- At this assignment, I would like to report with screenshots. I got help mostly at the
  websites (<a href="https://swcarpentry.github.io/shell-novice/">https://swcarpentry.github.io/shell-novice/</a>), and
  (<a href="https://www.runoob.com/linux/linux-command-manual.html">https://www.runoob.com/linux/linux-command-manual.html</a>), or just tried by myself.
- 1.1. 'ln -s' means soft link, and the first one argument is the target folder, and the second is name of the link.

```
[ese-hejl@login02 ~]$ ls
data_demo exam
[ese-hejl@login02 ~]$ ln -s data_demo/ data_demo_link
[ese-hejl@login02 ~]$ ls
data_demo data_demo_link exam
```

1.2. A '~' means home directory.

```
[ese-hejl@login02 ~]$ echo ~
/work/ese-hejl
```

1.3. 'touch filename' means creating a file with the filename.

```
[ese-hejl@login02 ~]$ cd data_demo/molecules/
[ese-hejl@login02 molecules]$ ls
cubane.pdb ethane.pdb methane.pdb octane.pdb pentane.pdb propane.pdb
[ese-hejl@login02 molecules]$ touch test.pdb
[ese-hejl@login02 molecules]$ ls
cubane.pdb methane.pdb pentane.pdb test.pdb
ethane.pdb octane.pdb propane.pdb
```

1.4. 'find . -type f' returns a list of all of the files in different rows, so we can use 'wc -l' to count the rows number which equals to files number.

```
[ese-hejl@login02 ~]$ cd data_demo/data/elements/
[ese-hejl@login02 elements]$ ls
        Bk.xml Cs.xml Ga.xml
                                Kr.xml
                                        Nb.xml
                                                Pd.xml
                                                        Rn.xml
                                                                 Tb.xml
                                                                        Yb.xml
Ag.xml Br.xml Cu.xml
                                                                 Tc.xml
                        Gd.xml
                                K.xml
                                        Nd.xml
                                                Pm.xml
                                                        Ru.xml
                                                                        Y.xml
                                                Po.xml
Al.xml B.xml
                C.xml
                                La.xml
                                                        Sb.xml
                                                                 Te.xml
                                                                        Zn.xml
                        Ge.xml
                                        Ne.xml
Am.xml Ca.xml
               Dy.xml
                                                Pr.xml
                                                        Sc.xml
                                                                Th.xml
                                                                        Zr.xml
                        He.xml
                               Li.xml
                                        Ni.xml
Ar.xml Cd.xml Er.xml
                        Hf.xml
                                Lr.xml
                                        No.xml
                                                Pt.xml
                                                        Se.xml
                                                                 Ti.xml
                                        Np.xml
                                                Pu.xml
As.xml
       Ce.xml
                Es.xml
                        Hg.xml
                                Lu.xml
                                                        Si.xml
                                                                 Tl.xml
At.xml
       Cf.xml
                Eu.xml
                        Ho.xml
                                Md.xml
                                        N.xml
                                                P.xml
                                                        Sm.xml
                                                                 Tm.xml
        Cl.xml
                Fe.xml
                        H.xml
                                Mq.xml
                                        0s.xml
                                                Ra.xml
                                                        Sn.xml
                                                                U.xml
Au.xml
Ba.xml
        Cm.xml
                Fm.xml
                        In.xml
                                Mn.xml
                                        0.xml
                                                Rb.xml
                                                        Sr.xml
                                                                V.xml
                Fr.xml
                                        Pa.xml
Be.xml
        Co.xml
                        Ir.xml
                                Mo.xml
                                                Re.xml
                                                        S.xml
                                                                W.xml
Bi.xml Cr.xml F.xml
                                        Pb.xml Rh.xml
                        I.xml
                                Na.xml
                                                        Ta.xml Xe.xml
[ese-hejl@login02 elements]$ find . -type f | wc -l
```

1.5. 'diff file1 file2' means comparing file1 and file2.

```
[ese-hejl@login02 ~]$ cd data_demo/data/pdb/
[ese-hejl@login02 pdb]$ ls
                                                               strychnine.pdb
aldrin.pdb
                    cyclopropane.pdb
                                           methanol.pdb
ammonia.pdb
                    ethane.pdb
                                           mint.pdb
                                                               styrene.pdb
ascorbic-acid.pdb
                    ethanol.pdb
                                           morphine.pdb
                                                               sucrose.pdb
benzaldehyde.pdb
                    ethylcyclohexane.pdb mustard.pdb
                                                               testosterone.pdb
camphene.pdb
                    glycol.pdb
                                           nerol.pdb
                                                               thiamine.pdb
cholesterol.pdb
                    heme.pdb
                                           norethindrone.pdb
                                                               tnt.pdb
                    lactic-acid.pdb
cinnamaldehyde.pdb
                                           octane.pdb
                                                               tuberin.pdb
citronellal.pdb
                    lactose.pdb
                                           pentane.pdb
                                                               tyrian-purple.pdb
codeine.pdb
                    lanoxin.pdb
                                           piperine.pdb
                                                               vanillin.pdb
                                                               vinyl-chloride.pdb
count.sh
                    lsd.pdb
                                           print.sh
cubane.pdb
                    maltose.pdb
                                           propane.pdb
                                                               vitamin-a.pdb
cyclobutane.pdb
                    menthol.pdb
                                           pyridoxal.pdb
                    methane.pdb
cyclohexanol.pdb
                                           quinine.pdb
[ese-hejl@login02 pdb]$ diff ethane.pdb ethanol.pdb
1,11c1,12
< COMPND
              ETHANE
< AUTHOR
              DAVE WOODCOCK 95 12 18
                                  -0.752
                                            0.001
< ATOM
                                                    -0.141
                                                            1.00
                                                                  0.00
              C
< ATOM
            2
              C
                            1
                                   0.752
                                           -0.001
                                                     0.141
                                                            1.00
                                                                  0.00
< ATOM
            3 H
                            1
                                   -1.158
                                            0.991
                                                     0.070
                                                            1.00
                                                                  0.00
            4
< ATOM
               Н
                                   -1.240
                                           -0.737
                                                    0.496
                                                            1.00
                                                                  0.00
            5
                            1
                                           -0.249
< ATOM
                                   -0.924
                                                    -1.188
                                                            1.00
                                                                  0.00
                            1
                                           -0.991
< ATOM
            6
                                   1.158
                                                    -0.070
                                                            1.00
                                                                  0.00
< ATOM
            7
                                    0.924
                                            0.249
                                                    1.188
                                                            1.00
                                                                  0.00
               н
< ATOM
            8
                                    1.240
                                            0.737
                                                    -0.496
                                                            1.00
               Н
                                                                  0.00
            9
< TER
> COMPND
              ETHANOL
 AUTHOR
              DAVE WOODCOCK 96 01 03
 MOTA
                                   -0.426
                                           -0.115
                                                   -0.147
                                                            1.00
                                                                  0.00
            1
               C
 MOTA
            2
               0
                                   -0.599
                                            1.244
                                                   -0.481
                                                            1.00
                                                                  0.00
            3
                                                   -0.981
                                           -0.738
                                                            1.00
                                   -0.750
 ATOM
               Н
                                                                  0.00
            4
                            1
                                   -1.022
                                           -0.351
 MOTA
                                                    0.735
                                                            1.00
                                                                  0.00
 MOTA
                                   -1.642
                                            1.434
                                                    -0.689
                                                            1.00
                                                                  0.00
            6
                                            -0.383
                                                     0.147
 ATOM
               C
                                    1.047
                                                            1.00
                                                                  0.00
 MOTA
                            1
                                    1.370
                                            0.240
                                                     0.981
                                                            1.00
                                                                  0.00
                                           -0.147
            8
 ATOM
                                    1.642
                                                    -0.735
                                                            1.00
                                                                  0.00
            9
               Н
                                    1.180
                                           -1.434
                                                     0.405
                                                            1.00
                                                                  0.00
  MOTA
  TER
           10
```

1.6. 'grep str file' means searching for str in the file, and '-c' means returning the counts of all of the results.

```
[ese-hejl@login02 data]$ grep -c 'But she' LittleWomen.txt
15
```

1.7. 'du' returns the size of the working folder, and my working folder is data demo/data/.

```
[ese-hejl@login02 data]$ du 1281 .
```

1.8. 'cp -r folder newfolder' means copying folder to newfolder. 'zip -q -r file.zip' means compressing all of the files in the working folder with a name 'file.zip'.

```
[ese-hejl@login02 ~]$ cp -r data_demo/writing/ data_demo/writing_new
[ese-hejl@login02 ~]$ cd data_demo/writing
[ese-hejl@login02 writing]$ ls
data haiku.txt thesis tools
[ese-hejl@login02 writing]$ cd ../writing_new/
[ese-hejl@login02 writing_new]$ ls
data haiku.txt thesis tools
```

```
[ese-hejl@login02 writing_new]$ zip -q -r writing_new.zip * [ese-hejl@login02 writing_new]$ ls data haiku.txt thesis tools writing_new.zip
```

'unzip file.zip' means decompressing the file.zip. At this time because of the same names of the files, I renamed some of them, and files with '\_d' are decompressed files. Other I didn't rename.

```
[ese-hejl@login02 writing_new]$ unzip writing_new.zip
```

```
[ese-hejl@login02 writing_new]$ ls
data empty-draft_d.md haiku.txt one_d.txt tools writing_new.zip
data_e haiku_d.txt LittleWomen_d.txt thesis two_d.txt
```

1.9. 'chmod 750 directory' means changing the permissions flags of directory to 750, and 750 corresponds with 'drwxr-x---'.

```
[ese-hejl@login02 data_demo]$ ll
total 133
drwxr-xr-x 2 ese-hejl ese-ouycc
                                 4096 Nov 24 19:21 creatures
drwxr-xr-x 5 ese-hejl ese-ouycc
                                 4096 Nov 24 19:21 data
drwxr-xr-x 2 ese-hejl ese-ouycc
                                 4096 Dec 2 15:20 molecules
                                   22 Nov 24 19:55 my_file_new
-rw-r--r-- 1 ese-hejl ese-ouycc
drwxr-xr-x 3 ese-hejl ese-ouycc
                                 4096 Nov 24 19:21 north-pacific-gyre
-rwxr-xr-x 1 ese-hejl ese-ouycc
                                   69 Nov 24 19:21 notes
-rwxr-xr-x 1 ese-hejl ese-ouycc
                                   32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-hejl ese-ouycc 21583 Nov 24 19:21 solar.pdf
drwxr-xr-x 2 ese-hejl ese-ouycc
                                4096 Nov 24 19:57 test
drwxr-xr-x 5 ese-hejl ese-ouycc
                                 4096 Nov 24 19:21 writing
drwxr-xr-x 5 ese-hejl ese-ouycc
                                 4096 Dec 2 16:09 writing_new
[ese-hejl@login02 data_demo]$ chmod 750 writing_new/
[ese-hejl@login02 data_demo]$ ll
total 133
drwxr-xr-x 2 ese-hejl ese-ouycc
                                 4096 Nov 24 19:21 creatures
drwxr-xr-x 5 ese-hejl ese-ouycc
                                 4096 Nov 24 19:21 data
drwxr-xr-x 2 ese-hejl ese-ouycc
                                 4096 Dec 2 15:20 molecules
                                   22 Nov 24 19:55 my_file_new
-rw-r--r-- 1 ese-hejl ese-ouycc
                                 4096 Nov 24 19:21 north-pacific-gyre
drwxr-xr-x 3 ese-hejl ese-ouycc
-rwxr-xr-x 1 ese-hejl ese-ouycc
                                   69 Nov 24 19:21 notes
-rwxr-xr-x 1 ese-hejl ese-ouycc
                                   32 Nov 24 19:21 pizza.cfg
-rwxr-xr-x 1 ese-hejl ese-ouycc 21583 Nov 24 19:21 solar.pdf
drwxr-xr-x 2 ese-hejl ese-ouycc
                                 4096 Nov 24 19:57 test
drwxr-xr-x 5 ese-heil ese-ouycc
                                 4096 Nov 24 19:21 writing
                                 4096 Dec 2 16:09 writing new
drwxr-x--- 5 ese-hejl ese-ouycc
```

1.10. 'history 10' returns the last 10 commands I made.

```
[ese-hejl@login02 data demo]$ history 10
  340
       rm data e
  341
       ls
  342
       ш
       cd ..
  343
  344
  345
       chmod 750 writing new/
  346
       u
  347
       history
  348
       history | tail 10
  349
       history
```

2. I writed a for loop at demo.sh. 'du -b \$f' returns all of the sizes of files with '.pdb' in this

folder in bytes. '-b' means sizes in bytes at this case. And it would print line by line.

```
GNU nano 2.3.1 File: demo.sh

for f in *.pdb
do
du -b $f
done
```

And I changed the permissions flags.

```
[ese-hejl@login02 pdb]$ chmod 750 demo.sh
```

## Then I ran it.

```
[ese-hejl@login02 pdb]$ ./demo.sh
1516
        aldrin.pdb
306
        ammonia.pdb
        ascorbic-acid.pdb
1444
1030
        benzaldehyde.pdb
        camphene.pdb
1830
5049
        cholesterol.pdb
1090
        cinnamaldehyde.pdb
1694
        citronellal.pdb
2452
        codeine.pdb
1158
        cubane.pdb
895
        cyclobutane.pdb
        cyclohexanol.pdb
1384
695
        cyclopropane.pdb
622
        ethane.pdb
690
        ethanol.pdb
2396
        ethylcyclohexane.pdb
765
        glycol.pdb
4209
        heme.pdb
1064
        lactic-acid.pdb
2562
        lactose.pdb
11193
        lanoxin.pdb
3395
        lsd.pdb
2562
        maltose.pdb
2164
        menthol.pdb
422
        methane.pdb
490
        methanol.pdb
1869
        mint.pdb
2288
        morphine.pdb
2123
        mustard.pdb
1680
        nerol.pdb
        norethindrone.pdb
2729
1828
        octane.pdb
        pentane.pdb
1226
2287
        piperine.pdb
825
        propane.pdb
1256
        pyridoxal.pdb
        quinine.pdb
3303
2675
        strychnine.pdb
1159
        styrene.pdb
2562
        sucrose.pdb
```

2787	testosterone.pdb
2196	thiamine.pdb .
1508	tnt.pdb
2395	tuberin.pdb
2103	tyrian-purple.pdb
1361	vanillin.pdb
423	vinyl-chloride.pdb
2894	vitamin-a.pdb