Topic 2:

Unix and Programming for Biologists

Included in this topic

… and the things that I think are most important

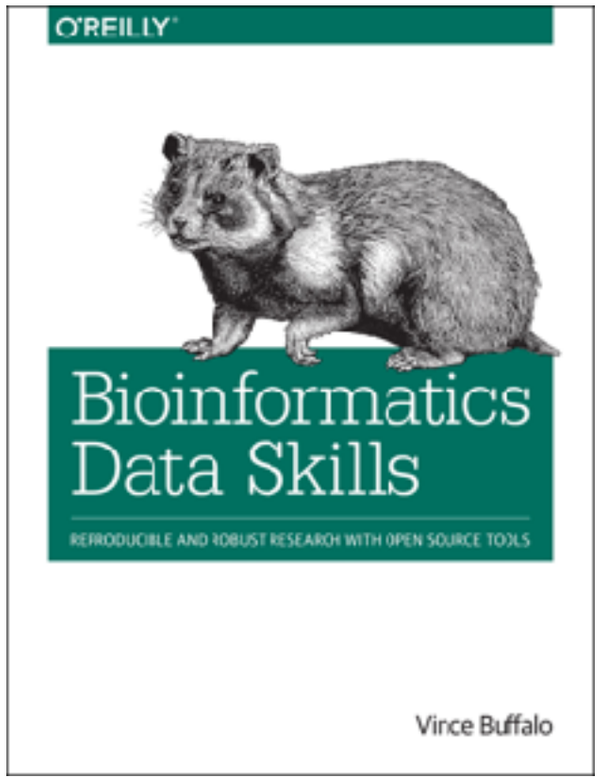
- Reproducibility
- The command line environment
- Paths (absolute versus relative)
- Modularity
- Metacharacters
- Different programming languages and why
- Learn a good text editor!

Ask for help!

There are lots of sources of help around - make use of them!

Sometimes the solution to a problem is simply knowing the right terms to Google or to search on StackOverflow

I highly recommend Vince Buffalo's "Bioinformatic Data Skills"



ChatGPT
although I hate it

stack overflow

Non-command line options

There are a number of non-command line options out there

For example

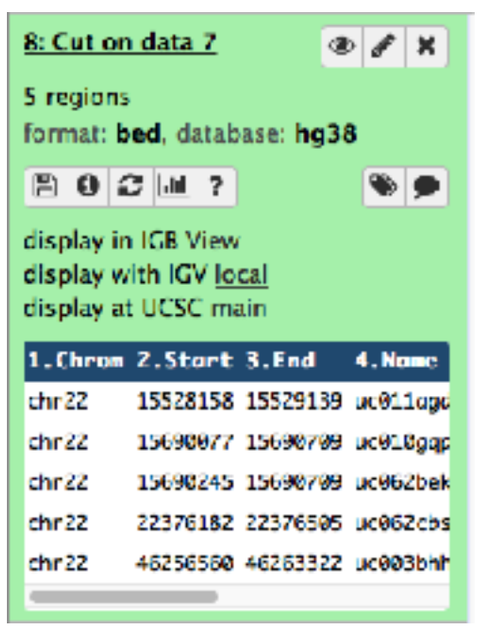
- Galaxy (https://www.galaxyproject.org/)
  Open Source, runs many of the common tools

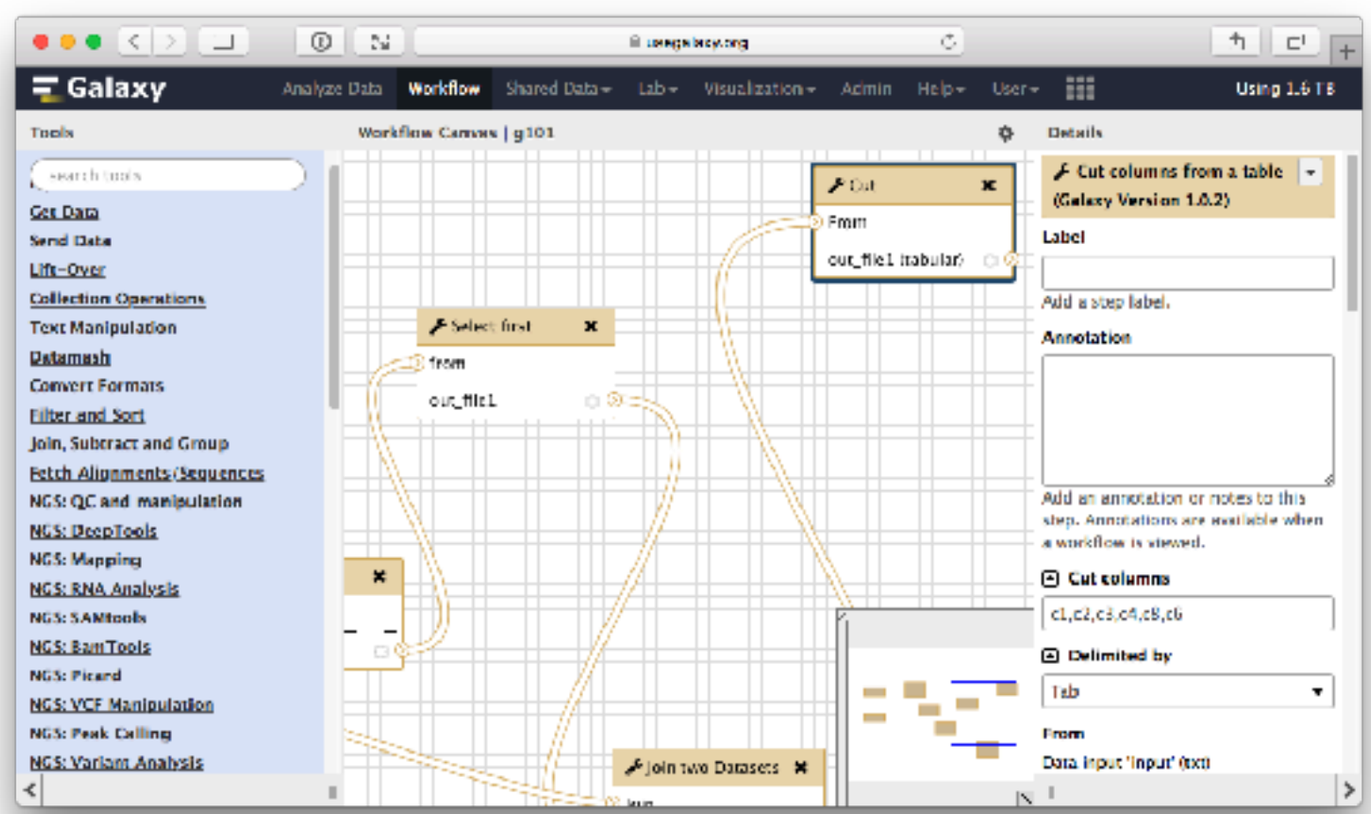
- geneious
  Commercial (a license costs $200 per year for a student)

GUI = Graphical User Interface

Galaxy

- Run pre-established tools, setup is form-based
- Jobs submitted to a cluster of servers (running the software stack)





Tons of features and supports most of the common types of analyses

- *Assembly*
- *Alignment*
- *Primer design, probe design*
- *Variant calling*
- *Annotation*
- *Even phylogenetics!*

So why use the command line?

So why use the command line?

- Efficiently work with large files
- Steps recorded, repeatable, auditable
- Powerful text editing tools. Powerful code revision tools
- Generally faster than GUI based methods
- Most scientific programs do not have a GUI (necessity)
- Highly portable and communicable
- Allows different programs to be combined arbitrarily
- It’s free and makes you feel like a hacker

Typical things that you might do at the command line

- Download and install packages
- Download, decompress and validate datasets
- Run software
  - Fine tune parameters
  - Analyse data

Reproducibility

One of our responsibilities as scientists is to present our methods so that others could reproduce them

In bioinformatics, keeping a record of what you do at the computer is as important as keeping detailed notes in your lab book

Your worst enemy when working on a computer is yourself from one year ago

Reproducibility

There are many ways to practice reproducibility

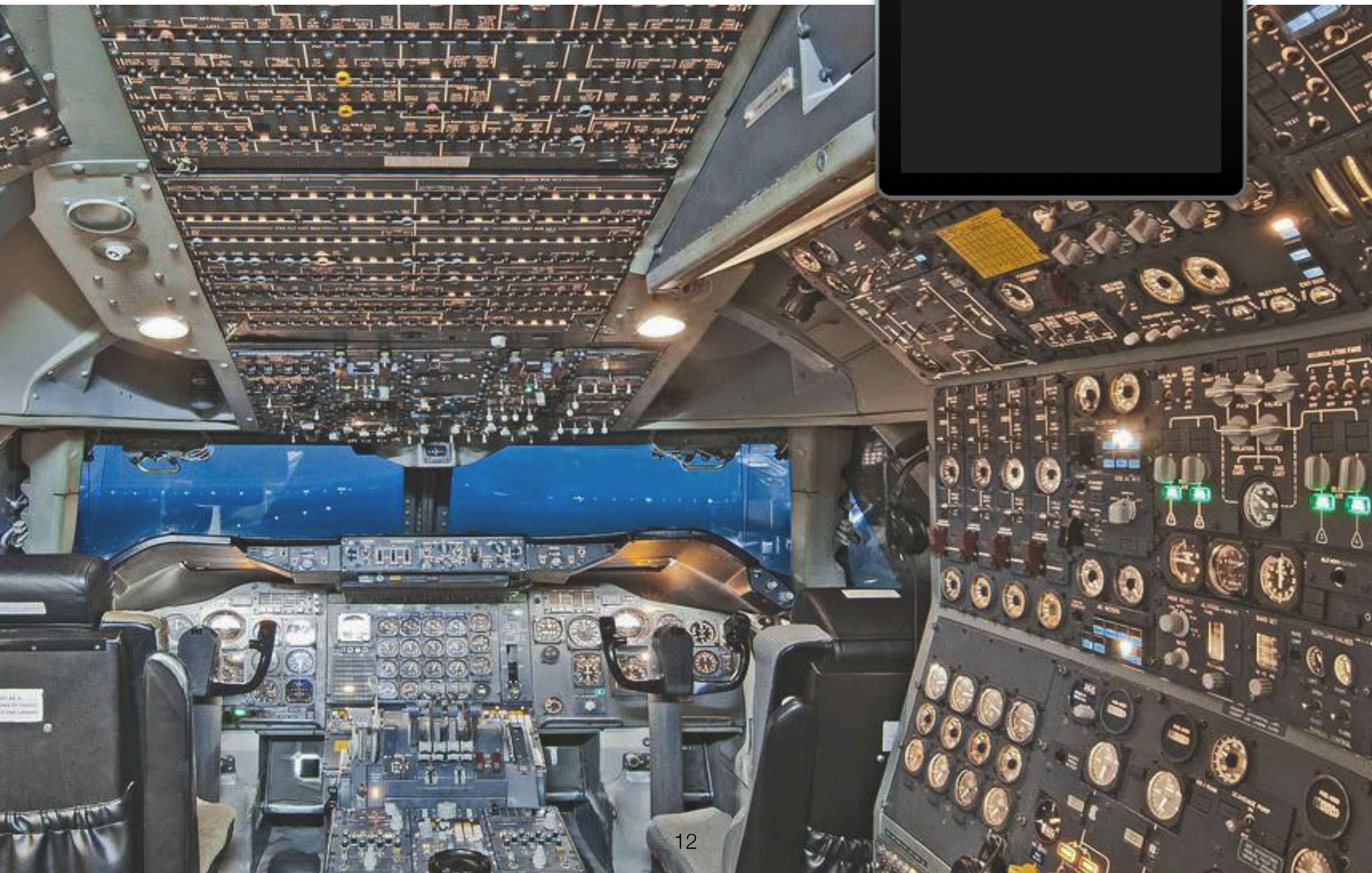
Clearly identify programs and dependencies

Documented shell scripts

Variable labels for all inputs

Version control

The UNIX SHELL



Part 1:Interface

1.1 Prompt or command line

When you open the Terminal on Mac or Linux systems or open a shell instance through Putty you'll get faced with something like this:

Prompt

Part 1:Interface

1.1 Prompt or command line

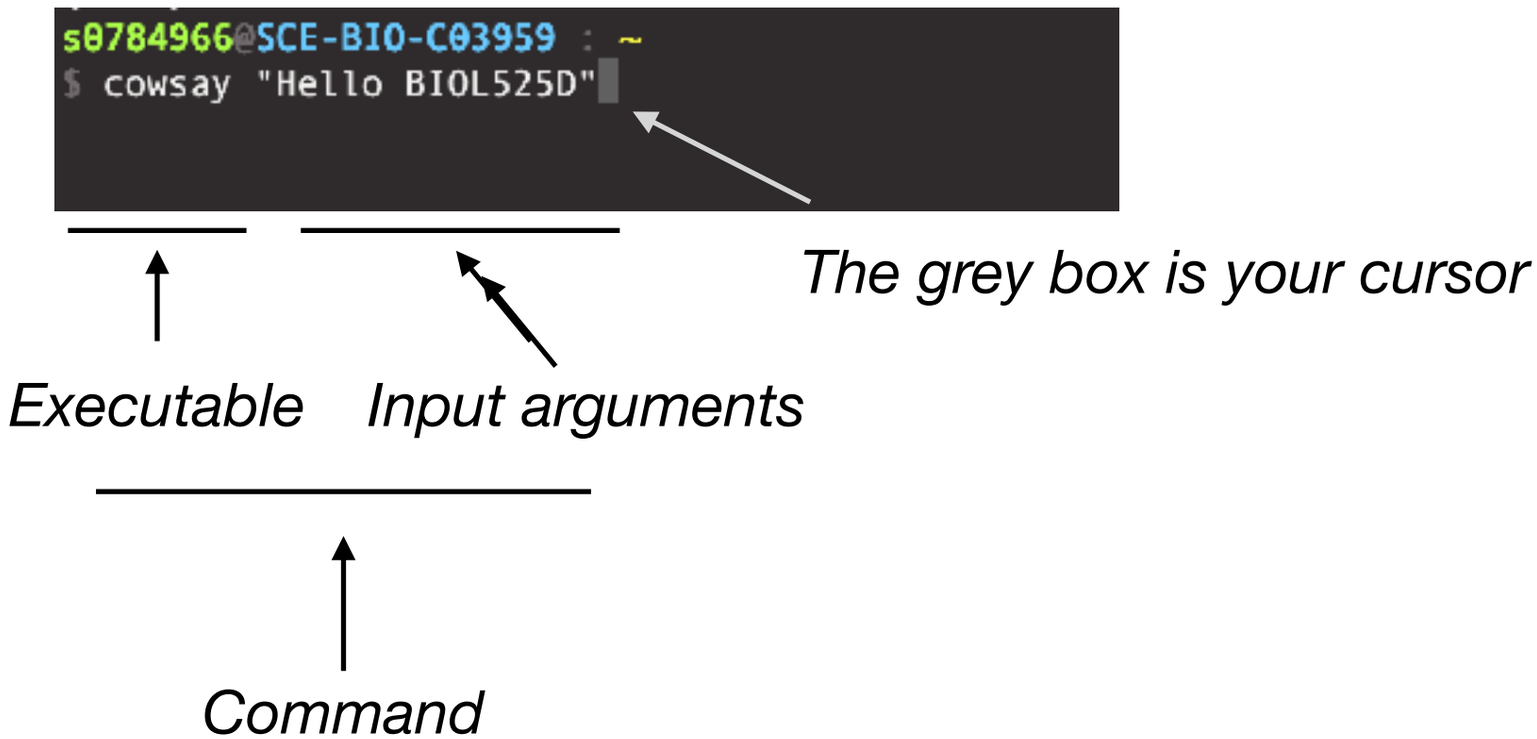
When you open the Terminal on Mac or Linux systems or open a shell instance through Putty you'll get faced with something like this:

Using the command line,
log in to the Virtual Machine you have been allocated to

Part 1:Interface

1.1 Prompt or command line

When you open the Terminal on Mac or Linux systems or open a shell instance through Putty you'll get faced with something like this:



Part 1:Interface

1.1 Prompt or command line

Try playing with the program called ***cowsay***

```
s0784966@SCE-BIO-C03959 : ~
$ cowsay "Hello BIOL525D"
```

The grey box is your cursor

Executable

Input arguments

Command

Part 1:Interface

1.2 Output

```
s0784966@SCE-BIO-C03959 : ~
$ cowsay "Hello BIOL525D"
 _________________
< Hello BIOL525D >
 -----------------
        \   ^__^
         \  (oo)\_______
            (__)\       )\/\
                ||----w |
                ||     ||
(base)
```

Output (STDOUT)

Programs generate output, what you do with the output varies

In a little bit we'll interact with some output

Part 1:Interface

1.3 Arguments

```
s0784966@SCE-BIO-C03959 : ~
$ cowsay "Hello BIOL525D"
 _______________
< Hello BIOL525D >
 ---------------
        \   ^__^
         \  (oo)\_______
            (__)\       )\/\
                ||----w |
                ||     ||
(base)
s0784966@SCE-BIO-C03959 : ~
$ cowsay -t "I'm tired now"
 ______________
< I'm tired now >
 --------------
        \   ^__^
         \  (--)\_______
            (__)\       )\/\
                ||----w |
                ||     ||
(base)
s0784966@SCE-BIO-C03959 : ~
$ cowsay -e'$$' -W 5 "I'm a high roller"
 _____
/ I'm  \
| a    |
| high |
| roll |
\ er   /
 ------
        \   ^__^
         \  ($$)\_______
            (__)\       )\/\
                ||----w |
                ||     ||
(base)
```

The “man” (short for manual) command gives you details about each program e.g. “$ man cowsay”

The “-t” option specifies that the cow should be sleepy

The “-e’$$’” option specifies that the cow should have dollar signs for eyes

The “-W 5’” option specifies that the text should be ‘wrapped’ every 5 characters (or so)

Part 1:Interface

Grammer and GNU syntax

Programs take options and parameters. For example:

rm -i -f --one-file-system --interactive=always A.txt B.gz

rm: the executable/program. always first. the other arguments are specific to that program.

-i -f: short options. single `-`. relative order is generally unimportant.collapsible, e.g-if

--one-file-system: long options. double `-`. some short and long forms are equivalent.

=always: some options take a param value. `=` introduces the value applied to the preceding long option. Short options can take a parameter, but without `=`, e.g.: `tar -cfF.gz mydir`

•**A.txt B.gz** Positional parameters. Variable number of them can be provided. Depending on the program order matters.

Some common commands

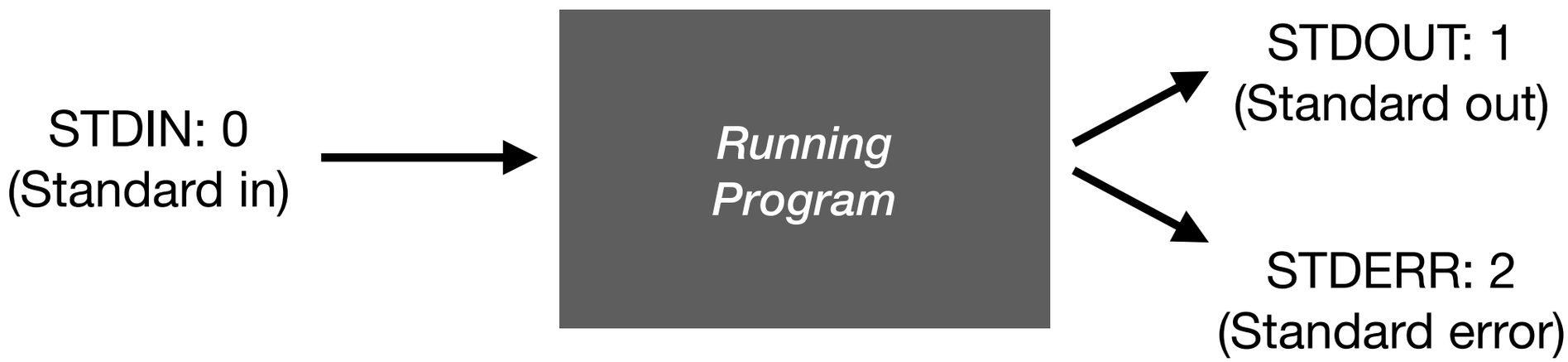
There are many, many UNIX commands to learn and get used to.

Here's a list of programs that I use a lot, for example

ls	cd	wc	top	cp
ps	cat	mkdir	head	mv
less	more	which	pwd	rm
grep	awk	sed	chmod	ssh
seq	echo	who	kill	passwd

Interface: stdio

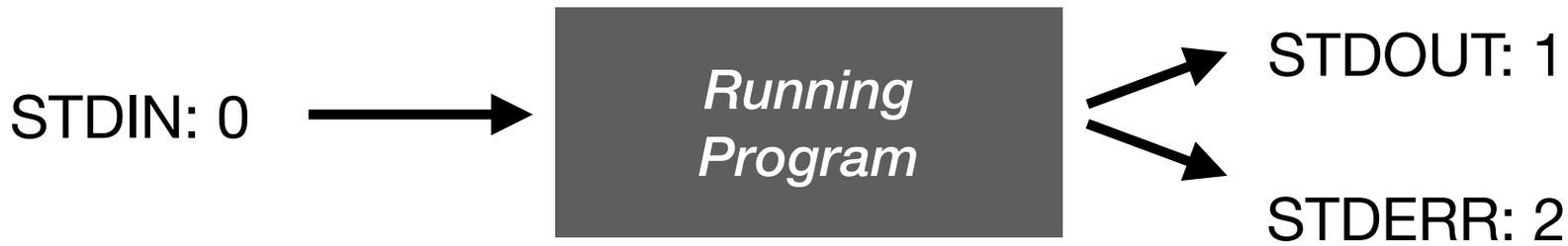
There are three files (or streams) that programs have access to



Under UNIX (the ancestor of Linux, MacOS android)
EVERYTHING IS A FILE

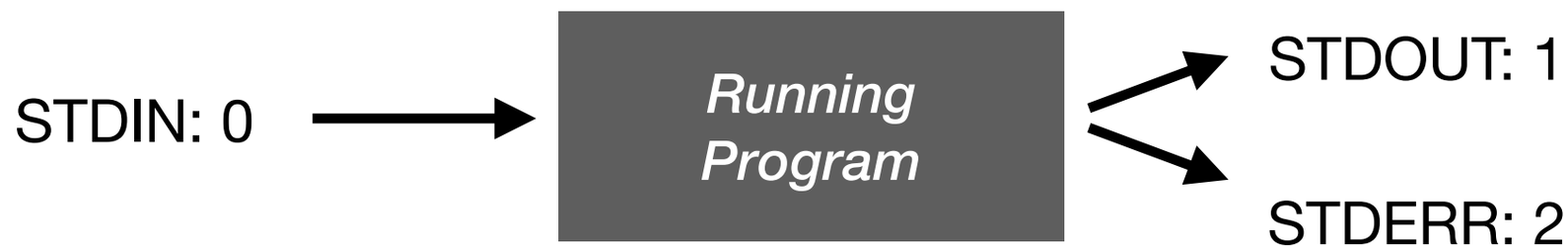
Programs, user input, output, directories (folders) and files are all files and have specific locations

Redirect and pipes



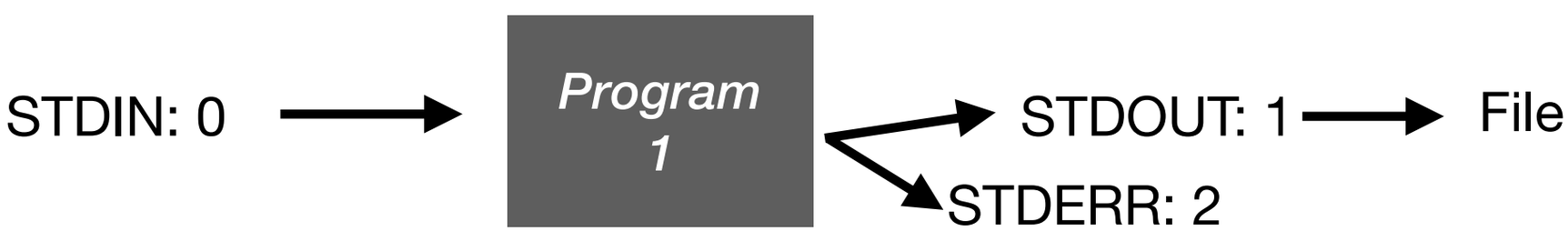
You can manage the different streams using
“redirects” (**>**) and “pipes”(**|**)

Redirect and pipes



You can manage the different streams using
"redirects" (>) and "pipes"(|)

The ">" symbol redirects STDOUT



$ ./program1 > File

The "<" symbol redirects STDIN

$ ./program2 < File

Redirect and pipes

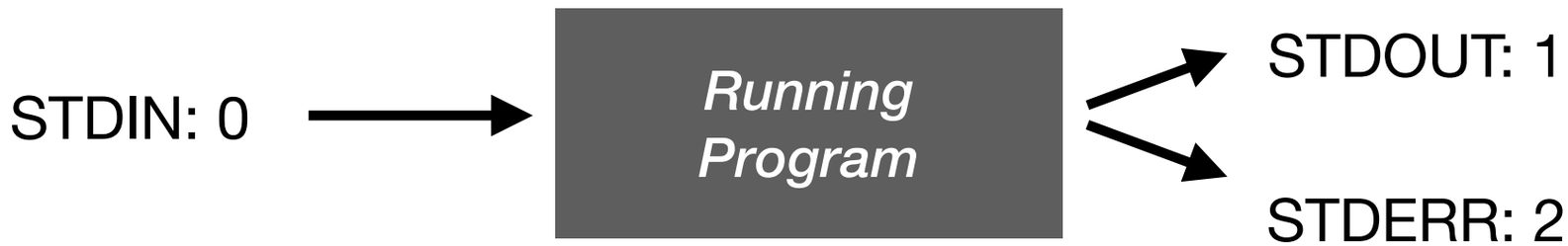
```
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls
./              CoolFile1.txt  temp1.txt      temp1b.txt     temp2.txt
../             CoolFile2.txt  temp1a.txt     temp1c.txt     temp3.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls > fileList.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$ cat fileList.txt
./
../
CoolFile1.txt
CoolFile2.txt
fileList.txt
temp1.txt
temp1a.txt
temp1b.txt
temp1c.txt
temp2.txt
temp3.txt
(base)
```

Use **ls** to list all the files present

Redirect **ls** to “fileList.txt” to keep a record of the files present

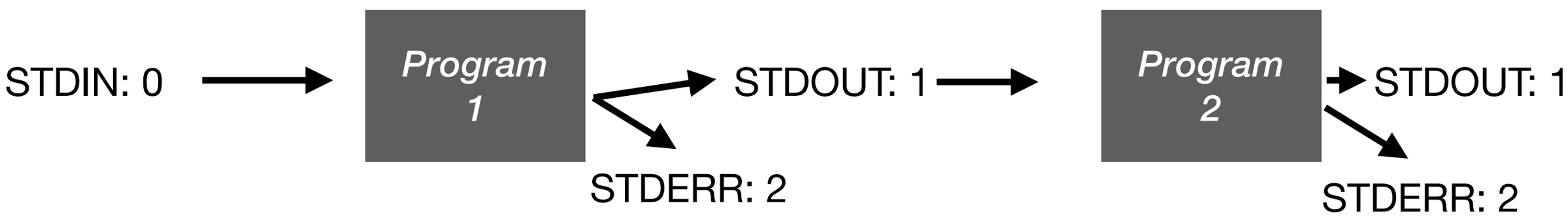
Inspect the contents of “fileList.txt”

Redirect and pipes



You can manage the different streams using
“redirects” (**>**) and “pipes”(**|**)

Pipes sets the STDOUT of one process to STDIN for another



Redirect and pipes

Pipe example

```
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls
./              CoolFile1.txt  temp1.txt      temp1b.txt     temp2.txt
../             CoolFile2.txt  temp1a.txt     temp1c.txt     temp3.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls | sort -r
temp3.txt
temp2.txt
temp1c.txt
temp1b.txt
temp1a.txt
temp1.txt
CoolFile2.txt
CoolFile1.txt
./
../
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls | sort -r | head -n2
temp3.txt
temp2.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$
```

List files using **ls**

Pipe the output of **ls** to **sort** and use the reverse order option

Pipe the output of **ls** to **sort** and use the reverse order option then pipe to **head** to display the first 2 items

Metacharacters

The pipe and redirect symbols (|, > and <) are special characters (called meta characters)

When working at the command line, there are a number of other metacharacters that you should be aware of

Metacharacters

The asterix (*)

- Used to match any and all characters

The question mark (?)

- Used to match a specific character

```
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls
./                  temp1.txt       temp2.txt
../                 temp1a.txt      temp3.txt
CoolFile1.txt       temp1b.txt
CoolFile2.txt       temp1c.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls temp*
temp1.txt    temp1b.txt   temp2.txt
temp1a.txt   temp1c.txt   temp3.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls temp?.txt
temp1.txt   temp2.txt   temp3.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$
```

Metacharacters

Brackets [ ]

- Used to match a specific set of parameters

Hyphen -
(*when within brackets*) -

- Used to specify an alphanumeric range

```
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls
./                temp1.txt       temp2.txt
../               temp1a.txt      temp3.txt
CoolFile1.txt     temp1b.txt
CoolFile2.txt     temp1c.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls temp1[a,b]*txt
temp1a.txt  temp1b.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls temp[1-2]*txt
temp1.txt   temp1b.txt  temp2.txt
temp1a.txt  temp1c.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$ ls temp1[b-c]*txt
temp1b.txt  temp1c.txt
(base)
s0784966@SCE-BIO-C03959 : ~/temptemp
$
```

Metacharacters

When working at the command line, there are a number of special characters (called metacharacters) that you should be aware of

Ampersand - “&”

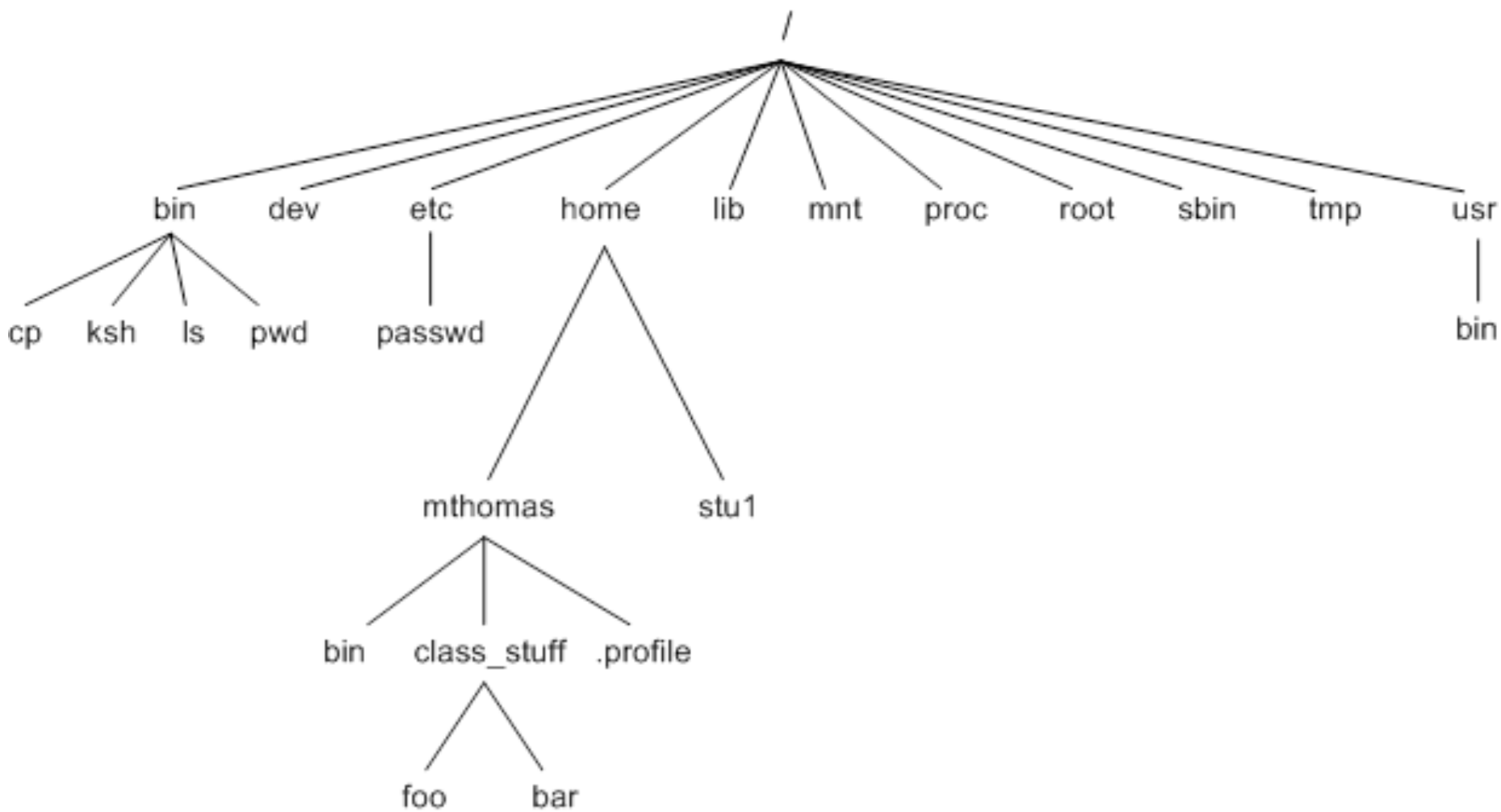
- Used to “background” a process

This leaves a process running in the background allowing you to keep working on other things while it finishes

We’ll make use of this in the tutorial

The UNIX Filesystem

EVERYTHING IS A FILE!



<u>Learning to navigate this file hierarchy is critical</u>

Paths: relative v. absolute

Most files that you will analyse have a location (path) in the hierarchy of files

You can specify the location of a file using it's full address (absolute path) or where it is in relation to your current location (the relative path)

Paths: relative v. absolute

```
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff
$ ls
./              .DS_Store       BIOL525D/       VEG/
../             Admin/          ComputerSetup/  mac/
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff
$ pwd
/Users/s0784966/UBC/ZoologyStuff
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff
$ cat BIOL525D/mycmd.sh
#!/bin/sh

age=31

echo "I am $age years young"
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff
$ cat /Users/s0784966/UBC/ZoologyStuff/BIOL525D/mycmd.sh
#!/bin/sh

age=31

echo "I am $age years young"
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff
$ cd
(base)
s0784966@SCE-BIO-C03959 : ~
$ cat BIOL525D/mycmd.sh
cat: BIOL525D/mycmd.sh: No such file or directory
(base)
s0784966@SCE-BIO-C03959 : ~
$ cat /Users/s0784966/UBC/ZoologyStuff/BIOL525D/mycmd.sh
#!/bin/sh

age=31

echo "I am $age years young"
(base)
s0784966@SCE-BIO-C03959 : ~
$
```

ls (**l**ist)
tells you the files present in your current location

---

pwd -(**p**rint **w**orking **d**irectory)
tells you where you are in the file system

I can access a file in the “BIOL525D” folder using it’s relative path (i.e. making use of my current location)

Or, I can access a file in the “BIOL525D” folder using it’s absolute path (i.e. making use of the file’s location)

If I leave the /Users/s0784966/UBC/ZoologyStuff directory, the relative path I used before no longer works

---

The absolute path works wherever you are though

Paths: relative v. absolute

The text “./“ refers to the directory that you are in

The text “../“ refers to one directory back in the file system

“../“ can be chained together to refer back multiple locations

```
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D
$ ls
./              .DS_Store       AllFiles/       Topic_1/        biol525d/       mycmd.sh*
../             2020_profiles/  Images/         Topic_2.key*    biol525d 2/     software/
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D
$ cd software/
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D/software
$ cat mycmd.sh
cat: mycmd.sh: No such file or directory
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D/software
$ cat ../mycmd.sh
#!/bin/sh

age=31

echo "I am $age years young"
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D/software
$
```

Here’s the contents of the “BIOL525D" directory

I’ll move into the “software” directory

I can not access the “mycmd.sh” file

I can refer to the “mycmd.sh” file if I tell the system that it is one directory back in the file system

Interface: permissions

```
drwxr-xr-x 12 niteshb users 4.0K Apr  8 20:51 testdir
|[-][-][-]    [-----] [---]
| |  |  |        |       |
| |  |  |        |       +-----------> Group
| |  |  |        +-------------------> Owner
| |  |  +----------------------------> Others Permissions
| |  +-------------------------------> Group Permissions
| +----------------------------------> Owner Permissions
+----------------------------------> File Type
```

Each file has a set of permissions that dictate what can and can’t be done to that file, and by whom

r - permission to read a file (i.e. see it’s contents)
w - permission to write to the file (i.e. to change it in some way)
x - permission to execute the file…

Executable files

If a file is marked as “executable” then you can run it as a standalone program

```
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D
$ ls -l mycmd.sh
-r--r--r--  1 s0784966  staff  48 24 Nov 09:44 mycmd.sh
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D
$ cat mycmd.sh
#!/bin/sh

age=31

echo "I am $age years young"
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D
$ ./mycmd.sh
-bash: ./mycmd.sh: Permission denied
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D
$ chmod u=rwx mycmd.sh
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D
$ ls -l mycmd.sh
-rwxr--r--  1 s0784966  staff  48 24 Nov 09:44 mycmd.sh*
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D
$ ./mycmd.sh
I am 31 years young
(base)
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D
$
```

Check permissions

Inspect the contents of the file

Attempt to run file - failure

Alter permissions

Check permissions again

Attempt to run file - success!

Executable files

If a file is marked as “executable” then you can run it as a standalone program

```
s0784966@SCE-BIO-C03959 : ~/UBC/ZoologyStuff/BIOL525D
$ cat mycmd.sh
#!/bin/sh

age=31

echo "I am $age years young"
(base)
```

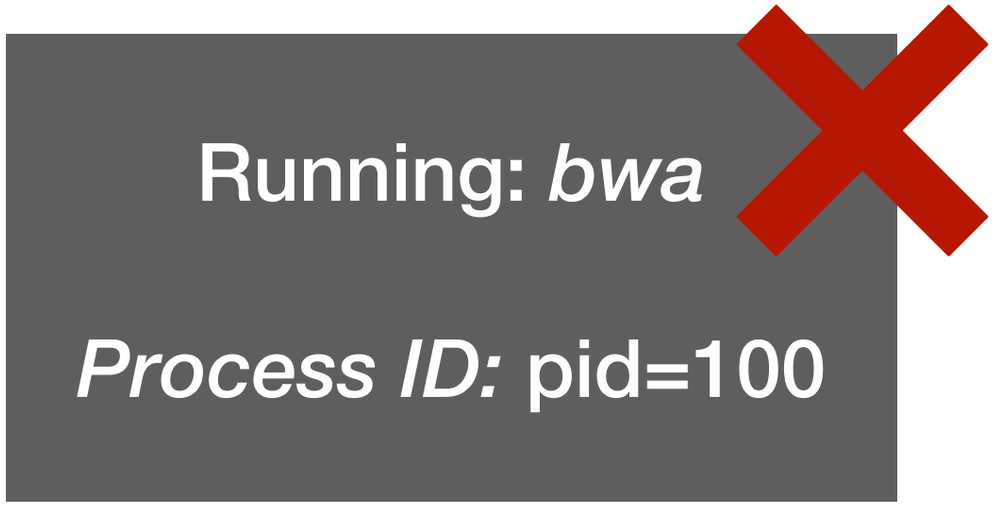
This piece of text “#!/bin/sh” is called a shebang

It tells the system where to look for the interpreter to run this script

On my computer, the “sh” command is located in “/bin/“

Interface: signals

$ kill -KILL 100



Signals are one-way messages sent to control running programs

SIGINT (interrupt) (CTRL-C on terminal)

SIGSTOP(pause) / SIGCONT (CTRL-Z on terminal / fg)

SIGKILL (kill the process immediately) (use "kill -9 PID”)

Compute Canada servers

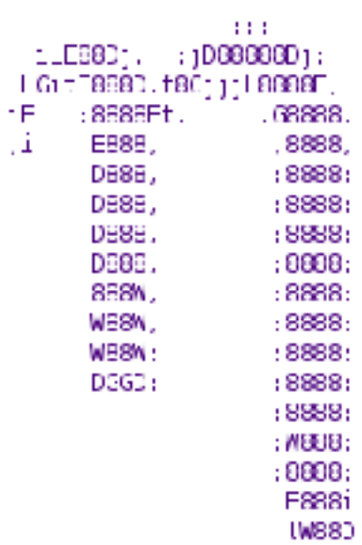
- Use a scheduling system
- Tasks must be submitted in specific bash scripts and will run when they get priority
- You have to specify how much RAM and time you need and how many CPUs you want to use.
- You can get an interactive job, which is like working on your server (e.g. the *salloc* command)

Learn a text editor!!

Working at the command line, you often need to edit text files

There are numerous command line text editors, you should invest some time in learning one

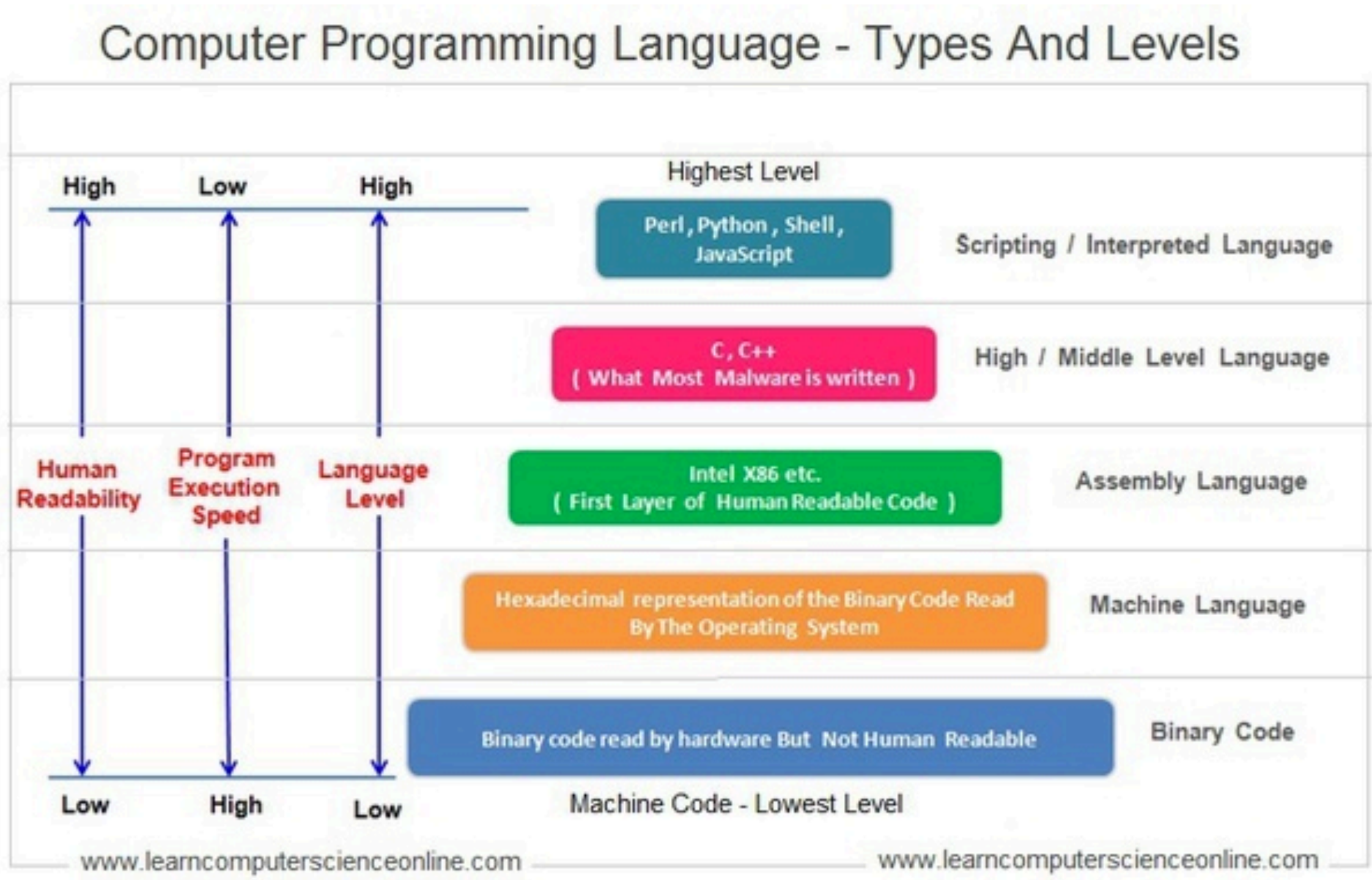
Three common ones to take a look at:



Nano ***Vim*** ***Emacs***

A *very* short introduction to programming

Programming Languages



Programming Languages

That you might come across in Bioinformatics

C/C++ (.cpp)

Shell scripting (.sh)

Perl (.pl)

Python (.py)

R (.r)

The text in parentheses refer to the commonly used file extensions for scripts written in the corresponding languages

	C++	Shell	Perl	Python	R
Speed to run					
Easy to code					
Plotting					
Data Structures					
Modular					
Handles large data well					
Prepackaged functions					

Bad | Intermediate | Good

**This is probably a very controversial slide*

Recommendations

Genomic dabbler

- Shell and R

Genomic scientist

- Shell, R and Python/Perl

Bioinformatician

- Shell, R, Python/Perl and C++

Recommendations

Numerous repetitive tasks demand speed

Software development demands time

General order:

1. Make it work

2. Make it go fast

3. Make it pretty

Language choice considerations:

- Meld with existing codebase

- Your current and future colleagues' expertise

Take homes

If you are new to UNIX, there has been a lot of information thrown at you very fast and I think it's better to focus on concepts rather than specific commands

- Reproducibility
- The command line environment
- Paths (absolute versus relative)
- Modularity
- Metacharacters
- Different programming languages and why
- Learn a good text editor!

(do bioinformatics at)

How do you get to ^Carnegie Hall?

(do bioinformatics at)

How do you get to Carnegie Hall?

Practice, practice, practice!!

I know this seems like a cop out, but there is really no better teacher than experience

You'll develop your skills much faster when you have a project that you are working towards

---

ROSALIND

"Fun" coding/bioinformatics problems to test your skills

http://rosalind.info/problems/locations/

PYTHON FOR BIOLOGISTS .COM

A Python course tailored to Biologists (I personally recommend it)

https://pythonforbiologists.com/

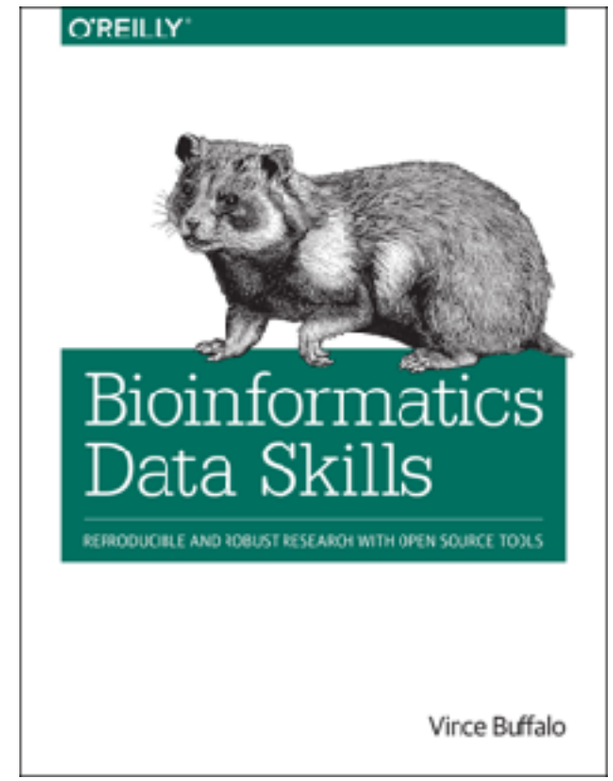
Apologies for the terrible joke

Ask for help!

There are lots of sources of help around - make use of them!

Sometimes the solution to a problem is simply knowing the right terms to Google or to search on StackOverflow

I highly recommend Vince Buffalo's "Bioinformatic Data Skills"

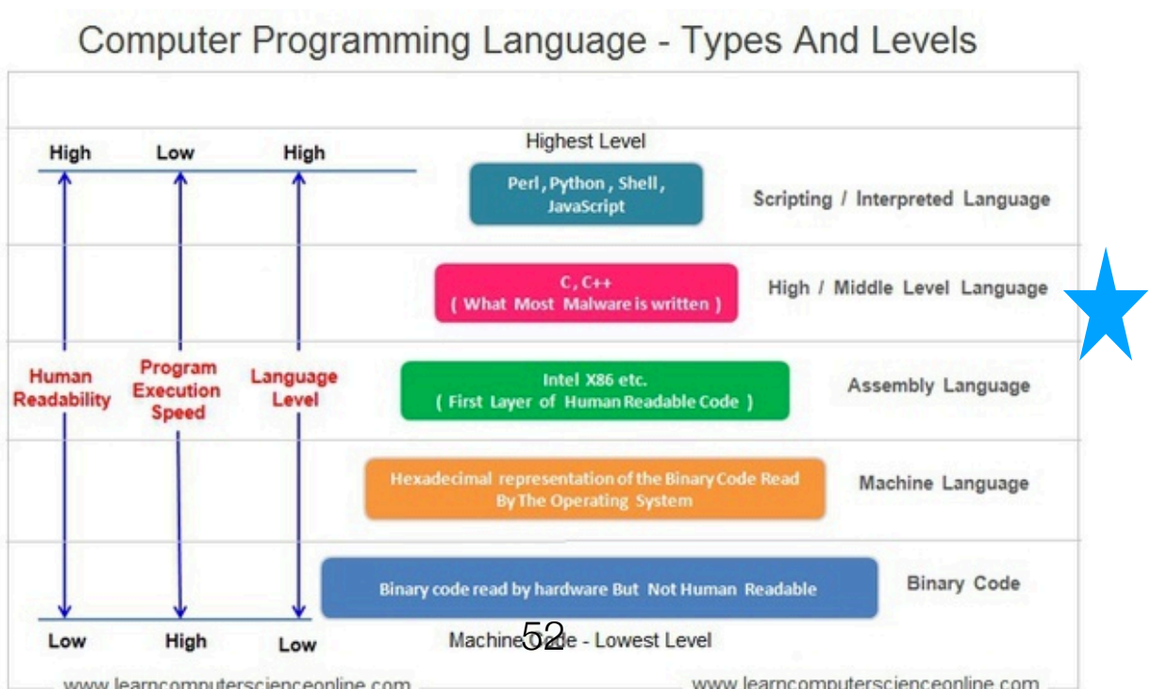


stack overflow

C++

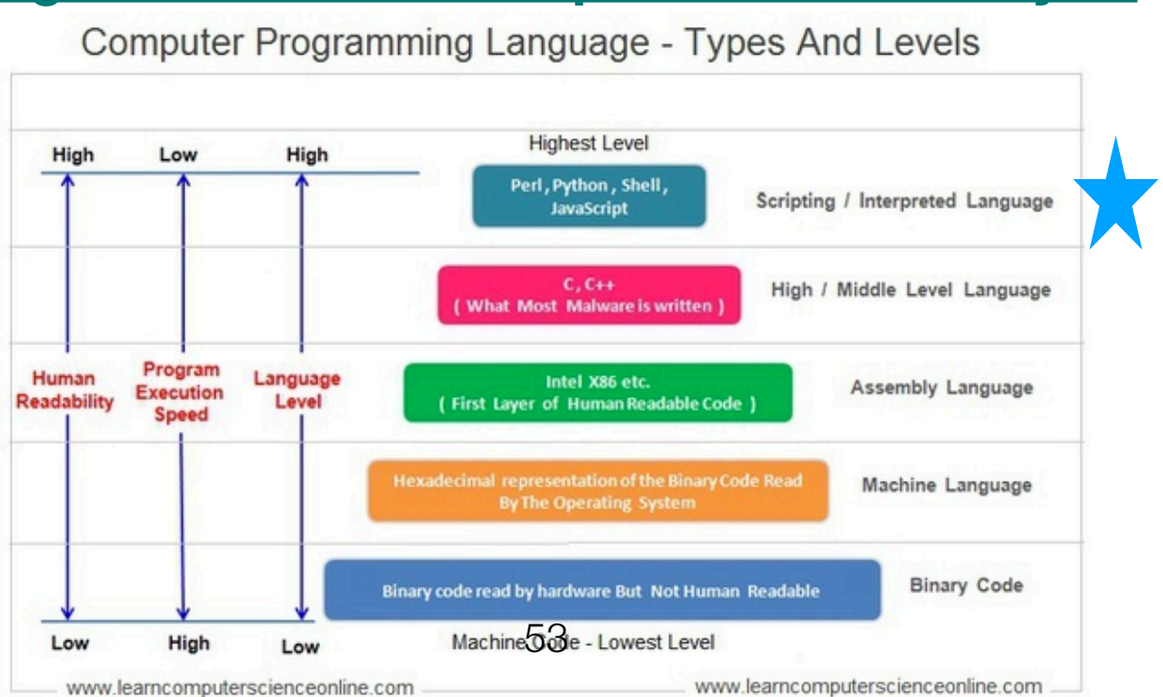
- *Compiles into very fast executable binary files*

- **There are very few prepackaged tools**
  - *This gives you detailed control*
  - **<u>But requires more specialised knowhow and takes longer to write</u>**
  - **<u>Harder to tweak and debug (because you have to compile before running</u>**
  - *Good for making low-level tools/libraries*



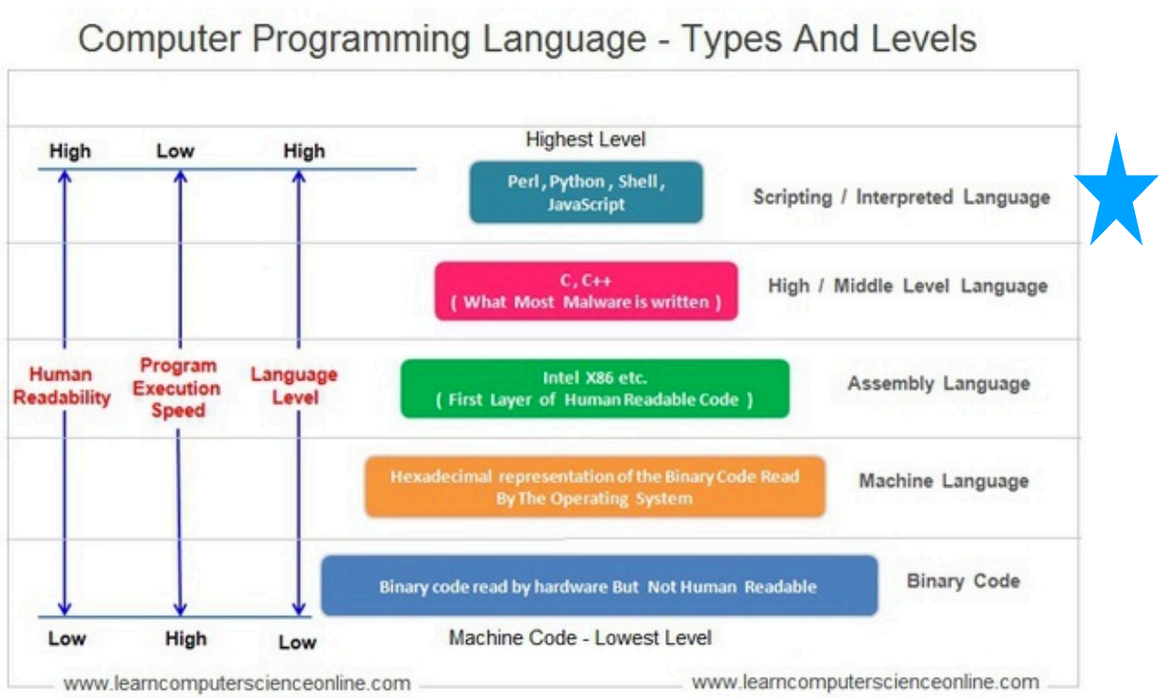
Shell scripting

- ***Chain together command line arguments to make repeatable and reusable scripts***
- ***Easy to write***
- ***Provides the glue between programs written in different languages***
- ***Connects naturally with external programs (e.g. sed awk, grep)***
- **Needs external programs for data manipulation and analysis**



Perl

- ***Excels at text processing***
- ***Some prepackaged functions***
- **Lacks complicated data structures**
- ***Very concise*** **(but at the expense of readability)**
- ***Fast for a high level language***



Python

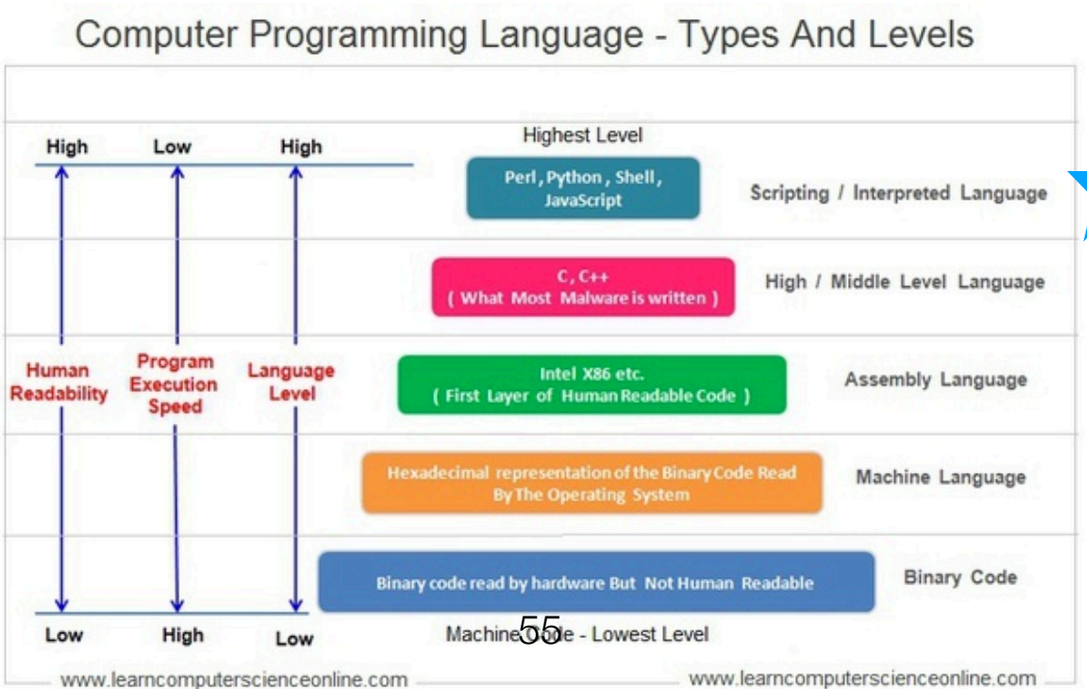
Slightly slower than Perl.

Batteries included. Scientific methods and plotting

Most popular language in the world right now, so there's lots of forum support

Allows rapid development and prototyping.

Good for reformatting data. Good data structures (e.g. handles CSV files well)



*My personal favourite!

R

Many packages for specific scientific tasks and statistics

Great at plotting

Harder to use with big data (GB+ files), although work arounds exist

Slowest option