Unix training

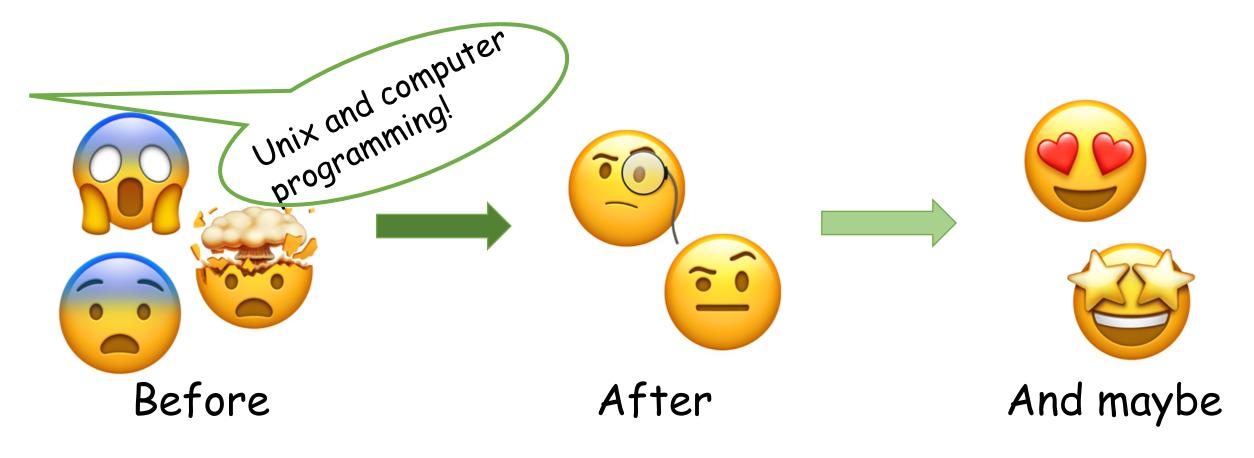
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General concepts of Computer programming

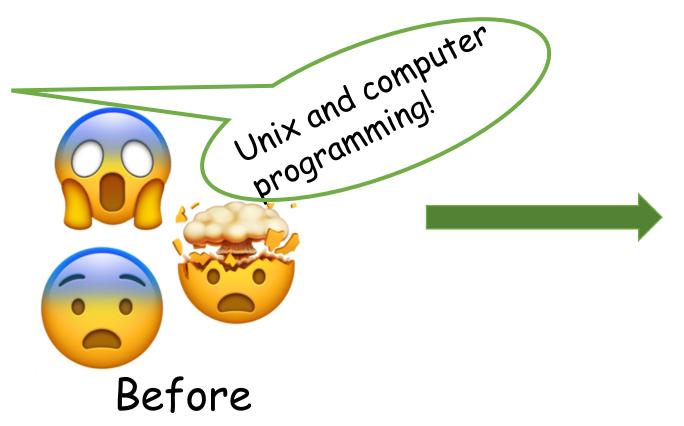
- Programming is a language for talking to computer.
- Language has grammar (syntax) and vocabs (commands = noun + verb (+ adjective)).
- Computer often reads from top line and go downward.
- Computer will do EXACTLY as you tell them, and sometimes will over-write things without asking for a confirmation
- Commands and names are case-sensitive.
- You can name objects anything you like, but
 - Use **meaningful** names
 - Avoid using function name as object name
 - Special characters e.g. # \$ & space are not allowed in object names (or it will make life difficult)
- Google is your friend, and so are BioStar,
 StackExchange, ResearchGate

 People often have the
 same question as you do

What this session is



What this session is **NOT**





After

Basic bioinformatics files

- For any sequencing projects
- Or if you work with genome databases, nucleic acid and, protein sequences
- FASTQ .fastq .fq .fq.gz
- FASTA .fasta .fa .fa.gz .fasta.gz
- sam, bam, gff, vcf, etc.

https://bioinformatics.uconn.edu/resources-and-events/tutorials-2/file-formats-tutorial/#

FASTQ file

Header line: can contain various information about the sequence eg. coordinate on sequencing chip. Here, it shows accession number and read ID.

File name: data from paired-end sequencing will have _1 _2 at the end of their file name. These numbers correspond to reads from each end of the same sequenced fragment

Another header line for the same sequence. Sometimes there will be only the plus (+) sign.

Quality score: Each character represent a score

@ERR506076.1 1 length=100

TAAGAATTAATGTATTGAGCTACACGTAATGTGATGTGĆAACTCAATCAGATGAGTGAAATTGCCCAGAAACAAATCACCAAAGAAGGTACA
TATATGTA

+ERR506076.1 1 length=100 4

@ERR506076.2 2 length=100

GCCGAAATTAGTGTTGACGGTCCGTTAAGAATTAATGTATTGATACACGTAATGTGATGTGCAACTCAATCAGATGAGTGAAATTGCCCAGA AACAAATC

+ERR506076.2 2 length=100

... (and many more lines follow)

FASTA file

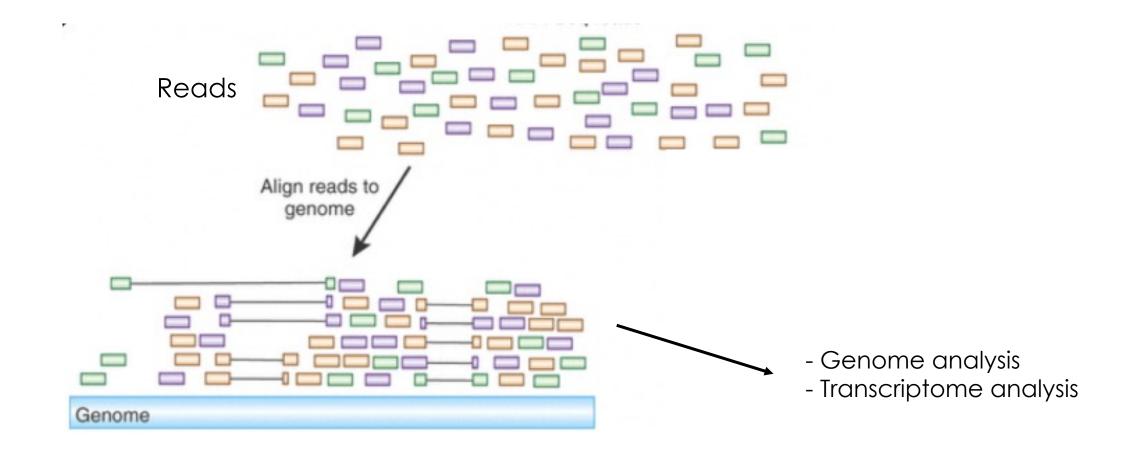
file name: .fa or .fasta

Header line: Information about the sequence. For genomic sequence, this is often contig ID or chromosome number. It can also contain other information such as contig length, species name, source of the information

>SM_V7_1 length=88881357

... (and many more lines follow)

SAM and BAM files sequence alignment/map, and binary version



SAM and BAM files sequence alignment/map, and binary version

Information about the mapping e.g. read ID, mapped position, mapping score

```
37M
                                                            15
1:497:R:-272+13M17D24M 113
                              chr1 497
                                                                       100338662 0
                                        0;==-==9;>>>>>>>>>>>>>>>>
CGGGTCTGACCTGAGGAGAACTGTGCTCCGCCTTCAG
                                                                                XT:A:U
                                                                                          NM: i:0
SM: i:37
          AM: i:0
                    X0:i:1
                              X1:i:0
                                        XM: i:0
                                                  X0:i:0
                                                            XG:i:0
                                                                      MD: Z: 37
19:20389:F:275+18M2D19M
                               99
                                        chr1
                                                  17644
                                                                       37M
                                                                                          17919
314
          TATGACTGCTAATAATACCTACACATGTTAGAACCAT
                                                  >>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>>
RG: Z: UM0098: 1
                                                                                          X0:i:0
                    XT:A:R
                              NM: i:0
                                        SM: i:0
                                                  AM: i:0
                                                            X0:i:4
                                                                      X1:i:0
                                                                                XM: i:0
XG: i:0
          MD: Z:37
19:20389:F:275+18M2D19M
                               147
                                        chr1
                                                  17919
                                                                      18M2D19M
                                                            :44999:499<8<8<<<8<<><<<><7<:<<<>><<
17644
                    GTAGTACCAACTGTAAGTCCTTATCTTCATACTTTGT
          -314
XT:A:R
          NM: i:2
                    SM: i:0
                              AM: i:0
                                        X0:i:4
                                                  X1:i:0
                                                            XM: i:0
                                                                      X0:i:1
                                                                                XG: i:2
                                                                                           MD:Z:
18^CA19
9:21597+10M2I25M:R:-209
                                        chr1
                                                  21678
                                                                      8M2I27M
                    CACCACATCACATATACCAAGCCTGGCTGTGTCTTCT
                                                            <:9<<5><<<>>><>
21469
          -244
XT:A:R
                                                            XM: i:0
          NM: i:2
                    SM: i:0
                              AM: i:0
                                        X0:i:5
                                                  X1:i:0
                                                                      X0:i:1
                                                                                XG: i:2
                                                                                          MD:Z:35
```

GFF filesGenome annotation

Location on the genome, what feature(s) has it been annotated for, evidence, etc.

```
Schisto_mansoni.Chr_3.unplaced.SC_0083
                                                CDS 852574
                                                                                   ID=Smp_138770.1:exon:18;Parent=Smp_138770.1;isObsolete=false;timelastmodified=17.10.2011+10:47:01+BST
                                                             852785
                                       chado
Schisto_mansoni.Chr_3.unplaced.SC_0083
                                                                                   ID=Smp_138770.1:exon:17;Parent=Smp_138770.1;isObsolete=false;timelastmodified=17.10.2011+10:47:01+BST
                                       chado
                                                CDS 854903
                                                             854990
Schisto_mansoni.Chr_3.unplaced.SC_0083
                                                                                   ID=Smp_138770.1:exon:16;Parent=Smp_138770.1;isObsolete=false;timelastmodified=17.10.2011+10:47:01+BST
                                               CDS 857133 857186
                                       chado
                                                                                   ID=Smp_138770.1:exon:15;Parent=Smp_138770.1;isObsolete=false;timelastmodified=17.10.2011+10:47:01+BST
Schisto_mansoni.Chr_3.unplaced.SC_0083
                                       chado
                                                CDS 860632 860763
Schisto_mansoni.Chr_3.unplaced.SC_0083
                                                CDS 861448 861573
                                                                                   ID=Smp_138770.1:exon:14;Parent=Smp_138770.1;isObsolete=false;timelastmodified=17.10.2011+10:47:01+BST
                                       chado
```

VCF files Variant calling format

Position of genome, sequence on reference genome, sequence in mapped reads, other information

```
##fileformat=VCFv4.0
##fileDate=20090805
##source=mylmputationProgramV3.1
##reference=1000GenomesPilot-NCBI36
##phasing=partial
.....more header lines......
                   REF ALT QUAL FILTER INFO
#CHROM POS ID
                                                         FORMAT
                                                                    NA00001
                                                                               NA00002
                                                                                           NA00003
20 14370 rs6054257 G
                            29 PASS NS=3;DP=14;AF=0.5;DB;H2
                                                                GT:GQ:DP:HQ 0 | 0:48:1:51,51
1 | 0:48:8:51,51 1/1:43:5:.,.
                       3 q10 NS=3;DP=11;AF=0.017
  17330 . T A
                                                         GT:GQ:DP:HQ 0 | 0:49:3:58,50 0 | 1:3:5:65,3
0/0:41:3
    1110696 rs6040355 A
                        G,T 67 PASS NS=2;DP=10;AF=0.333,0.667;AA=T;DB GT:GQ:DP:HQ 1 | 2:21:6:23,27
20 1230237. T
                  . 47 PASS NS=3:DP=13:AA=T
                                                         GT:GQ:DP:HQ 0 | 0:54:7:56,60 0 | 0:48:4:51,51
0/0:61:2
    1234567 microsat1 GTCT G,GTACT 50 PASS NS=3;DP=9;AA=G
                                                                    GT:GQ:DP
                                                                               0/1:35:4
                                                                                         0/2:17:2
1/1:40:3
```

Working with bioinformatics files

- Mostly text files in specific format
- Can be over many gigabytes in size
- Can have millions of lines

• ... we won't work manually

Unix

What is Unix?

- An operating system (like Windows or OSX)
- Provides a way to interact with the computer
- Many versions, including Linux, which is a free version of Unix

Why use it?

- Output of biological research is often large text files
- Suitable for working with these files and very powerful
- Saves time
- Widely used by the scientific community
- Robust and stable

Unix is another (computer) language

Languages have syntax (grammar)

Languages have nouns

Languages have verbs

Unix is another (computer) language

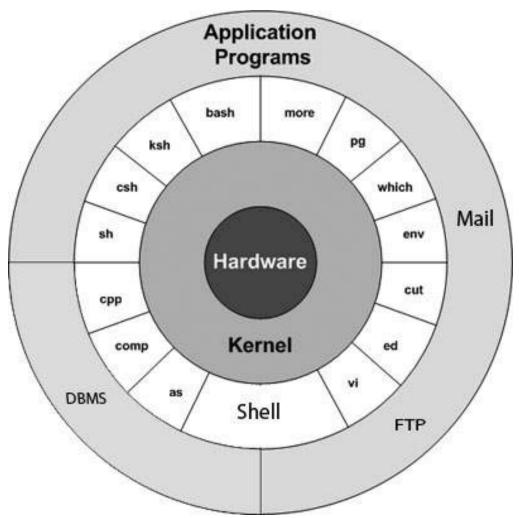
Languages have syntax (grammar)

Unix command line normally look like this...

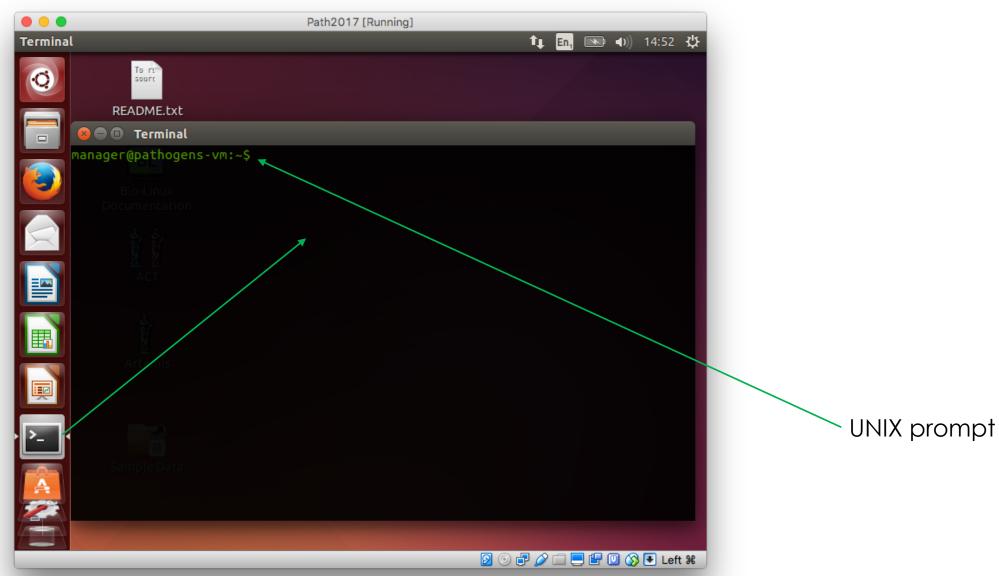
```
$ some command filename
                                        command (verb) follows by
                                        filename or location (noun)
$ some command location
                                         or additional information
                                            (arguments/options)
$ some command -i -a -x -n5 filename
$ some command filename anotherfile
 some command filename > newfilename
```

Unix

Operating system that underlies a lot of bioinformatics work, and system administration



Terminals and the Command Line



Unix Commands

Command What it does

Is List the contents of the current directory

cd Change directory

mv Moves a file

cp Copies a file

rm Deletes a file

less Displays the contents of a file

head Displays the first ten lines of a file

tail Displays the last ten lines of a file

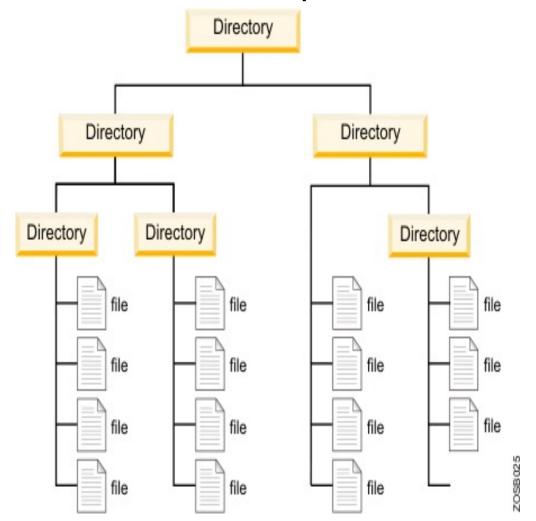
cat Concatenates files together

pwd Prints working directory

mkdir Makes a new directory

Computer file system

Folder is called "directory" in programming world You need to tell the computer the EXACT location of the file



File not found

There is no such file

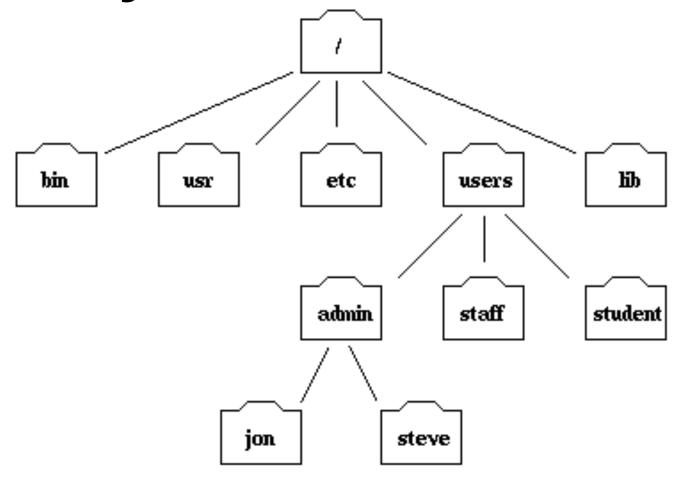
These are very common mistake.

Make sure you get the location

correct + the spelling

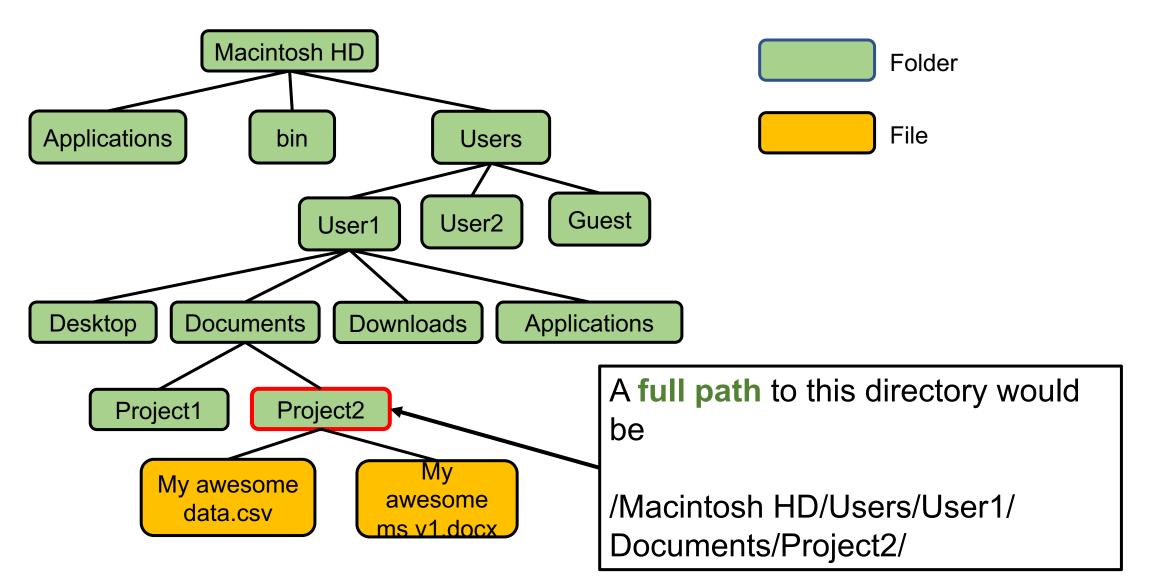
use TAB key

Unix file system

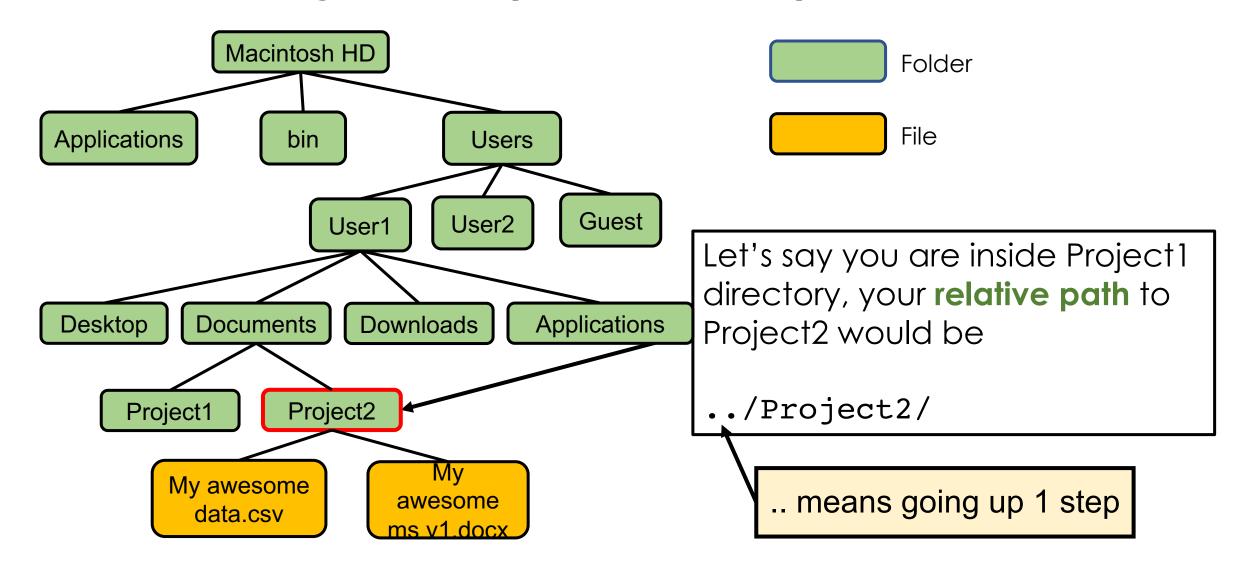


Part of the filesystem tree

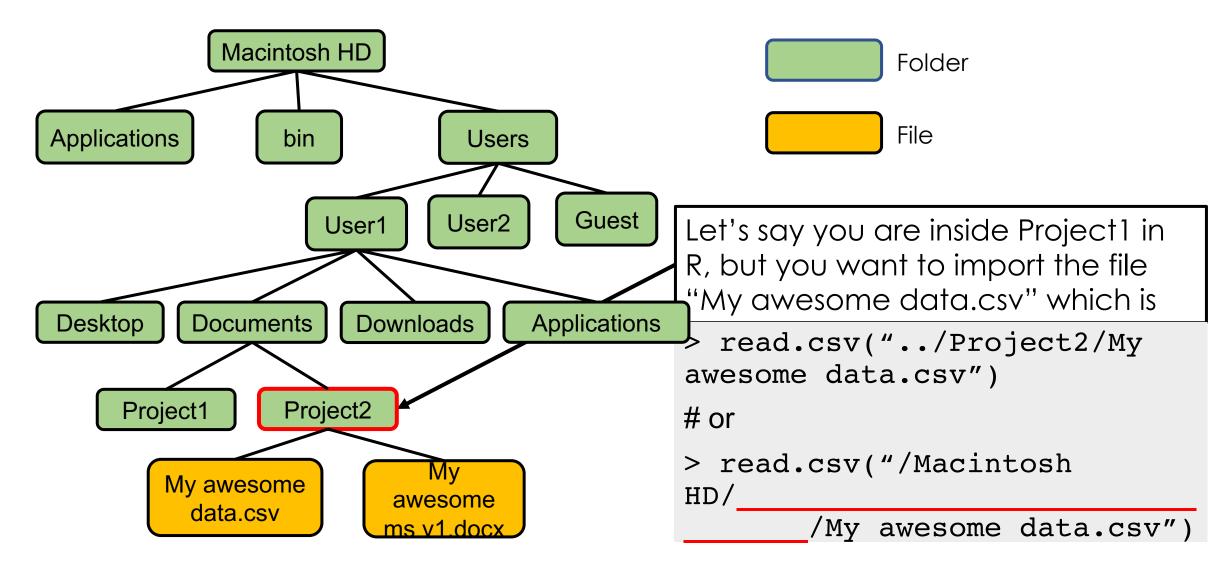
Mac file system (simplified)



Mac file system (simplified)



Mac file system (simplified)



Navigating

pwd

Is

cd

find

•

- -

Look into files

more

less

head

tail

cat (2 functions)

Extracting information from/about files

grep

WC

cut

sort

uniq

Creating/moving/copying/deleting files

touch

mkdir

mv

cp

rm

rmdir

Editing files

```
vim
chmod (and file permission)
cat
paste
>
>>
```

Special characters and wildcard characters

- output from command on the left become input for command on the right
- * any number of characters
- ? one character
- specify a range of characters
- specify a list of terms, separated by commas
- ! exclude this range of characters

And more complex (fancy/useful) commands

sed string editor

awk pattern search and more

```
Other useful things
history
man
which
tar
gunzip
diff/gdiff
command line options (- ...)
TAB and double TAB
"arrow up" press arrow up to get old commands
CTRL a Go to start of line
CTRL e Go to end of line
```

Reminders

- Unix is case sensitive
 - LS is not the same as Is
- Spaces must go between a command and the values passed to a command
 - mkdir newdir will work
 - mkdirnewdir will give an error
- Spelling must be correct. Mistyping a command or file name will give an error
- Use TAB key
- Don't fear the command line!

File permission (Is -I)

-rwxrw-r--, this means the line displayed is:

- a regular file (displayed as -)
- readable, writable and executable by owner (rwx)
- readable, writable, but not executable by group (rw-)
- readable but not writable or executable by other (r--)

Read	Write	Execute
4	2	1

If you want revision/extension on Unix

- http://www.ee.surrey.ac.uk/Teaching/Unix/
- http://swcarpentry.github.io/shell-novice/
- http://jnmaloof.github.io/BIS180L_web/2019/04/02/2Just_Enough_Unix/
- Look for Unix cheatsheet(s)