Computational Genomics

Part 1. Git & Unix

Professor Weigang Qiu
Hunter College of CUNY

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Kunming Institute of Zoology, CAS, China

Version Control with Git

1. **Download course repository**

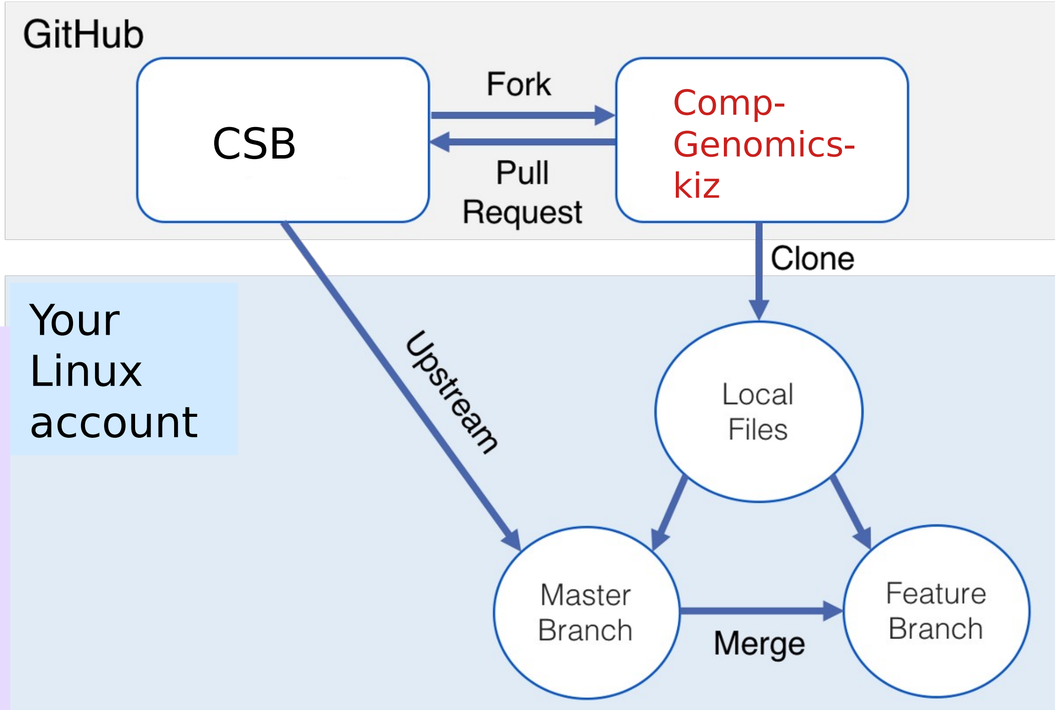
```
git clone
https://gitee.com/huntercollege/comp-genomics-kiz.git
```

2. **Pull the latest versions**

```
git pull
```

3. **Upload/Update file (ignore; not yet working; we will work on it later)**

```
git add <filename> # add a new file
git commit –m “message”
git push
```



GitHub

CSB

Fork

Pull Request

Comp-Genomics-kiz

Clone

Your Linux account

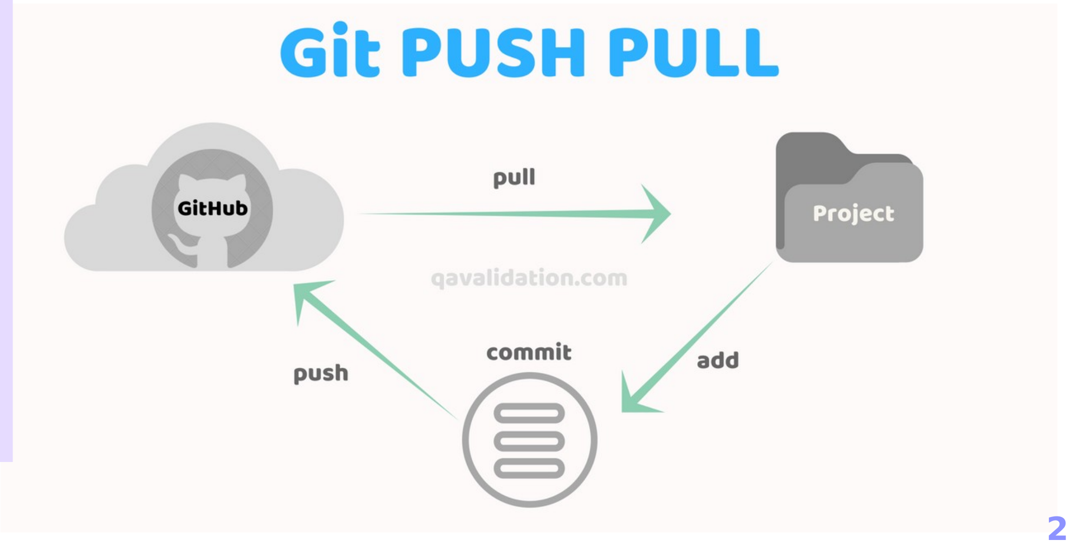
Upstream

Local Files

Master Branch

Merge

Feature Branch



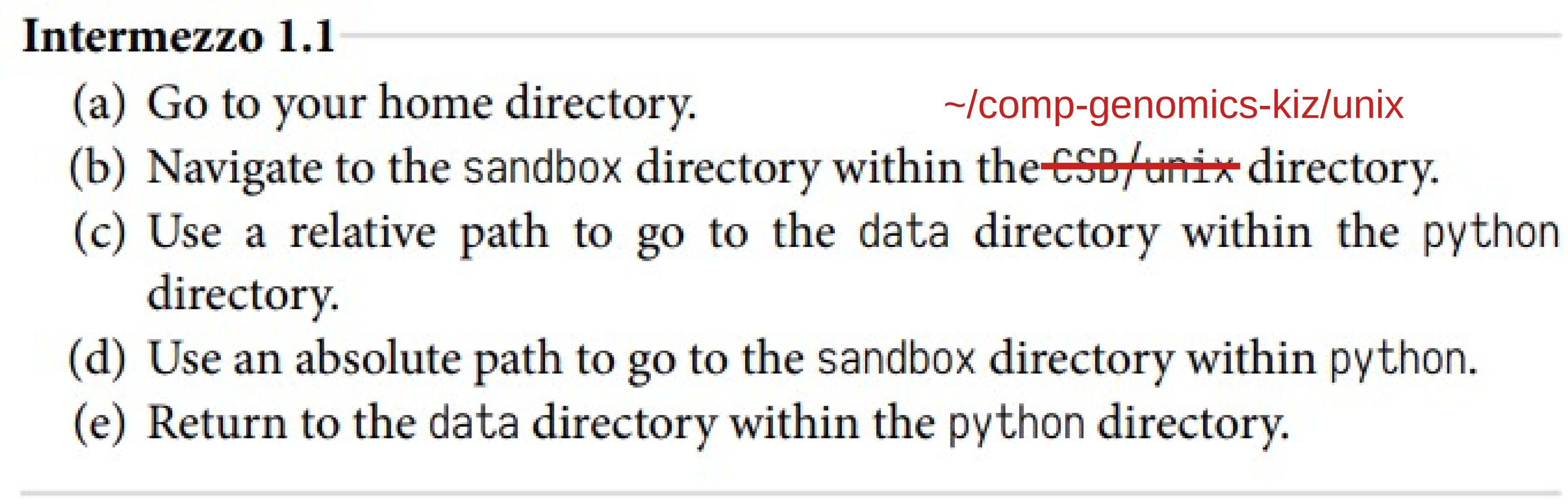
OVERVIEW

- Run “git pull” to get the latest files from the course repository
- Unix command line interface (CLI):
    - `$ command [--options] [arguments]`
    - High efficiency (faster than Python)
    - Faster than graphic user interface (GUI, point-and-click)
    - No need for programming for most of the text-wrangling
- Next week: Quiz #1, based on the following 4 exercises
    - 1.10.1 Next generation sequencing data
    - 1.10.2 Hormone levels in Baboons
    - 1.10.3 Plant-pollinator networks
    - 1.10.4. Data explorer

UNIX Basics (Chapter 1)

```
1. Directory listing & shorthand
    ls -lrth            # long, reverse, timestamp, human-readable
    pwd                 # present working directory
    ~                   # home directory
    .                   # current directory
    ..                  # parent directory
2. Keyboard shorthand (for command editing)
    Ctrl-a  # go to the beginning
    Ctrl-e  # go to the end
    Ctrl-l  # clear the screen
    Ctrl-u  # clear text before the cursor
    Ctrl-k  # clear text after the cursor
    Ctrl-c  # kill the (stalled) command
3. Directory navigation
    cd ~/comp-genomics-kiz/python/data    # absolute path
    Cd ../../unix/data                    # relative path
    cd -                          # toggle 2 directories
4. Use auto-completion & command history
    Tab                           # NEVER type out a full filename
    Arrow keys                    # EDIT & NEVER retype a command
    ls bad\ file\ name.txt        # NEVER use spaces in filenames
```

Exercise 1



Intermezzo 1.1

(a) Go to your home directory.

~/comp-genomics-kiz/unix

(b) Navigate to the sandbox directory within the ~~CSB/unix~~ directory.

(c) Use a relative path to go to the data directory within the python directory.

(d) Use an absolute path to go to the sandbox directory within python.

(e) Return to the data directory within the python directory.

UNIX Basics (Cont’d)

1. Copy files and directories

```
cp ~/comp-genomics-kiz/unix/data/Buzzard2015_about.txt ~/comp-genomics-kiz/unix/sandbox/
                                                                  # use absolute path
cd ~/comp-genomics-kiz/unix/sandbox/
cp ../data/Buzzard2015_about.txt .                                # use relative path
cp ../data/Buzzard2015_about.txt ./Buzzard2015_about2.txt         # copy & rename
cp -r ../data .                                                   # recursive copy
```

2. Move or rename a file

```
mv Buzzard2015_about2.txt ../data/                 # move file to a different directory
mv ../data/Buzzard2015_about2.txt ../data/Buzzard2015_about_new.txt  # move and rename
```

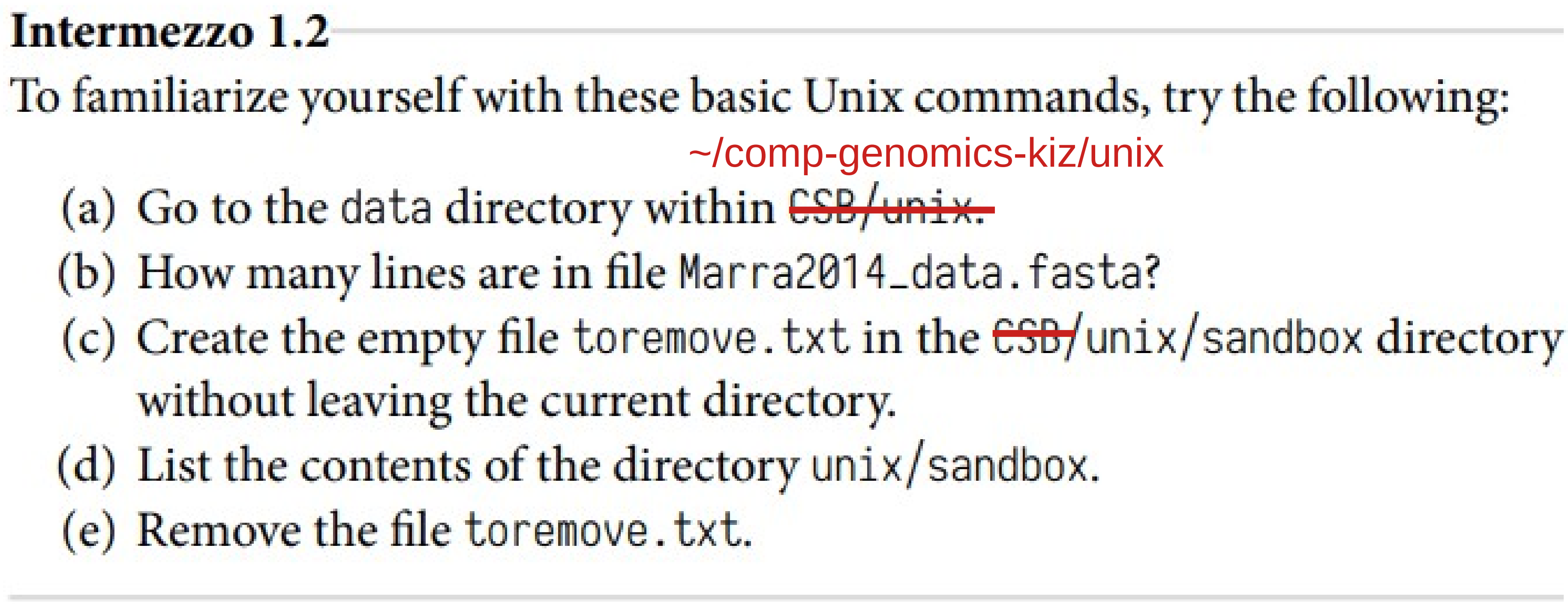
3. Remove file or directory

```
touch new_file.txt          # create an empty file (and update timestamp)
rm –i new_file.txt          # Proceed with caution; EXTREMELY destructive
mkdir –p d1/d2/d3           # make nested directories
rm –r d1                    # recursively remove a directory (and its sub-directories)
```

4. View & filter text files

```
cd      ~/comp-genomics-kiz/unix/data
less Marra2014_data.fasta   # spacebar to page down; b to page up; Q to quit
cat *.txt                   # concatenate all “.txt” files
wc *.txt                    # word count (all “.txt” files)
head Gesquiere2011_data.csv # show top lines
tail –n 2 Gesquiere2011_data.csv    # show tail two lines
sort Gesquiere2011_data.csv         # sort lines in a file (alphabetically)
sort –n Gesquiere2011_data.csv      # sort lines numerically
```

Exercise 2



Intermezzo 1.2

To familiarize yourself with these basic Unix commands, try the following:

~/comp-genomics-kiz/unix

(a) Go to the data directory within ~~CSB/unix.~~

(b) How many lines are in file Marra2014_data.fasta?

(c) Create the empty file toremove.txt in the ~~CSB~~/unix/sandbox directory without leaving the current directory.

(d) List the contents of the directory unix/sandbox.

(e) Remove the file toremove.txt.

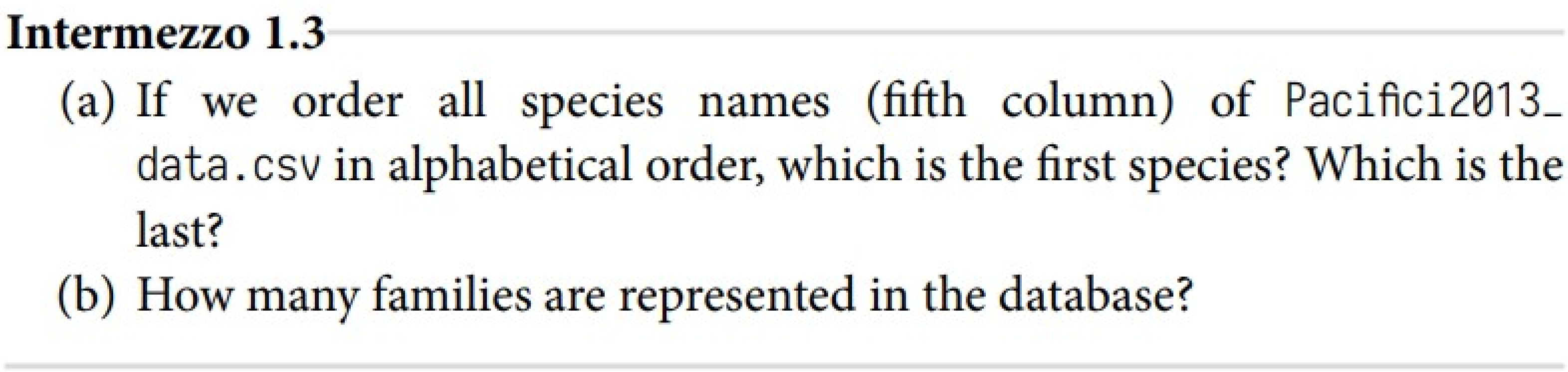
UNIX Advanced: “cut”

1. Redirect output (save output to file)

```
    cd ~/comp-genomics-kiz/unix/sandbox
    echo “My first line” > test.txt                    # redirect echo output to a new file
    echo “My second line” >> test.txt                  # append a second line
    cat test.txt                                       # show file content
    ls –lrt ../data/Saavedra2013 > filelist.txt        # list files and save to a file
    cat filelist.txt                                   # show file
    ls     ../data/Saavedra2013 | wc -l                # use pipe (|) to count # of files
```

2. Select columns using “cut”

```
    cd ~/comp-genomics-kiz/unix/data
    head Pacifici2013_data.csv                                      # show top 10 lines
    head Pacifici2013_data.csv | cut -d ";" -f 1                    # select 1st field, delimited by “;”
    head Pacifici2013_data.csv | cut -d ";" -f 1-4                  # select columns 1-4
    cut -d ";" -f 2 Pacifici2013_data.csv | tail –n +2              # select 2nd column, skip header (1st line)
    cut -d ";" -f 2 Pacifici2013_data.csv | tail –n +2 | sort | uniq          # show unique lines
```



Intermezzo 1.3

(a) If we order all species names (fifth column) of Pacifici2013_data.csv in alphabetical order, which is the first species? Which is the last?

(b) How many families are represented in the database?

UNIX Advanced: “tr” & “sed”

1. Character substitutions with “tr”

```
    echo “ACtGGcAaTT” | tr ‘actg’ ‘ACTG’         # lower to upper cases
    echo “ACtGGcAaTT” | tr 'a-z' 'A-Z'           # same as above
    echo “aaacttGGcaa” | tr –d ‘a’               # delete all ‘a’
    echo “aaacttGGcaa” | tr –s ‘a’               # squeeze consecutive ‘a’
```

2. Exercise: build a single command for the following tasks

```
    cd ~/comp-genomics-kiz/unix/sandbox
```

1. Remove header from the file “../data/Pacifici2013_data.csv”
2. Select columns 2-6 (Order, Family, Genus, Scientific_name, AdultBodyMass_g)
3. Substitute ‘;’ with a Tab (“\t”)
4. Sort by body mass, larger values first
5. Save to a file “BodyM.tsv”

3. String substitution with “sed”

```
    cd ~/comp-genomics-kiz/unix/data
    cat Bb-filelist.txt | sed "s/Borreliella/Borrelia/“        # substitute a word
    cat Bb-filelist.txt | sed "s/Borreliella/Borrelia/g“       # substitute globally
    cat Bb-filelist.txt | sed "s/ NCBI //“                     # remove a string
```

4. Use wildcards to process multiple files

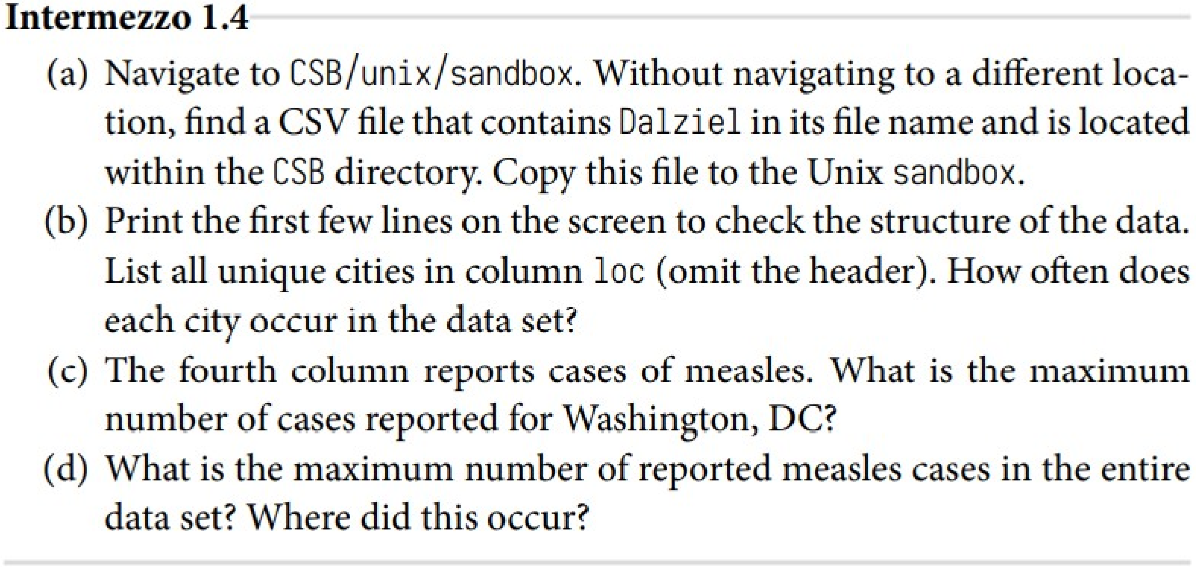
```
    cd ~/comp-genomics-kiz/unix/data/miRNA
    wc –l *.fasta                 # count # lines for all “.fasta” files
    head –n 2 pp*                 # show top two lines for all files starts with “pp”
    file *.???                    # find file types for files with 3-letter extensions
```

Exercise: find file type for all FASTA files; remove the string “_miR” from each line

UNIX Advanced: “grep”

```
cd ~/comp-genomics-kiz/unix/sandbox
grep “Vombatidae” BodyM.tsv                  # filter lines containing a term
grep --color “Vombatidae” BodyM.tsv          # color the term
grep –c “Vombatidae” BodyM.tsv               # count # of lines containing term
grep –w “Bos” BodyM.tsv                      # match only a full word
grep –i “Bos” BodyM.tsv                      # case-insensitive match
grep -B 2 -A 2 "Gorilla gorilla" BodyM.tsv   # include two lines before and after
grep -n "Gorilla gorilla" BodyM.tsv          # show line number of the match
grep Gorilla BodyM.tsv | grep -v gorilla     # show lines without a match (reverse)
grep -w "Gorilla\|Pan" BodyM.tsv             # “\|” to match any of multiple strings
```

```
find ~/comp-genomics-kiz –name “*Dalziel*”
```



Intermezzo 1.4

(a) Navigate to CSB/unix/sandbox. Without navigating to a different location, find a CSV file that contains Dalziel in its file name and is located within the CSB directory. Copy this file to the Unix sandbox.

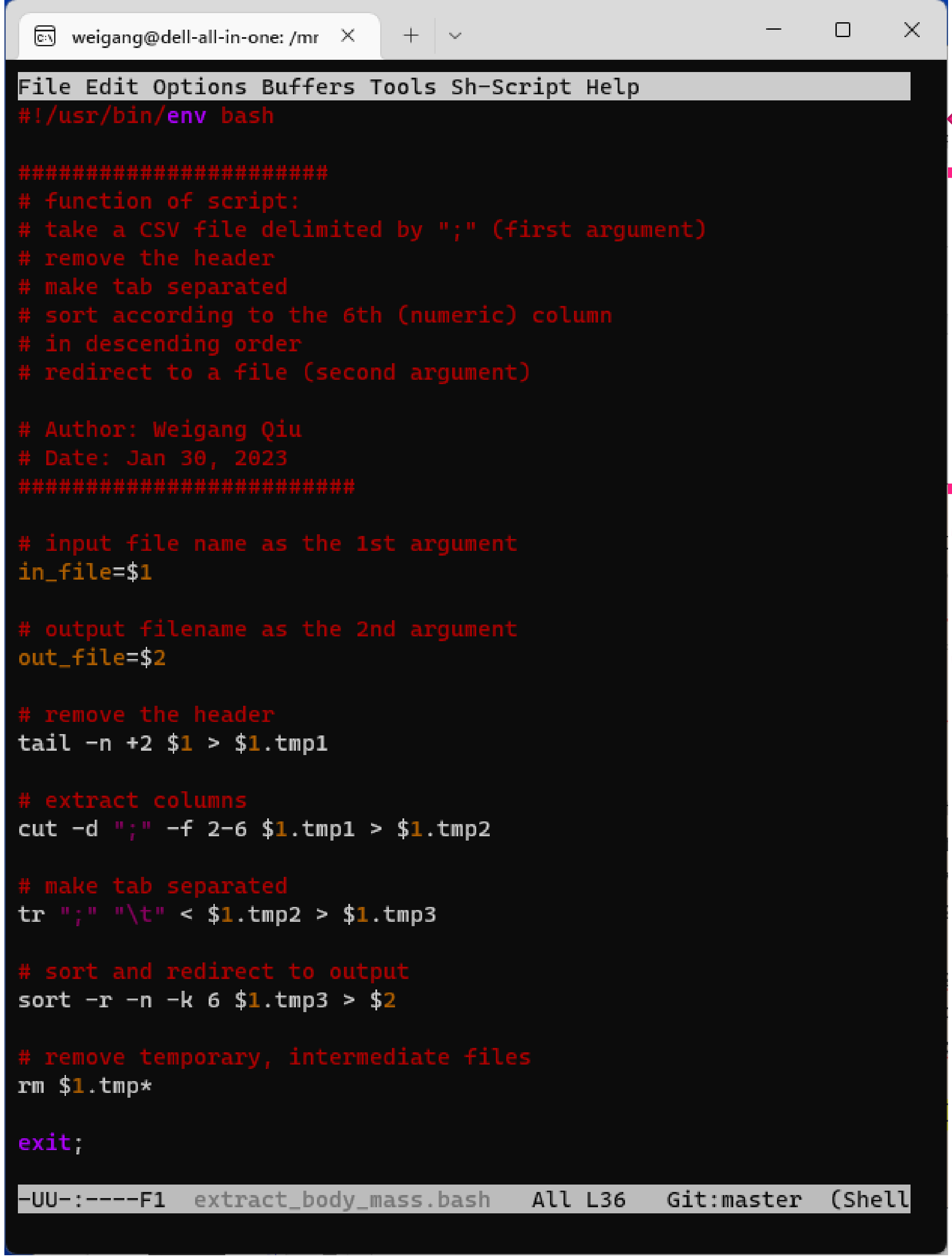
(b) Print the first few lines on the screen to check the structure of the data. List all unique cities in column loc (omit the header). How often does each city occur in the data set?

(c) The fourth column reports cases of measles. What is the maximum number of cases reported for Washington, DC?

(d) What is the maximum number of reported measles cases in the entire data set? Where did this occur?

UNIX Advanced: “for” loops & BASH scripting

```
1. Loop through files, strings, and numbers
    cd ~/comp-genomics-kiz/unix/data/miRNA              # microRNA data
    for file in *.fasta; do head –n 2 $file; done       # show top 2 lines for each file
    # find three miRNA across fasta files and save each to a new fasta file:
    for miR in     miR-208a miR-564 miR-3170; do grep $miR –A1 *.fasta > $miR.fasta; done
    # increment an index:
    for i in {1..10}; do echo $i; done                  # increment by 1
    for i in {1..10..2}; do echo $i; done               # increment by 2
2. BASH scripting
    1) Download, install & start an editor (vi, emacs, gedit, NotePad++)
    2) cd ~/comp-genomics-kiz/unix/sandbox
    3) Paste the following & save as “extract_body_mass.bash”: tail -n +2
       ../data/Pacifici2013_data.csv | cut -d ";“ -f 2-6 | tr “;” “\t" | sort -r -n -k 6 >
       BodyM.tsv
    4) bash extract_body_mass.bash          # Run script
    5) Add the bash path to the beginning & save: #!/usr/bin/env bash
    6) chmod +x extract_body_mass.bash      # change permission to make executable
    7) ./extract_body_mass.bash             # Run script again
    8) Make input and output filenames as arguments; Add comments (see next slide)
    9) ./extract_body_mass.bash ../data/Pacifici2013_data.csv BodyM.tsv
```


weigang@dell-all-in-one: /mr
File Edit Options Buffers Tools Sh-Script Help

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

#######################
# function of script:
# take a CSV file delimited by ";" (first argument)
# remove the header
# make tab separated
# sort according to the 6th (numeric) column
# in descending order
# redirect to a file (second argument)

# Author: Weigang Qiu
# Date: Jan 30, 2023
#########################

# input file name as the 1st argument
in_file=$1

# output filename as the 2nd argument
out_file=$2

# remove the header
tail -n +2 $1 > $1.tmp1

# extract columns
cut -d ";" -f 2-6 $1.tmp1 > $1.tmp2

# make tab separated
tr ";" "\t" < $1.tmp2 > $1.tmp3

# sort and redirect to output
sort -r -n -k 6 $1.tmp3 > $2

# remove temporary, intermediate files
rm $1.tmp*

exit;

-UU-:----F1  extract_body_mass.bash    All L36   Git:master  (Shell
```

Add the bash interpreter path as the first line

Add comments as documentation

Make input and output as arguments (Do not hard-code filenames within a script)

```
# save; make it executable
chmod +x extract_body_mass.bash

# Run with arguments:
./extract_body_mass.bash
../data/Pacifici2013_data.csv
BodyM.tsv
```

Build a (Complex) Unix Command

```
# The following command identifies modified CpG bases from sequencing
reads (FAST4 format) obtained using Nanopore technology

./ont-guppy/bin/guppy_basecaller    # program (with path)
-i Haplochromis_genome/fast5        # input folder
-s mod_out                          # output folder
-c ont-guppy/data/dna_r9.4.1_450bps_modbases_5mc_hac.cfg
                        # configuration file specifying CpG model
-x 'cuda:all’           # use GPUs (instead of CPUs)
--bam_out               # output in BAM format
--compress              # compress the output BAM files
--align_ref Haplochromis_genome/GCF_018398535.1_NCSU_Asbu1_genomic.fna
                        # reference genome (with path)
&                       # run in the background
```

- **NEVER type out a full path or filename. Tab for auto completion**
- **NEVER retype a command. Arrow keys to retrieve command history**