BCB/EEOB546: UNIX Exercise 1

While you may be able to complete this exercise without issue on your personal laptops using GitBash for Windows or in your Mac Terminal application, I would recommend copying the SNPs folder in the Week_01 folder to the student partion on the HPC cluster Nova. I have tested this assignment in this UNIX environment, and you should not run into problems there.

First, log into HPC Class on Nova by typing the following into your Terminal or GitBash application:

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ssh your_ISU_NETID@nova.its.iastate.edu
```

You will need to have an authenticator application on your mobile device to obtain your verification code. See instructions here:

https://www.hpc.iastate.edu/guides/nova/access-and-login

You will then need your ned-ID password.

The first time you login to hpc-class, it will respond with "host key not found, generate hostkey?(yes/no)". Answer yes.

To add the **SNPs** folder necessary for this exercise to HPC Class on Nova, let's clone the course repository in your directory:

git clone https://github.com/EEOB-BioData/BCB546_Spring2023

Now that you have the data you need, let's do something with it!

- Use the cd command to navigate your way into the SNPs folder
- Make sure you are inside the folder by using the pwd command
- Now use the <u>ls</u> (list) command to list the contents of the <u>SNPs</u> folder; you should see four yabbadabba-doo subfolders
- These folders each contain a single text file. Each of your collaborators (Fred, Wilma, Barney and Betty)
 have identified the number of SNPs in fifteen exons. Their files contain two columns: one with a unique ID
 for their exons and one with the number of SNPs/exon. Our goal is to determine which of the 60 exons
 investigated by our four collaborators has the most SNPs (and to learn some UNIX along the way!).

- from your current location in the SNPs folder, cd into the BarneySNPs folder
- use ls to observe the contents of the folder
- Use the cat (concatenate) command (cat BarneySNPs.txt) to print the entire contents of the text file
- try the head command on your text file (head BarneySNPs.txt) to print just the first portion of the file. How many lines of text are printed?
- Now try head -5. Any difference? How does this change if you vary the number? Understand what's going on here?
- Now let's try tail. What portion of the file is printed when you run this command on the text file?
- Modify your command to tail -n +2. This should print everything but the first row of your text file (*i.e.*, the header). This command will come in handy later on.
- Now let's cd back into the SNPs folder. If you type cd . , this will move you up one directory relative to your current directory; type pwd to verify this is the case; are you in the SNPs folder?
- It's a little messy with all these folders and files. First, let's move all our text files into a single new folder we will name AllSNPs. To create this folder use the command mkdir (make directory); type mkdir AllSNPs
- now use ls to see if your new directory has appeared
- you can copy all of your text files in the Flintstones' folders using the cp (copy) command in a single step by utilizing wild-card characters as follows:

cp *SNPs/*.txt AllSNPs/

- The wild asterisk matches all folders with names ending in "SNPs" and also the .txt files therein and these are then copied to the AllSNPs folder
- cd into your AllSNPs folder and with an 1s verify that all the text files are now there
- O.k., all of our files are now in a single folder, let's clean house. We're going to use a very handy but potentially dangerous command here, so be careful!
- First cd up a directory (you can use the cd .. syntax we learned above), when you 1s now you should see all those messy folders

- Try using the rmdir (remove directory) command on the BarneySNPs folder. Won't let you, will it? That's because rmdir only works on empty directories.
- There's a way around this. MAKE SURE you are in the SNPs folder by typing pwd. You should see:
 /home/<your user name>/SNPs. Now type: rm -r BarneySNPs. You just recursively removed BarneySNPs ...that means you removed that directory and all of its subdirectories and files (which is just a single text file here). Use the ls command to make sure BarneySNPs has disappeared. Now, imagine the carnage if you typed this command on your User directory on your personal machine!
 Goodbye years of hard work and data!!! Let's take a few deep breaths after imagining that and use this handy but scary command on Betty, Fred and Wilma. Finally, use ls to confirm all these folders have been removed.
- Now cd into the AllSNPs folder and print to your screen the contents of all files simultaneously by typing cat *
- We could just look through these data very carefully at this point and find the exon with the most SNPs, but let's eliminate potential human error by going a bit further; we want to produce a single file with everyone's data and sort this by the second column which includes the SNP data
- First, we need to remove the header line at the top of each file (the line with the column names). We'll do this with syntax that could greatly improve your quality of life, a for loop !
- Heres the syntax:

for i in *.txt; do tail -n +2 \$i >> \$i.tail; done

- And here's what it's doing: each of the files (matched with the wild asterisk, *.txt) is temporarily assigned to the variable i, then, in the do portion of the loop, the tail -n +2 command is applied (remember, that leaves us with everything but the header). The output of that command is then written to a new file that will have the same name as the original file but with .tail appended at the end. The loop will continue across all files matched by *.txt and then quit
- After running your for loop, type 1s and see if your brand new "headless" files are in your directory
- Check to see that the header has been removed by using cat on one of the .tail files
- Now let's combine these headless files into a single file by redirecting the output of cat to a text file. Here's the syntax:

cat *.tail > AllSNPs.txt

• The syntax above matches all files ending in .tail (the files we're interested in) and through cat

directs their content to the file we create called AllSNPs.txt

- Let's convince ourselves this has really worked using a new command: wc (stands for word count).
 Type wc * from your current directory; the first column of the output tells you how many lines there are in each file in your directory. How many lines does AllSNPs.txt have? Convinced?
- Great, we have the file we need to figure out which exon has the most SNPs, now we need to sort it. Let's use the sort command for this as follows:

sort -k2 AllSNPs.txt

- the -k2 argument tells your UNIX kernel to sort the file based on the second column (the SNP column);
 is this the sort we were after? NO! What's wrong? Sadly, we've sorted numbers as if they were text
- Let's try again, now with an additional argument:

sort -k2 -n AllSNPs.txt

the __n argument tells your UNIX kernel to sort these values numerically; bingo, that's what we wanted, but we had to scroll down through a bunch of values to find that Fred's eighth exon had the most SNPs (198). Let's use a pipe to get only the value we're after:

```
sort -k2 -n AllSNPs.txt | tail -1
```

- The pipe is the character []. This tells your UNIX kernel to take the output of your sort and send that to the tail -1 command which leaves you with only one exon; Fred wins with 198 SNPs in his eight exon....yabba dabba doo!!
- Congratulations, you're on your way with UNIX!