Prep-Course Informatics for Life Scientists

Introduction to Unix and the Command Line Interface

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  - Standard to interact with larger computer infrastructures (e.g. a compute server or cluster)
- The majority of bioinformatics tools have a CLI
  - We work with a high number of large files
  - Crunching that data requires high compute power $\Rightarrow$ compute server, cluster
  - Most file formats established in Bioinformatics are plain text

Basic Usage

- Enter a command and press the Return (↵) key

```
$ ls ↵
Desktop   Documents   Exercise
```

- To get help on how to use a particular command, try

```
$ ls --help ↵
$ man ls ↵
```

- The basic command syntax often follows this structure:

```
COMMAND [ARGUMENTS]
COMMAND [OPTIONS] [OPERANDS]
```

Basic Usage

- Often there are long (`--`) and short (`-`) versions of switches

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Exercise    Documents    Desktop
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```

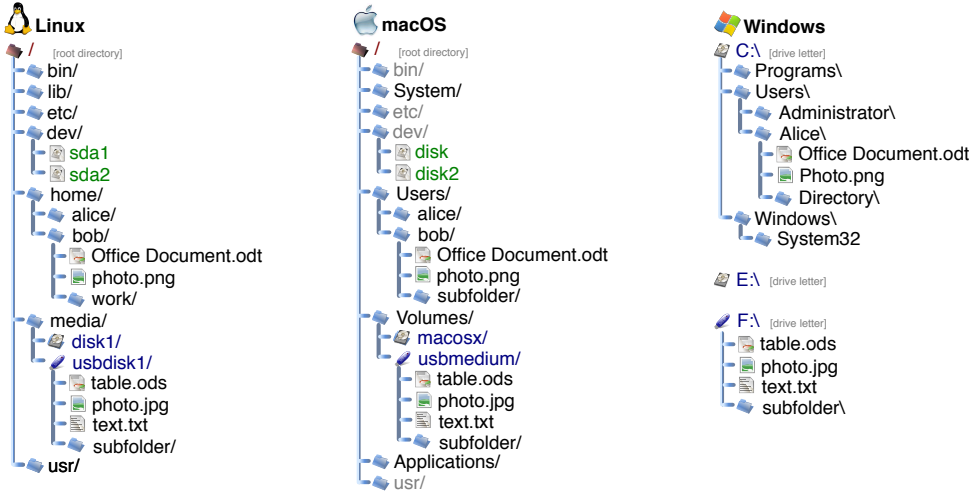
- Multiple switches can be specified together

```
$ ls -F -r ↵
Exercise/  Documents/  Desktop/
$ ls -Fr ↵
Exercise/  Documents/  Desktop/
```

File systems

File systems

A typical computer file system is structured like a tree



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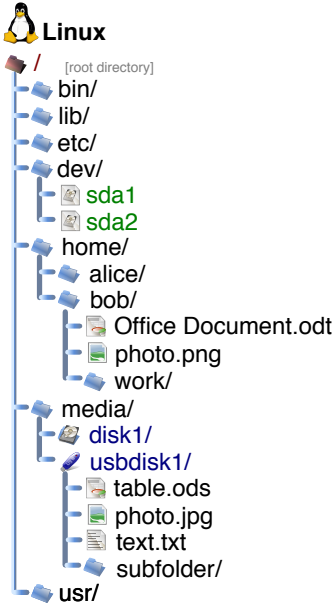
- When using the shell, one often says “I am in the directory xzy”.
- The working directory is not static, it can be changed throughout the runtime of a process.

File systems



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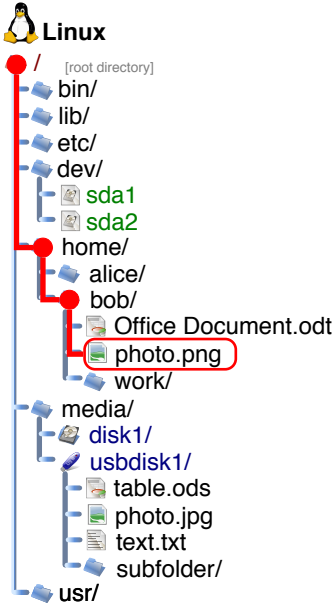

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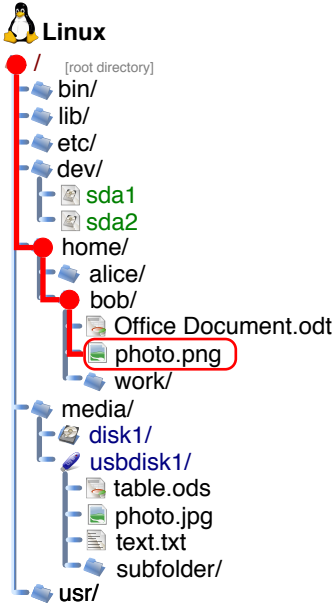

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  given that the current working directory is `/home`.

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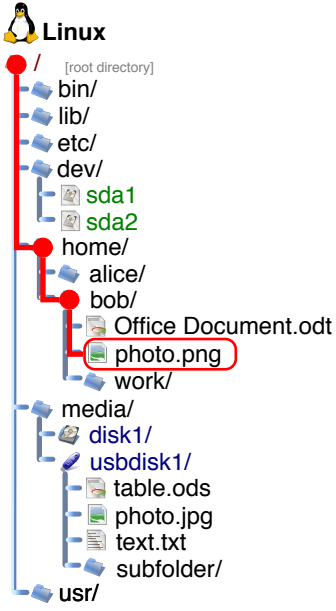

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- Relative paths start in the current working directory, for example

  `./bob/photo.png`

  given that the current working directory is `/home`.
- Every character sequence that does not start with a slash `/` character is interpreted as a relative path.

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  Displays the contents of folders (directories)
  - `ls -l` show details
  - `ls -lh` human readable file sizes
  - `ls -a` show hidden files and folders

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- **`cd` - change directory**
  Changes the current working directory

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    Required to copy directories with their contents.

- **`mv <source path> <destination path>` - move**
  Move files and folders **Overwriting targets cannot be undone!**

- **`rmdir <path>` - remove directory**
  Removes directories, but only if they are empty. Safe to use.

Working with the file system

- **`rm <path>` - remove**
  Remove files and folders. **Removing cannot be undone!**
  - **`rm -r` - recursive mode**
    Required to remove directories with their contents.

Getting started with plain text files

Inspecting plain text files

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- **`cat <path> [<path> ...]`** - **concatenate**
  Concatenates input files and prints them to the standard output (more on that later).

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- **`head <path>`**
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- **`tail <path>`**
  Output the last *n* lines of a plain text file.
  - **`tail -f`** - follow
    Keeps printing new lines as the file grows.

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- Well known graphical editors for for macOS: TextEdit and Atom
- Nano is a text editor that does not require a graphical user interface but works on the command line

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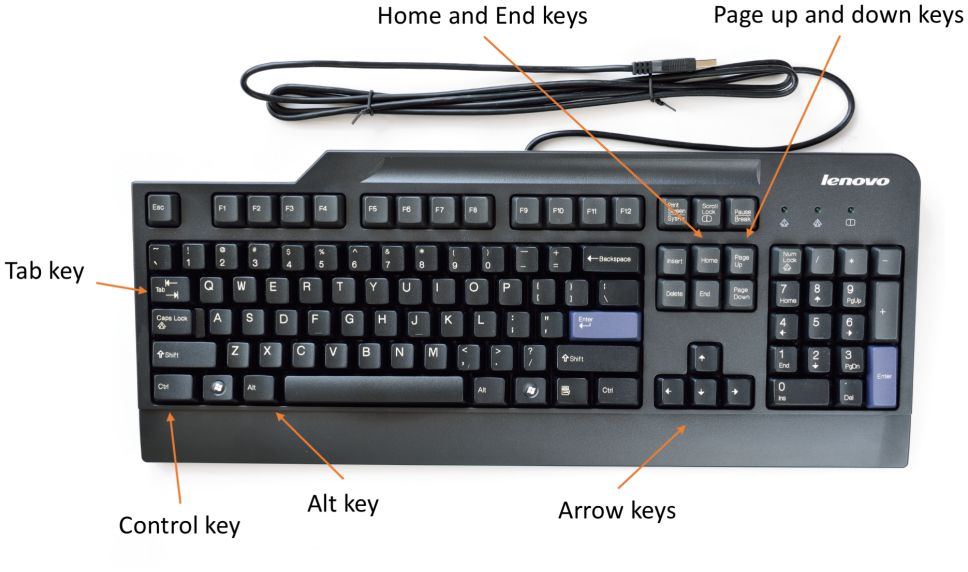
- **`CTRL-X`**
  Exits nano

Keyboard shortcuts

- **`TAB`**
  Autocomplete the command line
- **`TAB - TAB`**
  Show possible completions if not unique
- **`ALT-b`** and **`ALT-f`**
  Move one word backward (or forward) in the current command line
- **`Pos1`** or **`Home`**
  Move to the beginning of the current command line
- **`End`**
  Move to the end of the current command line

Keyboard shortcuts



Keyboard shortcuts

- **`Arrow Up`**
  Browse the shell history backward in time
- **`Arrow Down`**
  Browse the shell history forward in time
- **`CTRL-R`**
  Search the shell history backward in time
- **`CTRL-C`**
  Interrupt the current program.

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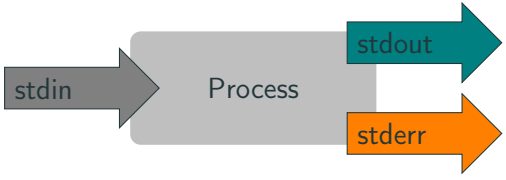

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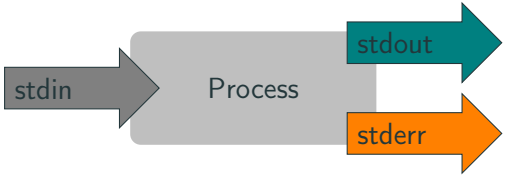

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```
$ ls -l doesnt.exist ↵
ls: cannot access 'doesnt.exist': No such file or directory
```

Process streams

- We can redirect streams into files using the **>** character

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Try the two examples above and check the contents of the two output files each time!

Process streams

- The **>** redirection overwrites the target file!
- Use **>>** to instead append the contents to the target file

Warm up

- ☞ Create a folder named `repetition`
- ☞ Create a file in that folder named `repetition.txt`
- ☞ Write the text `Hello World` into that file
- ☞ Copy the file to a new file named `repetition2.txt`
- ☞ Write the content of `repetition2.txt` twice into a new file `repetition3.txt`
- ☞ Print the content of the three files
- ☞ Delete the file `repetition.txt`
- ☞ Copy the folder `repetition` to the folder `repetition2` with all its contents
- ☞ Rename the folder `repetition` to `repetition_old`
- ☞ Remove the contents of the folder `repetition_old`
- ☞ Remove the folder repetition_old
- ☞ Remove the folder `repetition2`

Users, groups and permissions

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- On Linux systems users and groups are used to manage file permissions

Users, groups and permissions

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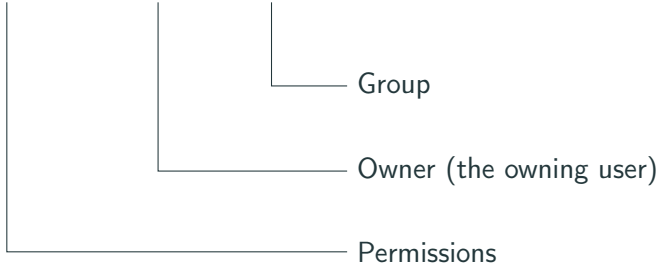

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- Symbol '-' indicates the absence of the corresponding permission

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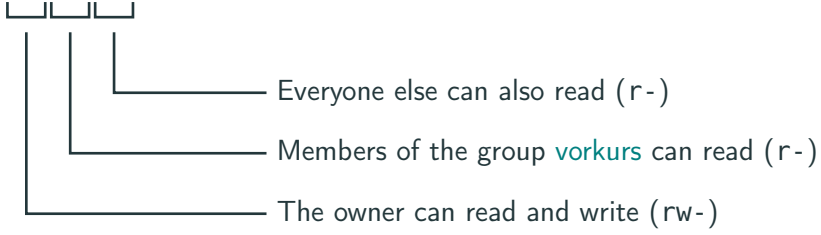

Users, groups and permissions

- Permissions are also used for directories (in fact they are also just files)
- However, interpretation of permissions for directories is slightly different
  - `r` determines whether the contents of a directory can be seen
  - `w` determines whether files can be created or deleted
  - `x` determines whether a user can change into the directory

- **`chown [owner]:[group] <path>` - change ownership**
  Changes the ownership and / or group association of a file or directory.
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- **`chmod <permissions> <path>` permissions** Changes the file permissions.
  - Symbol '+' to add permissions
  - Symbol '-' to remove permissions
  - Shortcuts for categories: (u)ser, (g)roup, (o)thers, (a)ll at once
  - Shortcuts for permissions: (r)ead, (w)rite, e(x)ecute

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- What is the next command doing?:
  `chmod u+rwx,g+rw,o+r <path>`

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Add write permission to everyone:

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$ chmod a+w Exercise/data/clinvar_20180225.vcf.gz  ↵
$ ls -l Exercise/data ↵
total 13960
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```

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- Permissions can be combined in a single-digit number via summation
- Triplet of single-digit numbers can specify the permissions for all categories
- Example: **`chmod 750 <path>`**
  - Owner: $7 = 4 + 2 + 1$ (all permissions 'rwx')
  - Group: $5 = 4 + 1$ (read and execute permissions 'r-x')
  - Other: 0 (no permissions '---')

Downloading data from the internet

Downloading data from the internet

- **`wget <url>`**

  Downloads a remote file. Supports HTTP(S) and FTP.

  - Option -c (--continue):
    Continue downloading a file that was already partially downloaded
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- **`curl -LO <url>`**
  - Another command line tool to download remote files, similar to wget.
  - Usually installed on macOS

Downloading data from the internet

Example **wget** invocation:

```
$ wget https://bioinfprep.github.io/assets/material.zip  ↵
--2020-10-21 08:00:04--  https://bioinfprep.github.io/assets/material.zip
Resolving bioinfprep.github.io... 185.199.111.153, 185.199.110.153, 185.199.108.153, ...
Connecting to bioinfprep.github.io|185.199.111.153|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 10586 (10K) [application/zip]
Saving to: 'material.zip.3'

material.zip.3               100%[=========================================>]
10.34K  --.-KB/s    in 0.001s

2020-10-21 08:00:04 (13.8 MB/s) - 'material.zip.3' saved [10586/10586]
```

Downloading data from the internet

Example **`curl`** invocation:

```
$ curl -LO https://bioinfprep.github.io/assets/material.tar.gz ↵
  % Total    % Received % Xferd  Average Speed   Time    Time     Time  Current
                                 Dload  Upload   Total   Spent    Left  Speed
100 10586  100 10586    0     0  57532      0 --:--:-- --:--:-- --:--:-- 57532
```

File compression and file archives

File compression and file archives

- The most common compressed archive file formats are .tar.gz and .zip
- tar is an archive format to reversibly combine multiple files into one file
- gz (gzip) is a data compression tool
- Often you find the combination of an archive with compression: .tar.gz
- zip is an "all in one" solution, i.e. does archiving and compression

ZIP file handling

- **`unzip -l <path>`**
  Shows the contents of a zip file
- **`unzip <path>`**
  Unpacks the contents of a zip file
- **`zip -r <outputpath> <contentpath> [<contentpath> ...]`**
  Add content to a zip file recursively. Creates the zip file if it does not exist.

ZIP file handling

```
$ unzip -l material.zip   ↵
Archive:  material.zip
  Length      Date    Time    Name
---------  ---------- -----   ----
        0  03-29-2017 09:36   material/
       51  03-22-2017 10:59   material/test_file_1.txt
       69  03-22-2017 10:59   material/test_file_2.txt
    34753  03-22-2017 12:36   material/large.fasta
       67  03-22-2017 12:39   material/small.fasta
      595  03-28-2017 08:58   material/duplicated_file.txt
       35  03-29-2017 09:29   material/my_diff_2.txt
       46  03-29-2017 09:29   material/my_diff_1.txt
       35  03-29-2017 09:34   material/my_sort_1.txt
      557  03-29-2017 09:36   material/tmp.txt
      557  03-29-2017 09:36   material/my_sort_2.txt
---------                     -------
    36765                     11 files
```

ZIP file handling

```
$ unzip material.zip ↵
Archive:  material.zip
   creating: material/
  inflating: material/test_file_1.txt
  inflating: material/test_file_2.txt
  inflating: material/large.fasta
  inflating: material/small.fasta
  inflating: material/duplicated_file.txt
 extracting: material/my_diff_2.txt
  inflating: material/my_diff_1.txt
  inflating: material/my_sort_1.txt
  inflating: material/tmp.txt
  inflating: material/my_sort_2.txt
```

ZIP file handling

```
$ unzip material.zip ↵
Archive:  material.zip
   creating: material/
  inflating: material/test_file_1.txt
  inflating: material/test_file_2.txt
  inflating: material/large.fasta
  inflating: material/small.fasta
  inflating: material/duplicated_file.txt
 extracting: material/my_diff_2.txt
  inflating: material/my_diff_1.txt
  inflating: material/my_sort_1.txt
  inflating: material/tmp.txt
  inflating: material/my_sort_2.txt
$ ls -F ↵
Desktop/  Documents/  Exercise/  material/  material.zip
```

ZIP file handling

```
$ unzip material.zip ↵
Archive:  material.zip
   creating: material/
  inflating: material/test_file_1.txt
  inflating: material/test_file_2.txt
  inflating: material/large.fasta
  inflating: material/small.fasta
  inflating: material/duplicated_file.txt
 extracting: material/my_diff_2.txt
  inflating: material/my_diff_1.txt
  inflating: material/my_sort_1.txt
  inflating: material/tmp.txt
  inflating: material/my_sort_2.txt
$ ls -F ↵
Desktop/  Documents/  Exercise/  material/  material.zip
$ ls material ↵
duplicated_file.txt  my_diff_1.txt  my_sort_1.txt  small.fasta      test_file_2.txt
large.fasta          my_diff_2.txt  my_sort_2.txt  test_file_1.txt  tmp.txt
```

ZIP file handling

```
$ zip -r new_material.zip material/ ↵
  adding: material/ (stored 0%)
  adding: material/my_diff_2.txt (stored 0%)
  adding: material/test_file_2.txt (deflated 41%)
  adding: material/duplicated_file.txt (deflated 92%)
  adding: material/test_file_1.txt (deflated 63%)
  adding: material/my_sort_1.txt (deflated 3%)
  adding: material/small.fasta (deflated 45%)
  adding: material/tmp.txt (deflated 52%)
  adding: material/my_sort_2.txt (deflated 51%)
  adding: material/my_diff_1.txt (deflated 4%)
  adding: material/large.fasta (deflated 77%)
```

GZIPed TAR file handling

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- **`tar xvzf <path>`**
  Unpacks the contents of a gzipped tar file.
  Overwrites existing output file paths!

- **`tar cvzf <outputpath> <contentpath> [<contentpath> ...]`**
  Add content to a gzipped tar file recursively.
  Overwrites an existing output zip file if it exists!

GZIPed TAR file handling

```
$ tar tzf material.tar.gz ↵
material/
material/test_file_2.txt
material/tmp.txt
material/my_sort_1.txt
material/test_file_1.txt
material/small.fasta
material/my_diff_2.txt
material/my_sort_2.txt
material/my_diff_1.txt
material/duplicated_file.txt
material/large.fasta
```

GZIPed TAR file handling

```
$ tar xvzf material.tar.gz ↵
material/
material/test_file_2.txt
material/tmp.txt
material/my_sort_1.txt
material/test_file_1.txt
material/small.fasta
material/my_diff_2.txt
material/my_sort_2.txt
material/my_diff_1.txt
material/duplicated_file.txt
material/large.fasta
```

GZIPed TAR file handling

```
$ tar cvzf new_material.tar.gz material/ ↵
material/
material/my_diff_2.txt
material/test_file_2.txt
material/duplicated_file.txt
material/test_file_1.txt
material/my_sort_1.txt
material/small.fasta
material/tmp.txt
material/my_sort_2.txt
material/my_diff_1.txt
material/large.fasta
```

GZIPed TAR file handling

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GZIPed TAR file handling

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- bzip2 compression with suffix `.tar.bz2`:
  use option `j` instead of `z`
- xz compression with suffix `.tar.xz`:
  use option `J` instead of `z`
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- **`tar xvf <path>`**
  Unpacks the contents of a compressed tar file

Standalone GZIP files

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- gzip is commonly used to compress all kinds of files
- **`gzip <path>`**
  Compresses the given file into `<path>.gz` and removes the original file
- **`gunzip <path>.gz`**
  Decompresses the given file into `<path>` and removes the compressed file

Standalone GZIP files

Download a compressed FASTQ file

```
$ curl -LO https://bioinfprep.github.io/assets/sequences.fastq.gz ↵
  % Total    % Received % Xferd  Average Speed   Time    Time     Time  Current
                                 Dload  Upload   Total   Spent    Left  Speed
100   330  100   330    0     0   6346      0 --:--:-- --:--:-- --:--:--  6470
100 13.5M  100 13.5M    0     0  9403k      0  0:00:01  0:00:01 --:--:-- 11.1M
```

Standalone GZIP files

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100 13.5M  100 13.5M    0     0  9403k      0  0:00:01  0:00:01 --:--:-- 11.1M
```

Inspect the downloaded file

```
$ ls -lh sequences.fastq.gz  ↵
-rw-r--r-- 1 vorkurs vorkurs 14M Apr  3  2018 sequences.fastq.gz
```

Standalone GZIP files

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Standalone GZIP files

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                                 Dload  Upload   Total   Spent    Left  Speed
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100 13.5M  100 13.5M    0     0  9403k      0  0:00:01  0:00:01 --:--:-- 11.1M
```

Inspect the downloaded file

```
$ ls -lh sequences.fastq.gz  ↵
-rw-r--r-- 1 vorkurs vorkurs 14M Apr  3  2018 sequences.fastq.gz
```

Decompress the downloaded file

```
$ gunzip sequences.fastq.gz  ↵
```

Inspect the decompressed file

```
$ ls -lh sequences.fastq ↵
-rw-r--r-- 1 vorkurs vorkurs 89M Apr  3  2018 sequences.fastq
```

File sizes

File sizes

- **`du <path>` - disk usage**
  Can be used to show individual file sizes or the total size of directories
  - **`du -h <path>`**
    Shows the sizes in a human readable format instead of kb
  - **`du -a <path>`**
    When applied on a directory, report sizes of all files, not only folders.

File sizes

- **du** and **ls** may report different sizes

```
$ du -h material.zip ↵
12K     material.zip
```

```
$ ls -lh material.zip ↵
-rw-r--r-- 1 vorkurs vorkurs 11K Apr  3 22:05 material.zip
```

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- The tools define the size of a file differently
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```

- The tools define the size of a file differently
  - **du** reports how much space the file consumes on the underlying storage
  - **ls** reports the size of the content stored inside the file
- **du** invoked with option --apparent-size also reports the size of the content

File comparison

File comparison

- **`diff <path1> <path2>`**
  Identifies differences between two plain text files and reports them as the smallest number of insertions and deletions required to transform one file into the other.
  - **`diff -i`** or **`diff --ignore-case`**
    Ignore case differences in the files contents
  - **`diff -w`** or **`diff --ignore-all-space`**
    Ignore all differences that involve only white space
  - **`diff -B`** or **`diff --ignore-blank-lines`**
    Ignore blank lines
  - **`diff -y`** or **`diff --side-by-size`**
    Output a human readable, side-by-side view instead of machine readable output

File comparison

☞ Use **`diff`** to identify the differences between the files `my_diff_1.txt` and `my_diff_2.txt`!

Sorting and Counting

Sorting and Counting

- **`sort <path>` - sort plain text**
  The **`sort`** tool can be used to sort plain text files line by line.
  - **`sort -b`** or **`sort --ignore-leading-blanks`**
    Ignore leading white space caracters
  - **`sort -n`** or **`sort --numeric-sort`**
    Interpret digits numerically instead of lexicographically
  - **`sort -r`** or **`sort --reverse`**
    Sort in reverse order
  - **`sort -u`** or **`sort --unique`**
    Output duplicate lines only once

Sorting and Counting

- **`uniq <path>`**
  Collapse consecutive identical lines into one line.
  - **`uniq -c`** or **`uniq --count`**
    Report the number of occurrences with each line
  - **`uniq -i`** or **`uniq --ignore-case`**
    Ignore case differences when comparing lines

Sorting and Counting

- `wc <path>` - **word count**
  Count words (or lines, characters, bytes) in plain text
  - `wc -c`
    Report the number of characters
  - `wc -l`
    Report the number of lines
  - `wc -w`
    Report the number of words
  - `wc -c`
    Print all three numbers

Sorting and Counting

- ☞ Sort the file `my_sort_1.txt`!
- ☞ Sort the file `my_sort_2.txt` in reverse numerical order!
- ☞ Which lines in `duplicated_file.txt` are duplicated and how often do they occur?
- ☞ Are all globally redundant lines collapsed by **`uniq`**?

Searching patterns in plain text

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- **`grep <pattern> <path> [<path> ...]`**
  Prints all lines of the input that match the given regular expression pattern
  - **`grep -v <pattern> <path> [<path> ...]`**
    Inverse mode, print all lines that do *not* match the given pattern
  - **`grep -l <pattern> <path> [<path> ...]`**
    Print only the names of files that the pattern matches against
  - **`grep -n <pattern> <path> [<path> ...]`**
    Print the line numbers along with the matches
  - **`grep --color <pattern> <path> [<path> ...]`**
    Highlight the pattern occurrence

Searching patterns in plain text

```
$ grep --color -n is sortme.txt ↵
1:This is an example file with content
2:that may be sorted. If you sort this file
4:because the line order is critical. None
5:of this makes any sense!
```

Process streams II

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- The | (pipe) symbol redirects the standard output stream (stdout) of one process to the standard input stream (stdin) of another process

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- Remember the common structure of commands that we have seen often today:

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COMMAND [OPTIONS] [INPUT FILE PATH]
```

Process streams II

- The | (pipe) symbol redirects the standard output stream (stdout) of one process to the standard input stream (stdin) of another process
- Remember the common structure of commands that we have seen often today:

```
COMMAND [OPTIONS] [INPUT FILE PATH]
```

- Most programs we have seen today would process data from stdin if no input file path is given!

Process streams II

Without stream redirection:

```
$ ls -l 1> temp.txt ↵
$ wc -l temp.txt ↵

15 temp.txt
```

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```

Process streams II

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15
```

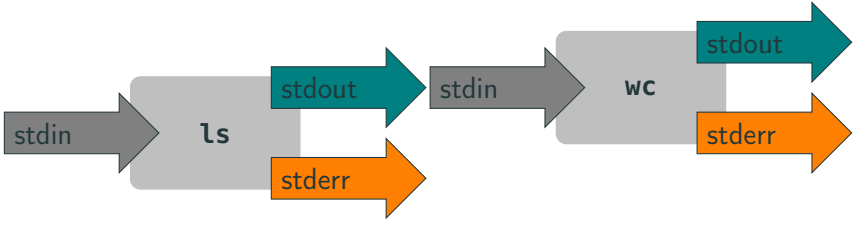

Process streams II

Recall:

```
$ uniq -c duplicated_file.txt  ↵
     22 bla
     28 blabla
      1 this line is not duplicatedbla
     21 bla
     28 blabla
```

Combining **sort** and **uniq**:

```
$ sort duplicated_file.txt | uniq -c ↵
     43 bla
     56 blabla
      1 this line is not duplicatedbla
```

Process streams II

What is the following command doing and why?

```
$ gunzip -c material.tar.gz | tar t ↵
```

Final Task

https://bioinfprep.github.io/task/unix1.html