and shortcuts

While working with the command-line there are many tips and tricks we can use to describe or identify files or directories we are searching for. These wildcards are somewhat like regular expressions and let us substitute directly or indirectly for single or multiple filenames.

Command	Description
*	Universal wildcard; anything, any number of times (or nothing)
?	Universal wildcard; anything, once
[a-z]	Any letter or number in range
{a, b}	Any letter or number in list
\	Escape character; ignore special meaning
!	Invert a search

Aside from wildcards, there are also meta-characters or symbols that are used to represent simple ideas or locations when navigating the file system.

Command	Description	
	Current directory	
	Parent directory (one directory above in hierarchy)	
~	Root directory (home)	

Following these command symbols there are additional key strokes or characters that allow us to alter commands, how they are run, or stop them completely. Along with this list, we have quick keys and commands that can be used to navigate the terminal commands themselves.

Command	Description	
	Pipe output from the left-side command into right-side command	
&	Runs command in the background when placed at the end of the command	
>	Save the output of a command to a file (e.g. ls -la > allFilesList.txt)	
>>	Append the output of a command to a file (e.g. ls -la/ > allFilesList.txt)	
[Tab]	Auto complete	
[Tab+Tab]	List all auto completed files in your path	
[Ctrl+C]	Cancel a process that is currently running	
[Ctrl+Z]	Move operation into the background	
clear or [Ctrl+L]	Clear all commands and results from terminal window	
alias	Set a short form for a command or series of commands	
[↑/↓]	Scroll back through the commands you have already entered (aka History)	
[Home] or [End]	Scroll quickly to the beginning or end of a command, or character by character. Arrows	
[←/→]	can be combined with [Ctrl] for skipping between space-separated words.	

<sup>\*</sup> On Mac OS you may have to substitute the [Ctrl] for the [Cmd] key

# 1.0.2 Commands for accessing, creating, and removing content

Now that we've reviewed some basic commands syntax for identifying files and directory structures, we can look closely at the actual manipulation of directories and files.

Command/Switches	Description	
pwd	Print working directory	
ls	List files in a directory (e.g. ls –al). Run lshelp to access the manual for this command)	
-a	Include hidden files	
-1	Show dates and permissions (long listing format).	
-1	List all files on separate lines	
-S	List all files in order of descending size	
11	An aliased equivalent to the call ls -alF	
cd	Change directory – the primary way of changing your current working directory	
mkdir	Make new directory	
rmdir	Remove empty directory	
rm	Remove file	
-r	Recursive removal of all files in directory. This option may also be implemented in many	
	other Unix commands.	
-f	While removing files ignore non-existent files or arguments with prompts (or warnings)	
mv	Move a file or a folder to a new location or rename a file	
ср	Copy a file to a new location	
gzip	Compress files	
gunzip	Uncompress (extract) files	
tar	Create or expand a tar archive	
-c	Create an archive file	
-v	Verbosely show the progress	
-f	Filename of archive	
-r	Append to a specified archive	
-x	Extract an archive file	
-t	List files in an archive	
-z	Filter archive through gzip	
passwd	Change your password	
history	Access the commands that you have previously ran	
Ctrl + r	Search for a previously run command	

# 1.1.0 Explore your command-line directory with ls

Let's practice using some of these commands to navigate our directories in our home directory.

1.1.1 Open your command line prompt (Terminal or Bash) and get oriented in your file system using the pwd and 1s commands.

```
pwd
ls
ls -1  # That's a number
ls -1  # That's a letter
```

```
mokca@LAPTOP-7LF60G94:/mnt/c/FGDS$ 1s
mokca@LAPTOP-7LF60G94:/mnt/c/FGDS$ 1s
mokca@LAPTOP-7LF60G94:/mnt/c/FGDS$ 1s -1
mokca@LAPTOP-7LF60G94:/mnt/c/FGDS$ 1s -1
total 0
drwxrwxrwx 1 root root 4096 Nov 22 14:38
drwxrwxrwx 1 root root 4096 Nov 22 14:39
mokca@LAPTOP-7LF60G94:/mnt/c/FGDS$ 11
total 0
drwxrwxrwx 1 root root 4096 Nov 22 14:39
mokca@LAPTOP-7LF60G94:/mnt/c/FGDS$ 11
total 0
drwxrwxrwx 1 root root 4096 Nov 22 14:38
```

# 1.2.0 Move files and directories with mv

The mv command serves dual purposes, mainly for moving files from one place to another. As we'll see, during the process you must also specify a destination folder. You may, however, also define a destination filePath, essentially renaming the file or directory as you move it! The mv command takes on the form of:

```
mv filePathFrom filePathTo
```

Note that for directories, if your filePathTo exists, then the filePathFrom will be moved into that directory. If filePathTo does not exist, then the directory will be renamed as it is moved. Additionally, when moving files, destination files can be overwritten or replaced if filePathTo already exists!

1.2.1 If your "FGDS" directory is not already in your home directory, move it and all its contents there using the mv command.

If you are working on Windows10, you can access your entire Windows file structure from the "mnt" directory.

1.2.2 Move your FGDS directory if necessary

```
cd ~/  # Return to your home directory
mv /mnt/c/FGDS ./  # Move over the FGDS folder
```

```
mokca@LAPTOP-7LF60G94:~$ 11

total 12
drwxr-xr-x 1 mokca mokca 4096 Nov 22 14:42 ./
drwxr-xr-x 1 root root 4096 Nov 18 23:05 ../
-rw-r-r- 1 mokca mokca 4246 Nov 21 23:43 .bashrc
drwxr-xr-x 1 mokca mokca 4096 Nov 18 23:05 .cache/
drwxr-xr-x 1 mokca mokca 4096 Nov 19 16:23 .conda/
drwxr-xr-x 1 mokca mokca 4096 Nov 19 16:23 .java/
drwxr-xr-x 1 mokca mokca 4096 Nov 18 23:05 .landscape/
-rw-r-r- 1 mokca mokca 4096 Nov 18 23:05 .motd_shown
drwxr-xr-x 1 mokca mokca 4096 Nov 20 01:41 .parallel/
-rw-r-r- 1 mokca mokca 4096 Nov 20 01:41 .parallel/
-rw-r-r- 1 mokca mokca 4096 Nov 21 23:47 .sudo_as_admin_successful
drwxr-xr-x 1 mokca mokca 4096 Nov 22 14:38 .motd_as_admin_successful
drwxr-xr-x 1 mokca mokca 4096 Nov 22 10:36 anaconda3/
drwxr-xr-x 1 mokca mokca 4096 Nov 21 23:57 downloads/
mokca@LAPTOP-7LF6OG94:~$
```

# 1.3.0 Change your current directory with cd

A mainstay of moving through directories is the  $\underline{\mathbf{c}}$  hange  $\underline{\mathbf{d}}$  irectory command –  $\underline{\mathbf{cd}}$ . This will be an important tool in your belt unless you memorize the location of everything in your files.

1.3.1 Use the cd command to navigate into the **Module1** directory using an absolute path.

```
cd ~/FGDS/Module1
# The location of the FGDS folder will depend on how you've set it up
```

1.3.2 From the **Module1** directory navigate directly to the **Module3** directory using a relative path.

```
cd ../Module3
```

1.3.3 Return to the **home** directory.

```
cd ~/ # 'cd ~' will also work
```

## 1.4.0 Create new directories with mkdir

1.4.1 Create a new directory within **FGDS** for this module called **Module4**. This will require us to use the **ls**, **cd**, and **mkdir** commands, but we will also explore how the **rmdir** command works so that you know how to remove a directory. Notice your **Module4** directory is now available in our Finder/File Explorer

```
cd FGDS
ls
mkdir ModuleFour  # Make a directory
ls
rmdir ModuleFour  # Remove the directory (only if empty)
ls
mkdir Module4
ls
ls -la
cd Module4
ls
pwd  # print the current working directory
```

```
okca@LAPTOP-7LF60G94:~/FGDS$ 1s
 ookca@LAPTOP-7LF60G94:<mark>~/FGDS</mark>
ookca@LAPTOP-7LF60G94:<mark>~/FGDS</mark>
                                               $
                                                  mkdir ModuleFour
                                                  1s
 okca@LAPTOP-7LF60G94:<mark>~/FGDS</mark>
okca@LAPTOP-7LF60G94:~/FGDS
                                                  rmdir ModuleFour
                                                  ls
 okcaCLAPTOP-7LF60G94:
okcaCLAPTOP-7LF60G94:
                                                  mkdir Module4
total Ø
                                                  Nov
                                                         22
22
lrwxrwxrwx 1 mokca mokca 4096
                                         4096
                                                  Nov
drwxr-xr-x
                     mokca mokca
                                                         22
22
22
22
22
drwxrwxrwx 1 mokca mokca 4096
drwxrwxrwx 1 mokca mokca 4096
drwxrwxrwx 1 mokca mokca 4096
                                                  Nov
Nov
Nov
                                                              14:38
drwxr-xr-x 1 mokca mokca 4096
                                                  Nov
 io kca@LAPTOP
                                                  cd Module4
 nokca@LAPTOP-7LF60G94:
nokca@LAPTOP-7LF60G94:
/home/mokca/FGDS/Module4
mokca@LAPTOP-7LF6OG94:~/FGDS/Module4$
```

# 1.5.0 Copy files with cp

You should now be in the **Module4** directory. Copy **HinfKW20\_genomic.fna**, **HinfKW20\_cds.fna**, **HinfKW20\_protein.faa**, and **HinfKW20\_features.txt** files from your **Module1** directory into your **Module4** directory.

In doing so, you will experiment with the **mv**, **cp**, and **rm** commands. We will also explore how to do this all at once with wildcards. Note that both the . and [tab] meta-characters and commands can make your life a lot easier here by specifying your current location in the filesystem and auto-filling filenames, respectively. You can also scroll up and down previous commands that you want to repeat using the up  $\uparrow$  and down  $\downarrow$  arrows.

#### 1.5.1 Copy files individually from **Module1** over to **Module4**

```
pwd  # Make sure you are in the Module4 directory!
ls
ls ../Module1
cp ../Module1/downloads/HinfKW20_genomic.fna .
cp ../Module1/downloads/HinfKW20_cds.fna .
cp ../Module1/downloads/HinfKW20_rna.fna .
cp ../Module1/downloads/HinfKW20_protein.faa .
ls
```

```
mokca@LAPTOP-7LF60G94: "/FGDS/Module4$ pwd
/home/mokca/FGDS/Module4$ ls
mokca@LAPTOP-7LF60G94: "/FGDS/Module4$ ls
mokca@LAPTOP-7LF60G94: "/FGDS/Module4$ ls ../Module1

downloads/MinfKW20_genomic.fna .
mokca@LAPTOP-7LF60G94: "/FGDS/Module4$ cp ../Module1/downloads/HinfKW20_cds.fna .
mokca@LAPTOP-7LF60G94: "/FGDS/Module4$ cp ../Module1/downloads/HinfKW20_rna.fna .
mokca@LAPTOP-7LF60G94: "/FGDS/Module4$ cp ../Module1/downloads/HinfKW20_protein.faa .
mokca@LAPTOP-7LF60G94: "/FGDS/Module4$ cp ../Module1/downloads/HinfKW20_protein.faa .
mokca@LAPTOP-7LF60G94: "/FGDS/Module4$ ls
HinfKW20_cds.fna HinfKW20_genomic.fna HinfKW20_protein.faa HinfKW20_rna.fna
mokca@LAPTOP-7LF60G94: "/FGDS/Module4$ ls
```

#### 1.5.2 Remove the Module4 directory and remake it

```
cd ..  # Return to ~/FGDS/
rmdir Module4  # What happens when we use this command?
rm -r Module4
ls
```

```
mokca@LAPTOP-7LF60G94:~/FGDS$ rmdir Module4
rmdir: failed to remove 'Module4': Directory not empty
mokca@LAPTOP-7LF60G94:~/FGDS$ rm -r Module4
mokca@LAPTOP-7LF60G94:~/FGDS$ ls
mokca@LAPTOP-7LF60G94:~/FGDS$ mkdir Module4
mokca@LAPTOP-7LF60G94:~/FGDS$ cd Module4
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$
```

1.5.3 Copy all of the .fna and .faa files over from **Module1**.

```
ls

ls ../

mv HinfKW20_rna.fna ../

ls

ls ../

mv ../HinfKW20_rna.fna .

ll

mokca@LAPTOP-7LF60G94:"/FGDS/Nodule4$ cp ../Module1/downloads/HinfKW20_*.fla,nla .

mokca@LAPTOP-7LF60G94:"/FGDS/Module4$ ls

HinfKW20_cds.fna HinfKW20_genomic.fna HinfKW20_protein.faa HinfKW20_rna.fna

mokca@LAPTOP-7LF60G94:"/FGDS/Module4$ mv HinfKW20_protein.faa

mokca@LAPTOP-7LF60G94:"/FGDS/Module4$ ls

HinfKW20_cds.fna HinfKW20_genomic.fna HinfKW20_protein.faa

mokca@LAPTOP-7LF60G94:"/FGDS/Module4$ ls ../

HinfKW20_rna.fna munual munual mokca@LAPTOP-7LF60G94:"/FGDS/Module4$ mv ../HinfKW20_protein.faa

mokca@LAPTOP-7LF60G94:"/FGDS/Module4$ mv ../HinfKW20_protein.fna .

mokca@LAPTOP-7LF60G94:"/FGDS/Module4$ mv ../HinfKW20_genomic.fna .

mokca@LAPTOP-7LF60G94:"/FGDS/Module4$ l1

total 4772

drwxr-xr-x 1 mokca mokca 4096 Nov 22 15:16 //

drwxr-xr-x 1 mokca mokca 4875338 Nov 22 15:15 HinfKW20_genomic.fna*

-rwxr-xr-x 1 mokca mokca 665876 Nov 22 15:15 HinfKW20_genomic.fna*

-rwxr-xr-x 1 mokca mokca 665876 Nov 22 15:15 HinfKW20_protein.faa*

-rwxr-xr-x 1 mokca mokca 33031 Nov 22 15:15 HinfKW20_protein.faa*

mokca@LAPTOP-7LF60G94:"/FGDS/Module4$ protein.faa*

mokca@LAPTOP-7LF60G94:"/FGDS/Module4$ protein.faa*
```

# 1.6.0 Create a compressed archive with tar or gzip

You might recall that through working with our data in **Module1-3**, many of our downloads come in compressed and/or archived files. It's time for us to practice using some of the command-line tools to create and work with these space-saving files. The tar (tape archive) command provides a way to create and extract from archive files but does not *directly* compress them. The tar command takes the form of:

tar -switches archiveName archiveContents

Some useful tar command switches:

Switch/flag	Description
-ffile	The file or archive you want to specify
-tlist	List the files present in an archive
-ccreate	Create an archive
-xextract	Rather than build an archive, you can use this tag to <i>extract</i> an archive.
-vverbose	Display all of the file names in the archive
-zgzip	Filter the archive through gzip (especially great for tar.gz files). Both for compression and
	decompression depending on other flags!
-kkeep-old-files	Don't replace existing files when extracting

1.6.1 Create a **tar** archive that contains all the gene, rna, and protein sequence information that you just moved to your **Module4** directory.

```
11
tar --help
tar -cvf HinfKW20_sequences.tar HinfKW20_*
# So we want to create an archive with the specified file name
# Note how the f is on the end!
11
```

```
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$ tar -cvf HinfKW20_sequences.tar HinfKW20_*
HinfKW20_cds.fna
HinfKW20_protein.fna
HinfKW20_protein.faa
HinfKW20_protein.faa
Mokca@LAPTOP-7LF60G94:~/FGDS/Module4$ 11
total 9124
drwxr-xr-x 1 mokca mokca
drwxrwxrwx 1 mokca mokca
-rwxr-xr-x 1 mokca mokca
4096 Nov 22 15:16
-rwxr-xr-x 1 mokca mokca
1875338 Nov 22 15:15 HinfKW20_cds.fna*
-rwxr-xr-x 1 mokca mokca
1853084 Nov 22 15:15 HinfKW20_genomic.fna*
-rwxr-xr-x 1 mokca mokca
33031 Nov 22 15:15 HinfKW20_protein.faa*
-rw-r--r- 1 mokca mokca
4433920 Nov 22 15:47 HinfKW20_sequences.tar
```

The gzip command has one function – to compress or expand files using the gzip algorithm. When we are using gzip on multiple files, it will accept them as input but it will individually compress them. By default, it will replace the original file(s) with the gzipped versions (.gz).

1.6.2 Create a compressed gzip version of HinfKW20\_cds.fna and HinfKW20\_genomic.fna. Take a look at the resulting files. Now decompress the same files with gunzip.

```
gzip --help
gzip HinfKW20_cds.fna HinfKW20_genomic.fna
ll
gunzip *.gz
```

1.6.3 Create a compressed **gzip** version of the tar archive. By archiving before compressing the file, everything is kept together as a group!

```
gzip HinfKW20_sequences.tar
11
```

```
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$ gzip HinfKW20_sequences.tar
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$ 11
total 1792
drwxr-xr-x 1 mokca mokca 4096 Nov 22 15:52 ./
drwxrwxrwx 1 mokca mokca 4096 Nov 22 15:16 //
-rw-r--r- 1 mokca mokca 1481565 Nov 22 15:47 HinfKW20_sequences.tar.gz
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$
```

1.6.4 Check how much our original archive folder was compressed vs the original version.

```
gzip -l HinfKW20_sequences.tar.gz
ls -l
```

1.6.5 Unarchive and decompress your tar.gz file by using tar and filtering it through gzip.

```
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$ tar -zxvf HinfKW20_sequences.tar.gz
HinfKW20_cds.fna
HinfKW20_genomic.fna
HinfKW20_protein.faa
HinfKW20_protein.faa
HinfKW20_protein.faa
Mokca@LAPTOP-7LF60G94:~/FGDS/Module4$ 11
total 6496
drwxr-xr-x 1 mokca mokca 4096 Nov 22 16:05 ./
drwxrwxrwx 1 mokca mokca 4096 Nov 22 15:16 __/
-rwxr-xr-x 1 mokca mokca 1875338 Nov 22 15:15 HinfKW20_cds.fna*
-rwxr-xr-x 1 mokca mokca 1853084 Nov 22 15:15 HinfKW20_genomic.fna*
-rwxr-xr-x 1 mokca mokca 665876 Nov 22 15:15 HinfKW20_protein.faa*
-rwxr-xr-x 1 mokca mokca 33031 Nov 22 15:15 HinfKW20_protein.faa*
-rw-r--r-- 1 mokca mokca 1481565 Nov 22 15:47 HinfKW20_sequences.tar.gz
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$
```

1.6.6 Prior to this we used both tar and gzip to accomplish the creation of a tar.gz file but much like our last call, we can create a compressed archive tar.gz file by using tar and filtering it through gzip.

```
ls -l
```

1.6.7 How do we view the contents of a tar.gz file? We already know how to do it with a .gz file. Let's compare

# 2.0.0 Viewing and manipulating file contents

Now that you have a sense of how you can move around your file system to create and remove content, let's look at some important commands for viewing and manipulating file contents. There are different terminal commands that can be used to quickly view, edit, summarize, combine, and search content.

## 2.1.0 Use the less command to view content

The **less** command allows you to view the contents of a file by moving through it both forward and backwards. It comes equipped with hot-keys or commands that make it easy to navigate your text files one at a time.

Keys	Description	
[Arrow keys],	Navigate around the page in a forwards or backwards direction	
[space], [page-up],		
[page-down]		
b	Return to previous page	
Line_numg	Jump to a line number, default is the start of the file (e.g. 1000g)	
Line_numG	Jump to a line number, default is the end of the file (e.g. 46G)	
/	Search for text in the file (e.g. /ribonuc)	
n	Find next occurrence	
?	Find previous occurrence	
-N	Display the line numbers in your file	
q	Exit the file	

- 2.1.1 Copy the **HinfKW20\_features.txt** file from your **Module1** directory into your **Module4** directory with the cp command. Then create a copy of this file titled **HinfKW20\_features\_copy.txt**
- 2.1.2 Explore the **HinfKW20\_features\_copy.txt** file with the **less** command. Jump to line **1000** and then search for the genes **mutS** and **2-isopropylmalate**.

```
less HinfKW20 features copy.txt
                                                            # Display line numbers in the file
        -N
        1000g
                                                            # Go to line 1000
                                                            # Look for the mutS gene
        /mutS
        /2-isopropylmalate
                                                            # Look for 2-isopropylmalate
                                                            # quit less
                                                                                        L42023.1
                                                             chromosome
ropylmalate synthase (leuA)
                                                                                        L42023.1
                                                                   chromosome
HI_0987 1077
                                                              chromosome
opylmalate dehydrogenase (bet
                                                                                        L42023.1
                                                                                                      10462
                                                                   chromosome
HI_0988 1410
                                                                                                      10462
                                                     Assembly chromosome L42023.1
3-isopropylmalate dehydratase, alpha subunit (leuC)
                                                                                        L42023.1
                                                                                                      10476
```

2.1.3 Comprehension challenge: on what line would you find "galactoside ABC transporter, ATP-binding protein"?

# 2.2.0 Use vi to edit your text files

The text editor **vi** is a standard component of the Linux operating system and was created in 1976. While intimidating at first, this can be a very helpful editor when working with your files.

Key	Description
Arrow keys	Move around the file
i	Editing mode. This is great for preventing accidental changes to your file!
esc	Exit editing mode
:q	Quit – this will produce a warning if you made changes.
:q!	Quit the file and discard changes
:w filename	Save to filename
:w! filename	Overwrites to filename
:wq	Save and exit the file
:colorscheme[space][tab]	Get a selectable list of colour themes
:color <theme></theme>	Directly select a colour theme

2.2.1 Open up the file in vi and delete the header of the file **HinfKW20\_features\_copy.txt**. Save it and compare file sizes with the original.

```
Move around the file with arrow keys, ctrl and shift

i  # Enter edit mode

Remove some of the header line with [backspace]

[Esc]  # Exit editing mode

dd  # delete the entire header line
:wq  # Save changes and quit vi

ll

mokcaelAPTOP-7LF60G94: */FGDS/Module45 11

total 6692
drwxr-xr-x 1 mokca mokca 4096 Nov 22 18:49
drwxr-xr-x 1 mokca mokca 466933 Nov 22 15:15
-rwxr-xr-x 1 mokca mokca 466933 Nov 22 15:15
-rwxr-xr-x 1 mokca mokca 466933 Nov 22 18:49
-rwxr-xr-x 1 mokca mokca 466933 Nov 22 15:15
-rwxr-xr-x 1 mokca mokca 665876 Nov 22 15:15
-rwxr-xr-x 1 mokca mokca 665876 Nov 22 15:15
-rwxr-xr-x 1 mokca mokca 665876 Nov 22 15:15
-rwxr-xr-x 1 mokca mokca 1853084 Nov 22 15:15
-rwxr-xr-x 1 mokca mokca 1855056 Nov 22 15:15
-rwxr-xr-x 1 mokca mokca 185506 Nov 22 15:15
```

# 2.3.0 Concatenate files directly with cat

The cat command is useful when working with multiple files (like sequencing data) that you'd like to combine into a single file. Likewise, header-less data sets can be combined without opening an editor, copying, pasting, saving, etc.

2.3.1 Concatenate the **HinfKW20\_cds.fna** and **HinfKW20\_rna.fna** files together to get all these sequences into a single file.

# 2.4.0 Use grep to search through a file

We spent some time in Module 1 going over regular expressions when editing text. We saw how powerful it could be to use this language to search through our text files. grep is an essential command-line utility which has its origins in Unix but is now available for all Unix-like systems and exists in variant forms even in the Windows environment and many programming languages. grep generally takes the form of:

grep	-switches	"searchPattern"	filePath
------	-----------	-----------------	----------

Switches	Description	
-E	Use full regular expressions as defined in the bash shell	
-P	Use Perl-compatible regular expressions	
-i	Match without regard to case	
<b>-</b> ₩	Invert the search	
-c	Count the results in the file	
-1	List only file names containing matches	
-h	Hide filenames in the output	

2.4.1 Count all the *unique* lines containing occurrences of tRNA and rRNA from the **HinfKW20\_features\_copy.txt** file using the **grep** command and in doing so, explore the functionality of the > and >> redirectors.

```
ls -l *.txt
```

```
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$ 11 *.txt
-rwxr-xr-x 1 mokca mokca 466933 Nov 22 16:46 HinfKW20_features.txt*
-rwxr-xr-x 1 mokca mokca 466703 Nov 22 18:49 HinfKW20_features_copy.txt*
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$ grep -ci "tRNA" HinfKW20_features_copy.txt
67
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$ grep -ci "rRNA" HinfKW20_features_copy.txt
38
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$
```

2.4.2 Redirect the output of **grep** to a file using the > redirectors. Notice how the output of the grep command looks? The output highlights in red all occurrences of our search pattern, even if they should appear on multiple lines! Are we retrieving only **tRNA** features?

```
grep -in "tRNA" HinfKW20_features_copy.txt # Note the output!
grep -i "tRNA" HinfKW20_features_copy.txt > HinfKW20_tRNA_features.txt
ls -l *.txt
```

2.4.3 Append the output of grep to a file using the >> redirectors. Rather than overwriting our destination file, we can append to our HinfKW20\_tRNA\_features.txt using the correct redirection symbol. Then we'll rename the file with the mv command.

```
grep -i "rRNA" HinfKW20_features_copy.txt
mv HinfKW20_tRNA_features.txt HinfKW20_RNA_features.txt
```

```
less HinfKW20_RNA_features.txt
ls -l *.txt
```

2.4.4 How do we ensure we are counting only tRNA or rRNA features from our file? Based on our earlier grep output, it appears that feature types will either occur at the beginning of a line or in the second column. Here we can turn to Perl-compatible regular expressions with the -p switch. Remember what we learned earlier in **Module 1**?

**Stick with the -P!** By using PCRE we are able to use meta characters like tabs (\t) and spaces (\s)! There are other methods for utilizing tabs as well but they can be a little more complex. Using PCRE opens up additional features not provided by basic regular expressions (default) or even extended (-E) regular expressions.

# 2.5.0 Count words and lines with wc

Whenever you want to quickly investigate a file, the output of a command, or track how a file might be updating from another process, you can use the wc (word count) command to check the number of words, lines, or characters. This command generally takes the form of:

wc -switches filePath

Switches	Description
-1	Count the number of lines
-M	Count the number of words
-m	Count the number of characters

2.5.1 Count the number of words and lines in **HinfKW20\_cds.fna** using the wc command.

2.5.2 Count and compare the number of features in the <code>HinfKW20\_cds.fna</code>, the <code>HinfKW20\_rna.fna</code>, and the <code>HinfKW20\_protein.faa</code> files by combining the <code>grep</code> command and the <code>wc</code> command using <code>I</code>. The pipe symbol (<code>I</code>) redirects output from one command to the next, taking the place of input (ie <code>filePath</code> in this case).

Note that all fasta file entry headers start with the > symbol and that that grep -c ">" filename would also have worked here, but we wouldn't have gotten to see how I can be used to combine commands.

# 2.6.0 Quickly extract from tabular data with cut

When you generate data that might be in a tabular format, you may wish to look at specific columns or change the delimiter of the file (csv versus tsv, etc.). This may be after a series of commands or as part of a series where you wish to reformat or isolate output on the fly. The cut command takes the form of:

Cut	-switches	parameters	filePath
Cut	DWILCUILCD	Parameters	T T T C T a C I I

Key	Description
-f,fields=LIST	Specify columns to return (comma-separated list)
-d,delimiter=DELIM	Specify delimiter used to read/identify columns (tab is default)
-c,characters=LIST	Specify range of characters to use (don't use on tabular data!)
output-delimiter=STRING	Specify the type of delimiter to use for resulting output

2.6.1 Generate a simplified gene features file that only contains essential information regarding where and what each CDS feature is using the cut command. Call this new file HinfKW20\_features\_simple.txt.

```
ls -l *.txt
grep -i "CDS" HinfKW20_features_copy.txt
grep -i "CDS" HinfKW20_features_copy.txt |
grep -i "CDS" HinfKW20_features_copy.txt |
HinfKW20_features_simple.txt
less HinfKW20_features_simple.txt
ls -l *.txt
```

```
L42023.1 79805 80245 - predicted coding region HI0074 HI_0074
L42023.1 80526 82649 + anaerobic ribonucleoside-triphosphate reductase (nrdD) HI_0075
L42023.1 82667 83627 + acyl-CoA thioesterase II (tesB) HI_0076
L42023.1 83638 84504 + predicted coding region HI0077 HI_0077
L42023.1 84580 85959 - cysteinyl-tRNR synthetase (cysS) HI_0078
L42023.1 86062 86571 + peptidyl-prolyl cis-trans isomerase B (ppiB) HI_0079
L42023.1 86575 87006 + conserved hypothetical protein HI_0080
L42023.1 87148 87936 + conserved hypothetical protein HI_0081
L42023.1 88193 88459 + predicted coding region HI0082 HI_0082
```

# 2.7.0 Sort your data with sort

You want to quickly **sort** your tabular data in ascending or descending order. Again, this could be pre-, post-or mid-pipeline. The **sort** command takes the form of:

sort -switches parameters filePath

Switches	Description
-k	Specify specific column number to sort by
-t	Specify delimiter to separate columns
-n	Sort by numerical string value
-r	Sort in reverse order

2.7.1 Sort the output **HinfKW20\_features\_simple.txt** file by feature name rather than by their location in the genome using the **sort** command.

2.7.2 Sort the output **HinfKW20\_features\_simple.txt** file by column 3 using the **sort** command using both the string and numerical string values.

```
sort -k 3 HinfKW20_features_simple.txt | less
```

You may notice that there is a big difference between out two kinds of sorts. In the one instance, it's more of an alphabetical sort, not accounting for the context of non-leading 0 numbers. In the latter case, the -n switch attempts to give context to the column values by assuming these are numerical values!

# 3.0.0 Creating bash scripts and regulating access to files or programs

We are now going to learn how to combine commands into some simple scripts and how to regulate file access. This is where understanding your file system and directory tree really comes into play. Just like when you are in a Finder or File Explorer window, you can't open a file or run a program that is not in your current folder, but there are ways to manage this effectively. To begin, let's review some more helpful commands and files that are part of your Linux OS.

Command	Description	
bash	Execution command (e.g. bash script.sh).	
sudo	Super user permissions for system files (e.g. sudo rm systemfile.txt).	
\$PATH	Directories whose files or programs can be accessed from anywhere on your system.	
.bash_profile/	Configuration script file in your root directory that is run every time you enter the shell. It is used to modify your \$PATH (.bash profile for MAC and .bashrc for LINUX).	
.bashrc		

# 3.1.0 Alter file permissions with chmod

When working with files, there are three general tasks you'd like to do with your files: read, write, and execute (if they are programs). In order use any of these options, a file must have those specific permissions enabled. Furthermore, every file keeps track of the general types of people (levels) that can access it: you (user), groups who own/share the file with you (group), and world-wide access or other users on the system (other).

Switches/Syntax	Description	
+, -, =	Add, subtract, or set directly the permissions of a level	
u, g, o, a	Level tags for user, group, other, or all	
r, w, x	Permission tags to set for read, write, and execute	
4, 2, 1	The octal values for read, write, and execute. These can be added to make specific combinations of permissions ie 6 -> read and write, vs 7 -> read, write, and execute and are set in a three-digit value to represent user/group/other	

#### When using the chmod command, it takes the general form of

chmod options level=permissions, level2=permissions, level3=permissions filePath

or

chmod options 3-digit-octal filePath

Let's try some examples and see how it works in more detail.

3.1.1 **chmod** the permissions of all txt files to read for all levels and write only for the user.

```
11 *.txt
chmod u=rw,g=r,o=r *.txt
11 *.txt
```

3.1.2 **chmod** the permissions of all txt files with octal to read and write for user and group levels only and read access for other.

```
chmod 664 *.txt
11 *.txt
```

# 3.2.0 Generating your first bash script

A bash script is a plain text file that carries a series of commands that can be executed by the command-line. All the calls we have been working with, can be included in a bash script to run and manipulate our files. Any commands from your bash script can be run directly in the command-line interface. We combine these commands into a single bash script to save time and "automate" our commands.

3.2.1 Create a new file titled **bash\_script.sh** in a new directory titled **scripts**. This directory should be a subdirectory in the **Module4** directory. **sh** is an extension that is commonly applied to executable bash scripts. Make this file executable for all users with **chmod**. Note how the permissions on the file have changed.

```
mkdir scripts
cd scripts
vi bash_script.sh
    :wq
11
```

```
mokca@LAPTOP-7LF6OG94:~/FGDS/Module4$ mkdir scripts
mokca@LAPTOP-7LF6OG94:~/FGDS/Module4$ cd scripts
mokca@LAPTOP-7LF6OG94:~/FGDS/Module4/scripts$ vi bash_scripts.sh
mokca@LAPTOP-7LF6OG94:~/FGDS/Module4/scripts$ 11
total 0
drwxr-xr-x 1 mokca mokca 4096 Nov 23 12:44 ./
drwxr-xr-x 1 mokca mokca 4096 Nov 23 12:44 ../
-rw-r--- 1 mokca mokca 0 Nov 23 12:44 bash_scripts.sh
mokca@LAPTOP-7LF6OG94:~/FGDS/Module4/scripts$ chmod a+rwx bash_scripts.sh
mokca@LAPTOP-7LF6OG94:~/FGDS/Module4/scripts$ 1s -1
total 0
-rwxrwxrwx 1 mokca mokca 0 Nov 23 12:44 bash_scripts.sh
mokca@LAPTOP-7LF6OG94:~/FGDS/Module4/scripts$
```

# 3.3.0 Edit your bash script

Now that we have our bash script file, we can edit it again with vi to add some commands. We're going to include the following text in our bash script which will count the number of files in a directory and then count the number of lines, words, and characters in each file.

This script can then be run using the **bash** command. Recall that the **vi** command gets you into the script, the **i** key allows you to insert text into the file, the **esc** key cancels insert mode, and the **:wq** command sequence allows you to **w**rite (save) the script and **q**uit.

In many programming languages, everything to the right of a # (pound) sign within a script file is ignored (not interpreted nor executed). This feature allows us to add comments to our code to make more readable and easier to understand, without introducing bugs in our code

```
#! /bin/bash # this is called a shebang. Tells the system that this is a UNIX
    executable file

echo "This is how many files are in your directory:"
ls | wc -l # list files and pipes its output to count lines

echo "This is the number of lines, words, and characters in each file:"
# echo prints text into the console

for file in * # this is something called a for loop
do
wc -l $file # The $ refers to each file detected by out for loop
wc -w $file
wc -m $file
done
```

3.3.1 Open up vi, edit the file, insert the above code and save the file.

```
vi bash_script.sh
    i
    # copy and paste the above code into vi
    <esc>    # escape insert (writing mode)
    :wq    # save (write) changes and quit
less bash_script.sh
```

```
mokca@LAPTOP-7LF60G94:~/FGDS/Module4/scripts$ 11

total 0

drwxr-xr-x 1 mokca mokca 4096 Nov 23 13:19 ./

drwxr-xr-x 1 mokca mokca 4096 Nov 23 12:44 ../

-rwxrwxrwx 1 mokca mokca 384 Nov 23 13:18 bash_script.sh*

mokca@LAPTOP-7LF60G94:~/FGDS/Module4/scripts$ bash bash_script.sh

"This is how many files are in your directory:"

1

"This is the number of lines, words, and characters in each file:"
12 bash_script.sh
79 bash_script.sh
376 bash_script.sh
```

# 3.4.0 Run your bash script from other directories

Now try running the script from your **Module4** directory. This won't work unless you specify the absolute or relative path to your script. When you do specify the relative path, the script will run on your current directory. However, it won't be able to give you file sizes for any sub-directories like **scripts**.

3.4.1 Run your bash script from a different directory. You'll want to properly locate it by absolute or relative location.

```
nokca@LAPTOP-7LF60G94:^
                                                                                                                                                                                          <mark>le4</mark>$ bash bash_script.sh
  bash: bash_script.sh: No such file or directory
mokca@LAPTOP-7LF6OG94:~/FGDS/Module4$ bash scripts/bash_script.sh
"This is how many files are in your directory:"
This is how many files are in your directory:

'This is the number of lines, words, and characters in each file:

'This is the number of lines, words, and characters in each file:

195 HinfkW20_RNA_features.txt
12567 HinfkW20_RNA_features.txt
22557 HinfkW20_all.fna
36029 HinfkW20_all.fna
1908369 HinfkW20_cds.fna
36349 HinfkW20_cds.fna
35434 HinfkW20_cds.fna
35434 HinfkW20_cds.fna
35521 HinfkW20_features.txt
52198 HinfkW20_features.txt
466933 HinfkW20_features.txt
466933 HinfkW20_features.copy.txt
52177 HinfkW20_features_copy.txt
1709 HinfkW20_features_cimple.txt
14998 HinfkW20_features_simple.txt
14998 HinfkW20_features_simple.txt
14998 HinfkW20_features_simple.sortedbyproduct.txt
14998 HinfkW20_features_simple_sortedbyproduct.txt
14998 HinfkW20_features_simple_sortedbyproduct.txt
22878 HinfkW20_genomic.fna
22885 HinfkW20_genomic.fna
22885 HinfkW20_genomic.fna
22837 HinfkW20_protein.faa
22347 HinfkW20_protein.faa
2347 HinfkW20_protein.faa
3051 HinfkW20_protein.faa
3055 HinfkW20_protein.faa
3057 HinfkW20_protein.faa
3058 HinfkW20_protein.faa
3059 HinfkW20_protein.faa
3051 HinfkW20_protein.faa
    0 scripts
      c: scripts: Is a directory
    0 scripts
wc: scripts: Is a directory
    0 scripts
      nokcaCLAPTOP-7LF6OG94:~/FGDS/Module45
```

# 3.5.0 Add scripts to your \$PATH variable to access them anywhere

As you can see from our above example, when using the bash script we generated, it is important to know where the script is located. However, navigating to the location of a script when you are in a completely different directory can make your commands quite long. You can get around this by storing scripts close to the root or home directory OR you can make them part of your **SPATH** variable.

The **\$PATH** environmental variable is an **ordered** list of paths that Linux will search through for executables when running a command. You do not need to include the executable itself but just the directory where it is located.

3.5.1 Add the scripts directory to your **\$PATH** so that any script in the directory **scripts** can be run from anywhere on your system without having to specify the absolute or relative path to the script. You will need to edit your **\$PATH** through your **.bash\_profile** (Mac OS) or **.bashrc** (Windows/linux) to accomplish this.

# 3.5.2 Source your .bash\_profile or .bashrc file and confirm it has been changed.

```
source .bashrc  # macOS: source .bash_profile
echo $PATH
cd FGDS/Module4
bash bash_script.sh
```

```
nokadinPlOP-7LF60G94: "VEORS Modules" echo SPATH
/hone/moka-/anaconda3/condabin:/usr/local/sbin:/usr/local/sbin:/usr/bin:/usr/sbin:/usr/sbin:/usr/games:/usr/local/gam
es:/mnt/c/Program Files/WindowsApps/CanonicalGroupLinited.Ubuntu28.044n/Windows_2004.2021.825.0_x64_79rhkp1fndgsc:/mnt/c/Windows.common Files/oracle/Java/javapath:/mnt/c/WINDOWS/system32:/mnt/c/WINDOWS/system32/WindowsPowerShell/vi.0:/mnt/c/WINDOWS/system32:/mnt/c/WINDOWS/system32.WindowsPowerShell/vi.0:/mnt/c/WINDOWS/system32.VopenSSH:/mnt/c/Program Files/Intel/Winter/spare Files/Common Files/Intel/WintelssCommon-mnt/c/Program Files/Minter/bin/x64*/mnt/c/Program Files/Intel/Winter/spare Files/Intel/Intel(R) Management Engine
Components/DAL:/mnt/c/Users/mokca/AppData/Local/GitHubDesktop/
bin:/mnt/c/Program Files/Intel/Winter/mikter/spare/mokca/AppData/Local/GitHubDesktop/
bin:/mnt/c/Program Files/Intel/Winter/mikter/spare/mokca/AppData/Local/GitHubDesktop/
bin:/mnt/c/Program Files/Intel/Winter/mokca/AppData/Local/GitHubDesktop/
bin:/mnt/c/Program Files/Intel/Winter/mokca/AppData/Local/GitHubDesktop/
bin:/mnt/c/Program Files/Intel/Winter/mnt/c/Program Fil
```

# When you use CTRL + C instead of copying using right click



# 4.0.0 Running operations on a remote server

The last thing we are going to learn today is how to access data and perform operations on a remote server. Genomic data and analyses often occur on remote servers that have more storage and computing power than your personal computers. Here are some important commands for running operations on remote servers:

Switches/Syntax	Description	
ssh	Start a secure remote shell connection (e.g. ssh fgds@142.150.214.76 -p 24)	
-p	Specify the port to use	
	Start a file transfer remote shell connection	
sftp	(e.g. sftp -oPort=24 fgds@142.150.214.76)	
get	Transfer from the server to your computer (e.g. get HinfKW20_cds.fna)	
put	Transfer from your computer to the server (e.g. put HinfKW20_cds.fna)	
1	Place before any command to run it on your computer rather than the server (e.g. 1cd)	
quit	Close the sftp connection	
scp	Securely copy files to/from remote location (e.g. scp HinfKW20_cds.fna fgds@142.150.214.76/home/HinfKW20_cds.fna)	

# 4.1.0 Connect and explore with ssh

We can use the secure shell protocol to communicate between two computers. This is more commonly known as **ssh** and uses an encrypted connection that is suitable for even on insecure networks. We'll briefly explore the basics of using **ssh** to connect, alter and explore another system.

4.1.1 Connect to our course server through an ssh connection and create a new directory for yourself with an empty file using mkdir and vi. Make sure to replace the directory name with your own name after "cagef fgds". You will always disconnect from a server using the exit command.

```
ssh fgds@142.150.215.32
        PW = fall2022
mkdir cagef_fgds_your_name
cd cagef_fgds_your_name
vi myemptyfile.txt
        :wq
ls -l
exit
```

```
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$ ssh fgds@142.150.215.32
fgds@142.150.215.32's password:
Activate the web console with: systemctl enable —now cockpit.socket

Last login: Tue Nov 23 14:48:01 2021 from 76.69.117.7
[fgds@esc4037-hopper-guttman ~1$ mkdir cagef_fgds_calvinmok
[fgds@esc4037-hopper-guttman ~1$ cd cagef_fgds_calvinmok
[fgds@esc4037-hopper-guttman cagef_fgds_calvinmok]$ vi myemptyfile.txt
[fgds@esc4037-hopper-guttman cagef_fgds_calvinmok]$ ls -1
total 0
-rw-rw-r--. 1 fgds fgds 0 Nov 24 19:13 myemptyfile.txt
[fgds@esc4037-hopper-guttman cagef_fgds_calvinmok]$ exit
logout
Connection to 142.150.215.32 closed.
mokca@LAPTOP-7LF60G94:~/FGDS/Module4$
```

# 4.2.0 Send and retrieve files with sftp

The sftp or SSH File Transfer Protocol (aka Secure File Transfer Protocol) is another network protocol that uses ssh to facilitate file access, transfer, and management. This protocol uses the user-authenticated credentials required for an SSH connection.

4.2.1 Connect to our course server through a sftp connection and exchange content using the get and put commands. Note that all basic commands will apply to the server, but you can interact with your local computer by placing a "1" before the command when you're in a sftp connection.

```
cd cagef_fgds_your_name # replace with your own name
ls
get myemptyfile.txt # "get" downloads myemptyfile.txt
lls # the preceding "l" points to your local computer (e.g. your laptop)
put HinfKW20_rna.fna # "put" uploads HinfKW20_rna.fna to the server
ls
exit
```

#### That's it (for today)!



# 5.0.0 Class summary

That concludes our fourth lecture and introduction to the command-line tools and file structure. Next module we will take a closer look at installing programs in various ways through the command-line and contrast how some methods may be more appropriate to different needs of the data scientist. Altogether we've explored the following in this module:

- File and directory creation.
- Altering file content and file permissions.
- Running basic command-line tools for viewing and summarizing files.
- Creating your first bash script
- Setting up your **\$PATH** variables
- Connecting to remote systems with ssh and sftp

## 5.1.0 Post-lecture assessment (10% of final grade)

Soon after this lecture, a homework assignment will be made available on Quercus in the assignment section. It will build on the ideas and/or data generated within this lecture. Each homework assignment will be worth 10% of your final mark. If you have assignment-related questions, please try the following steps in the order presented:

- Check the internet for a solution read forums and learn to navigate for answers.
- Generate a discussion on Quercus outlining what you've tried so far and see if other students can contribute to a solution.
- Contact course teaching assistants or the instructor.

# 5.2.0 Suggested class preparation for Module 5

Next week we will begin exploring installations in the command-line interface and learning navigate our way through the spaghetti-string connections that result. There is nothing to help prepare for this except raw experience and lots of googling.

You will also have to install a package named Anaconda ahead of time. This will make your life much easier. Instructions will be sent through Quercus.



# Appendix 1: Shell (Terminal) Commands

From Haddock & Dunn. 2011. Practical Computing for Biologists. Sinauer Assoc. Sunderland MA

Terminal operations are described in Chapters 4–6, 16, and 20. Many of the built-in bash shell commands are summarized here for quick reference. To get more information about a command and its options, type man, followed by the name of the command. If you are not sure which command applies, you can also search the contents of the help files using man –k followed by a keyword term.

Command	Description	Usage
ls	List the files in a directory  Parameters that follow can be folder names (use * as a wildcard)  -a Show hidden files -1 Show dates and permissions -1 List the file names on separate lines. Useful as a starting point for regexp into a list of commands -G Enable color-coding of file types -F Show a slash after directory names	<pre>ls -la ls -1 *.txt ls -FG scripts ls ~/Documents ls /etc</pre>
cd	Change directory Without a slash, names are relative to the current directory With a preceding slash (/) names start at the root level Tilde (~/) starts at the user's home directory Two dots () goes "up" to the enclosing directory One dot refers to the current directory Minus sign goes to the previously occupied directory Use tab key (see below) to auto-complete partially typed paths Use backslash before spaces or strange characters in the directory name, or put the whole name in quotes	<pre>cd scripts cd /User cd ~/scripts cd My\ Documents cd 'My Documents' cd/ cd cd -</pre>

Command	Description	Usage		
pwd	Print the wo	Print the working directory (the path to the folder you are in)		
<b>↑</b>	↑ key to step back through previously typed commands  The cursor can be repositioned with the ← and → keys, and commands can then be edited  Press return from anywhere in the line to re-execute. On OS  X you can also reposition by option -clicking at a cursor location			
tab	Auto-compl line	ete file, folder, or script names at the command	cd ~/Doc tab	
less	Show contents of a file, page by page These commands also apply to viewing the results of man While less is running:		less data.txt	
	q	Quit viewing		
	space	Next page		
	b	Back a page		
	15 g	Go to line 15		
	G	Go to the end		
	↑ or ↓	Move up or down a line		
	/abc	Search file for text abc		
	n	After an initial search, find next occurrence of the search item		
	?	Find previous occurrence of the search item		
	h	Show help for less		
mkdir	Make a new	directory (a new folder)	mkdir scripts	
rmdir	Remove a d	irectory (folder must be empty)	rmdir ~/scripts	
rm	Remove file or files  Use the -f flag to delete without confirmation (careful!)  Use the -r flag to recursively delete the files in a directory and then the directory itself  rm test.txt  rm -f *_temp.dat			
man	Show the manual pages for a Unix command man mkdir Use -k to search for a term within all the manuals man -k date The result is displayed using the less command above, so the same shortcuts allow you to navigate through		man -k date	

Command	Description	Usage
ср	Copy file, leaving original intact Does not work on folders themselves Single period as destination copies file to current directory, using same name	<pre>cp test1.txt test1.dat cp temp/temp cp/test.py .</pre>
mv	Move file or folder, renaming or relocating it Unlike cp, this does work on directories	<pre>mv test1.txt test1.dat mv temp/temp2</pre>
1	Pipe output of one command to the input of another command	history   grep lucy
>	Send output of a command to a file, overwriting existing files  Do not use a destination file that matches a wildcard on the left side	ls -1 *.py > files.txt
>>	Send output of a command to a file, appending to existing files	echo "#Last line" >> data.txt
<	Send contents of a file into command that supports its contents as input	mysql -u root midwater < data.sql
./	Represents the current directory in a path—the same location as pwd  Trailing slash is optional  Can execute a file in the current directory even when the file directory is not included in the PATH	<pre>cp/*.txt ./ ./myscript.py</pre>
cat	Concatenate (join together) files without any breaks. Streams the contents of the file list across the screen	cat README cat *.fta > fasta.txt
head	Show the first lines of a file or command Use the -n flag to specify the number of lines	head -n 3 *.fasta ls *.txt   head
tail	Show the last lines of a file or output stream  Use the -n flag to specify the number of lines to show  With a plus sign, skip that number of lines and show to the end. Use -n +2 to show from the second line of the file to the end, skipping one header line	tail -n 20 *.fta tail -n +3 data.txt
wc	Count lines, words, and characters in an output stream or file	wc data.txt ls *.txt   wc
which	Show the location of executable files in the system path	which man

Command	Description Usage		
grep	Search for phrase in a list of files or pipe and show matching lines:  grep -E "searchterm" filelist  Often used in conjunction with piped output: command   grep searchterm  Use quotes around search terms, especially spaces or punctuation like >, &, #, and others  To search for tab characters, type ctrl V followed by tab inside the quotes  Optional flags:		
	-c Show only a count of the results in the file		
	<ul> <li>-v Invert the search and show only lines that do not match</li> <li>-i Match without regard to case</li> </ul>		
<ul> <li>Use full regular expressions Terms should be enclosed in quotes. Use [] to indicate a character range rather than the wildcards of Chapters 2 and 3 General wildcard equivalents: \s [[:space:]] \w [[:alpha:]] \d [[:digit:]] </li> <li>List only the filenames containing matches</li> </ul>			
	<ul><li>-n Show the line numbers of the match</li><li>-h Hide the filenames in the output</li></ul>		
agrep	Search for approximate matches, allowing insertions, deletions, or mismatched characters. (Must be installed separately.) See Chapter 21  Optional flags include:  -d ", " Use comma as delimiter between records  -2 Return results with up to 2 mismatches.  Maximum is 8 mismatches  -B -y Return the best match without specifying a number of mismatches  -1 Only list file names containing matches  -i Match without regard to case	agrep -d "\>" -B -y ATG seqs.fta agrep -3 siphonafore taxa.txt	
chmod	Change access permissions on a file (usually to make a script executable or Web accessible)  First option is one of u, g, o for user, group, other  Second option after the plus or minus is r, w, or x, for read, write, or execute. Can also use binary encoding as explained in Appendix 6	chmod u+x file.pl chmod 644 myfile.txt chmod 755 myscript.py	

Command	Description	on	Usage
set	Show environmental variables, including functions that have been defined		
\$HOME	The enviro	nmental variable containing the path user's home	echo \$HOME cd \$HOME
\$PATH		PATH variable, where the directories to search for ads are stored	export PATH=\$PATH:/usr/local/bin
nano	Invoke the	text editor. Control key sequences include:	nano filename.txt
	<i>ctrl</i> X	Exit nano (will be prompted to save)	
	ctrl O	Save file without exiting	
	<i>ctrl</i> Y	Scroll up a page	
	<i>ctrl</i> V	Scroll down a page	
	ctrl C	Cancel operation	
	ctrl G	Show help and list of commands	
ctrl C	Interrupt t	he current process	
sort	Sort lines of a file		sort -k 3 data.txt
	-k <i>N</i>	Sort using column number N instead of starting at the first character. Columns are delimited by a series of white space characters	<pre>sort -k 2 -t "," F1.csv sort -nr numbers.txt sort A.txt &gt; A_sort.txt</pre>
	-t ","	In conjunction with —k, use commas as the delimiter to define columns	
	-n	Sort by numerical value instead of alphabetical	
	-r	Sort in reverse order	
	-u	Return only one unique representative from a series of identical sorted lines	
uniq	in a file of anywher to the u	ingle line for each consecutive instance of that line or output stream. To remove all duplicates from re in the file, it must be sorted before being piped miq command g to return a count along with the repeated	uniq -c records.txt sort names   uniq -c

Command	Description	Usage
cut	<ul> <li>Extract one or more columns of data from a file</li> <li>-f 1,3 Return columns 1 and 3, delimited by tabs</li> <li>-d "," Use commas as the field delimiter instead of tabs. Used in combination with -f</li> <li>-c 3-8 Return characters 3 through 8 from the file or stream of data</li> </ul>	<pre>cut -c 5-15 data.txt cut -f 1,6 data.csv cut -f2 -d ":" &gt; Hr.txt</pre>
curl	Retrieve the contents of a URL from over the network. URL should be placed in quotes. Without additional parameters, will stream contents to the screen  For some Linux versions, wget offers similar functionality  See man curl for ways to send user login information at the same time  -o Set the name of the output file to save individual files for the data. See #1 below  -m 30 Set a time out of 30 seconds  [01-25] In the URL, substitute two digit numbers from 01 to 25 into the address in succession  {22,33} Substitute items in brackets into URL  {A,C,E}  #1 The substituted value, for use in generating the filename	<pre>curl "www.myloc.edu" &gt;   myloc.html curl "http://www.nasa.   gov/weather[01-12]   {1999,2000}" -m 30   -o weather#1_#2.dat</pre>
sudo	Run the command that follows as a superuser with privileges to write to system files	<pre>sudo python setup.py install sudo nano /etc/hosts</pre>
alias	Define a shortcut for use at the command line. To make alias cx='chmod u+x' persistent, add to startup settings file .bash_profile or equivalent	
function	Create a shell function—like a small script myfunction() { \$1 is the first user argument supplied after the command is typed # insert commands here echo \$1 \$0 is all the parameters—useful for loops as below Variable names are defined with the format NAME= with no spaces. They are retrieved with \$NAME Save it in .bash_profile to make it permanent	
;	In a command or script, equivalent to pressing return and starting a new line	date; ls

Command	Description	Usage
for	Perform a for loop in the shell. Can be useful in the context of a function	for ITEM in *.txt; do echo \$ITEM done
if	An if statement in a shell function:  if [ test condition ]  then  # insert commands  else  # alternate command  fi  Comparison operators are eq for equals, 1t for less than and gt for greater than	<pre>if [ \$# -lt 1 ] then   echo "Less than" else   echo "greater than 1" fi</pre>
` `	Backtick symbols surrounding a command cause the com- mand to be executed and then substitute the output into that place in the shell command or script	<pre>cd `which python`/ nano `which script.py`</pre>
host	Return IP number associated with a hostname, or the hostname associated with an IP address, if available	host www.sinauer.com host 127.0.0.1
ssh	Start a secure remote shell connection	ssh lucy@pcfb.org
scp	Securely copy files to or from a remote location	<pre>scp localfile user@host/path/remotefile scp user@host/home/file.txt localfile.txt</pre>
sftp	Start a file transfer connection to a remote site. The prompt changes to an ftp prompt, at which the following commands can be used:  open From the prompt, open a new sftp connection get Bring a remote file to the local server put Place a local file on the remote system cd Change directory on the remote server lcd Change directory on the local machine quit Exit the sftp connection	sftp user@remotemachine
gzip gunzip zip unzip	Compress and uncompress files	gzip files.tar gunzip files.tar.gz unzip archive.zip
tar	Create or expand an archive containing files or folders  -cf Create -xvf Expand -xvfz Expand and uncompress gzip	tar -cf archive.tar ~/scripts tar -xvfz arch.tar.gz

Command	Description	Usage
&	When placed at the end of a command, runs it in the back- ground	
ps	Show currently running processes. Flags controlling the output vary greatly by system. Usually a good starting point is -ax. See man ps for more	ps -ax   grep lucy
top	Show current processes sorted by various parameters, most useful of which is processor usage –u	top -u
kill -9	Terminate a process emphatically, using its process ID. Retrieve PID from the ps or top command	kill -9 5567
killall	Terminate processes by name	killall Firefox
nohup	Run command in background and don't terminate it when logging out or closing the shell window  Use in this odd format shown, to prevent program output to cause the command to quit	nohup command 2> /dev/ null < /dev/null &
ctrl Z	Suspend the operation to move it into the background or perform other operations	
jobs	Show backgrounded or suspended jobs, won't show normal active processes	
bg	Move a suspended process into the background. Optional number after it in the format %1 will specify the job number	
apt-get yum rpm port	Package installers for various Unix distributions. Search for and install remote software packages. Typically used with sudo	sudo apt-get install agrep yum search imagemagick