

Bioinformatics Preparatory Course

Basic Unix

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October 21, 2020

Why bother with the shell?

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 - Searching, organizing, transferring large numbers of files
 - Exploring and manipulating plain text files
 - Can be programmed

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 - Standard to interact with larger computer infrastructures (e.g. a compute server or cluster)

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 - SSH (secure shell) interface to access a Unix-like system remotely
 - 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

- 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 [OPTIONAL SWITCHES] [MANDATORY ARGUMENTS]
```

Basic Usage

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

```
$ ls ↵
```

```
Desktop  Documents  Exercise
```

```
$ ls -r ↵
```

```
Exercise  Documents  Desktop
```

```
$ ls --reverse ↵
```

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Exercise Documents Desktop
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```
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```
Exercise Documents Desktop
```

- Multiple switches can be specified together

```
$ ls -F -r ↵
```

```
Exercise/ Documents/ Desktop/
```

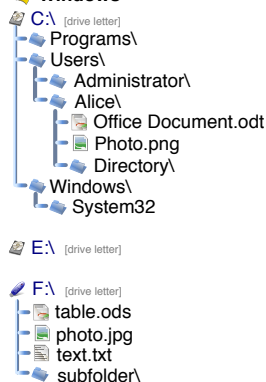
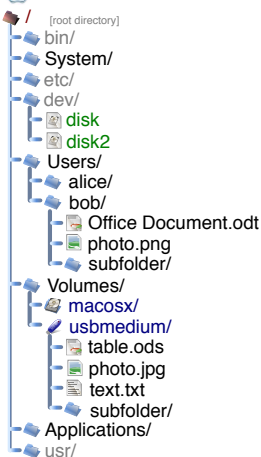
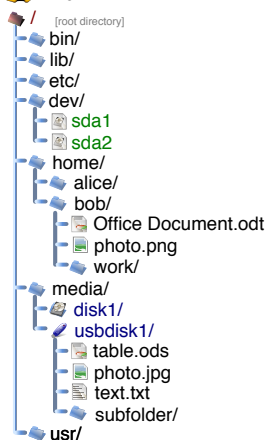
```
$ ls -Fr ↵
```

```
Exercise/ Documents/ Desktop/
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File systems

File systems

A typical computer **file system** is structured like a **tree**

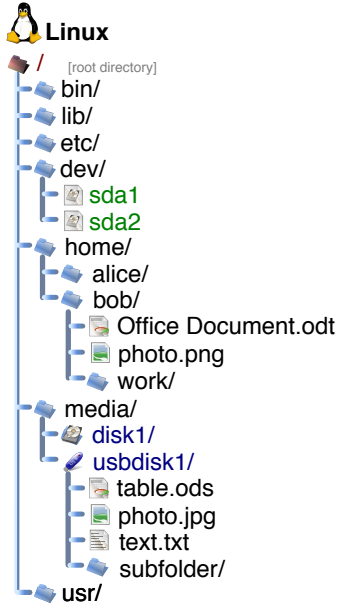


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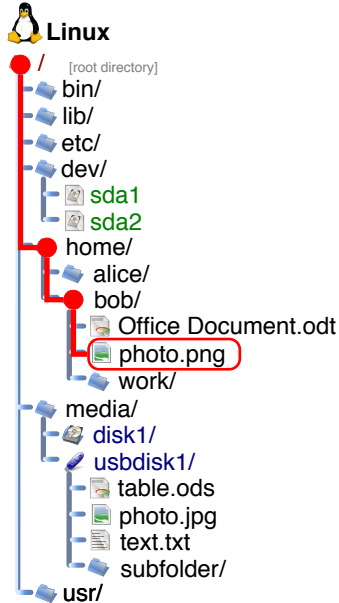
- Every running computer program, i.e. every process, including the **shell**, refers to one directory inside the file system tree as its **working directory**.
- When using the **shell**, one often says “I am in the directory xzy”.
- The **working directory** is not static, it can be changed throughout the runtime of a process.

File systems



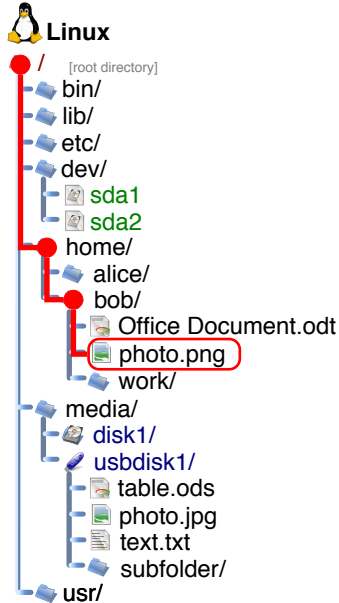
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File systems



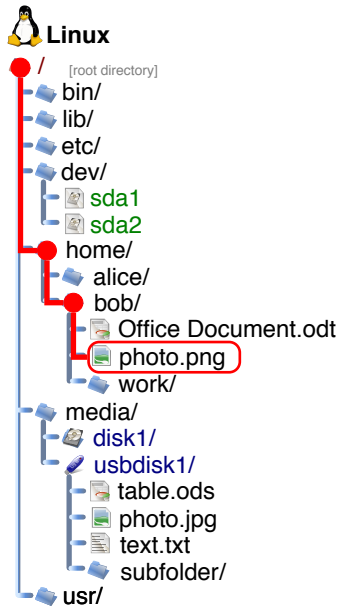
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- **Absolute paths** start in the root directory, for example
`/home/bob/photo.png`
- **Relative paths** start in the current working directory, for example
`./bob/photo.png`
given that the current working directory is `/home`.

File systems



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- **Absolute paths** start in the root directory, for example
`/home/bob/photo.png`
- **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.

Working with the file system

- **pwd** - print working directory
Prints the current working directory

Working with the file system

- **pwd** - print working directory
Prints the current working directory
- **ls** - list
Displays the contents of folders (directories)
 - **ls -l** show details
 - **ls -lh** human readable file sizes
 - **ls -l** show hidden files and folders

Working with the file system

- **pwd** - print working directory
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- **ls** - list
Displays the contents of folders (directories)
 - **ls -l** show details
 - **ls -lh** human readable file sizes
 - **ls -l** show hidden files and folders
- **cd** - change directory
Changes the current working directory

- **mkdir** **<path>** - make directory

Creates a new directory

Working with the file system

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Creates a new directory

- **cp <source path> <destination path>** - copy

Copies files and folders. **Overwriting targets cannot be undone!**

- **cp -r** - recursive mode

Required to copy directories with their contents.

Working with the file system

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- **mv <source path> <destination path>** - move

Move files and folders **Overwriting targets cannot be undone!**

Working with the file system

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- **cp -r** - recursive mode

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.

- **rm <path>** - remove

Remove files and folders. **Removing cannot be undone!**

- **cp -r** - recursive mode

Required to remove directories with their contents.

Getting started with plain text files

- **more <path>**

Page through text one page at a time

Inspecting plain text files

- **more <path>**

Page through text one page at a time

- **less <path>** - the opposite of more

More powerful than more, bidirectional, provides searching

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- **cat <path> [<path> ...]** - concatenate

Concatenates input files and prints them to the standard output (more on that later).

- **head <path>**

Output the first n lines of a plain text file.

Inspecting plain text files

- **head <path>**

Output the first n lines of a plain text file.

- **tail <path>**

Output the last n lines of a plain text file.

- **tail -f** - follow

Keeps printing new lines as the file grows.

- A **text editor** is a program used to edit plain text files

Creating and editing plain text files

- A [text editor](#) is a program used to edit plain text files
- Well known graphical editors are [Notepad](#) on Microsoft Windows and [TextEdit](#) on Apple macOS

Creating and editing plain text files

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- Well known graphical editors are [Notepad](#) on Microsoft Windows and [TextEdit](#) on Apple macOS
- [Nano](#) is a text editor that does not require a graphical user interface but works on the command line

- **nano <path>**

Opens the file specified by path. Can be used on non-existing paths to create new files.

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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.

Process streams

- Every **process** has three input / output streams
 - Standard input (stdin)
 - Standard output (stdout)
 - Standard error (stderr)

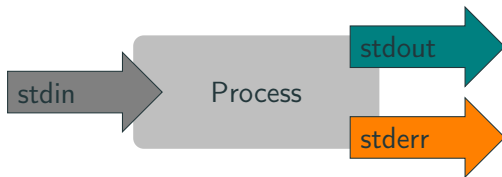
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- We have so far **only worked with stdout**.

- Normally, we cannot see the difference between `stdout` and `stderr`

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- This output is produced on `stdout`

```
$ ls -l Exercise/data ↵  
total 13960  
-rw-r--r-- 1 vorkurs vorkurs 14293917 Mar 27  
2018 clinvar_20180225.vcf.gz
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Process streams

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- This output is produced on `stderr`

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

- 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!

- 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`
- 👉 Duplicate the content of the file `repetition2.txt` and write it to the 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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- A user can be a real person or just be an arbitrary logical entity
- Groups are sets of users
- Every file has a single **owner** and is also associated with a single **group**

Users, groups and permissions

```
$ ls -l Exercise/data ↵
```

```
total 13960
```

```
-rw-r--r-- 1 vorkurs vorkurs 14293917 Mar 27 13:42 clinvar_20180225.vcf
```

Group

The file owner

- A set of **permissions** is associated with each file which determine who has what type of access to the file

Users, groups and permissions

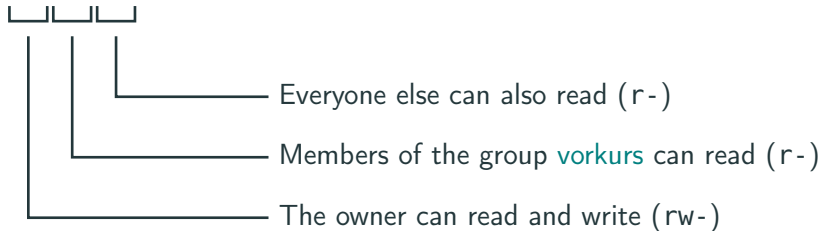
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- There are three access types:
 - **read**
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- There are three access types:
 - **read**
 - **write**
 - **execute**
- This triplet of permissions (**rwX**) is defined for three groups of users:
 - The owner
 - Members of the file's group
 - The rest of the world

Users, groups and permissions

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total 13960
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```



The interpretation of the permissions for **directories** is slightly different

- **read** determines whether the contents of a directory can be seen
- **write** determines whether files can be created or deleted
- **execute** determines whether a user can change (**cd**) into the directory

- **chown [owner][:group] <path>** - change ownership

Changes the ownership and / or group association of a file or directory. Only the **root** user is allowed to change the owner of a file.

Users, groups and permissions

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Changes the ownership and / or group association of a file or directory. Only the **root** user is allowed to change the owner of a file.

- **chmod** **<permissions>** **<path>** - change file mode bits, aka permissions

Changes the file permissions. Examples:

- **chmod g+w <path>**

Add write permissions to the group

- **chmod o-r <path>**

Remove read permissions for the rest of the world

- Shortcuts:

(o)wner, (g)roup, (o)thers, (a)ll at once

(r)ead, (w)rite, e(x)ecute

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```

Add the [write](#) permission to everyone:

```
$ chmod a+w Exercise/data/clinvar_20180225.vcf.gz ↵  
$ ls -l Exercise/data ↵  
total 13960  
-rw-rw-rw- 1 vorkurs vorkurs 14293917 Mar 27 13:42 clinvar_20180225.vcf
```

- Permissions can also be specified numerically
 - 4: read (r)
 - 2: write (w)
 - 1: execute (x)

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- Permissions can also be specified numerically
 - 4: read (r)
 - 2: write (w)
 - 1: execute (x)
- To combine permissions, the numbers are added
- Three digits specify the permissions for all three groups (owner, group, rest of the world) simultaneously:

chmod 750 <path>

- $7=4+2+1$: owner has all permissions (rwx)
- $5=4+1$: group members have read and execute permissions (rx)
- 0: rest of the world has no permissions

Downloading data from the internet

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- **wget <url>**

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

- **wget -c** or **wget --background**

Continue downloading a file that was already partially downloaded

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- **curl -LO <url>**

curl is another command line tool to download remote files, similar to **wget**.

Downloading data from the internet

Example **wget** invocation:

```
$ wget https://compbio.de/vorkurs/material.zip ↵
--2020-10-20 20:20:43-- https://compbio.de/vorkurs/material.zip
Resolving compbio.de (compbio.de)... 188.40.166.122
Connecting to compbio.de (compbio.de)|188.40.166.122|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 10586 (10K) [application/zip]
Saving to: 'material.zip'

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

2020-10-20 20:20:43 (15.3 MB/s) - 'material.zip' saved [10586/10586]
```

Downloading data from the internet

Example **curl** invocation:

```
$ curl -LO https://compbio.de/vorkurs/material.zip ↵
```

% Total	% Received	% Xferd	Average Speed	Time	Time	Time	Current
			Dload	Upload	Total	Spent	Left
100	10586	100	10586	0	0	57532	0
--:--:--	--:--:--	--:--:--	--:--:--	--:--:--	--:--:--	--:--:--	57532

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
- `zip` is an “all in one” solution, i.e. does archiving and compression

- **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
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ZIP file handling

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```
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    inflating: material/duplicated_file.txt
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```
 extracting: material/my_diff_2.txt
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```
    inflating: material/my_diff_1.txt
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```
    inflating: material/tmp.txt
```

```
    inflating: material/my_sort_2.txt
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```
$ ls -F ↵
```

```
Desktop/  Documents/  Exercise/  material/  material.zip
```

ZIP file handling

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```

```
    inflating: material/my_diff_1.txt
```

```
    inflating: material/my_sort_1.txt
```

```
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```

```
    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 -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%)
```

- **tar tzf <path>**

Shows the contents of a gzipped tar file

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Unpacks the contents of a gzipped tar file. **Overwrites existing output file paths!**

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Unpacks the contents of a gzipped tar file. **Overwrites existing output file paths!**

- **tar cvzf <outputpath> <contentpath> [<contentpath> ...]**

Add content to a zip file recursively. **Overwrites an existing output zip file if it exists.**

```
$ 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
```

```
$ 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
```

```
$ 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
```

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- TAR files are sometimes compressed with compression tools other than `gzip`.
- For `.tar.bz2` files, use the `j` switch instead of the `z` switch
- For `.tar.xz` files, use the `J` switch instead of the `z` switch
- In fact, recent versions of `tar` will detect the compression algorithm automatically:

```
$ tar xf material.tar.gz ↵
```


- To compress only a single file, a file archive is not necessary

Standalone GZIP files

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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 http://compbio.de/vorkurs/SRR6800317.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

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Inspect the downloaded file

```
$ ls -lh SRR6800317.fastq.gz ↵
```

-rw-r--r--	1	vorkurs	vorkurs	14M	Apr 3 2018	SRR6800317.fastq.gz
------------	---	---------	---------	-----	------------	---------------------

Standalone GZIP files

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```

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------------	---	---------	---------	-----	------------	---------------------

Decompress the downloaded file

```
$ gunzip SRR6800317.fastq.gz ↵
```

Inspect the decompressed file

```
$ ls -lh SRR6800317.fastq ↵
```

-rw-r--r--	1	vorkurs	vorkurs	89M	Apr 3 2018	SRR6800317.fastq
------------	---	---------	---------	-----	------------	------------------

File sizes

- **du <path>** - disk usage

Can be used to show the sizes of individual files or the total size of entire 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.

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

```
$ du -h material.zi ↵p
```

```
12K      material.zip
```

```
$ ls -lh material.zip ↵
```

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

File sizes

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

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```
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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
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File sizes

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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
- When **du** is invoked with the flag **--apparent-size**, it too reports the size of the content

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-side**

Output a human readable, side-by-side view instead of machine readable output

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

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 characters
- **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 redundant lines only once

- **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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Prints all lines of the input that match the given regular expression pattern

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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

```
$ 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

- The `|` (pipe) character can be used to **redirect** the **standard output** stream of one process to the **standard input** stream of another process

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- Remember the common structure of command line interfaces that we have seen often today:

```
COMMAND [OPTIONAL SWITCHES] [INPUT PATH]
```

Process streams II

- The | (pipe) character can be used to **redirect** the **standard output** stream of one process to the **standard input** stream of another process
- Remember the common structure of command line interfaces that we have seen often today:

```
COMMAND [OPTIONAL SWITCHES] [INPUT PATH]
```

- Most programs we have seen today would process data from the **standard input** stream 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
```

Process streams II

Without stream redirection:

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

With stream redirection:

```
$ ls -l | wc -l ↵  
15
```

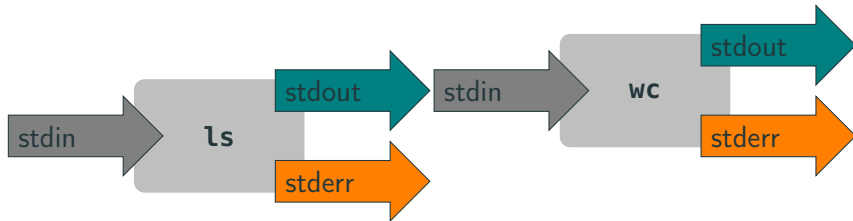

Process streams II

Without stream redirection:

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$ wc -l temp.txt ↵  
15 temp.txt
```

With stream redirection:

```
$ ls -l | wc -l ↵  
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
```

What does this do and why?

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