NSGP+GPP Data Science Setup

Introduction to Concepts and Strategies

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https://github.com/brownritt/nsgp_data_science

Expectations

"Everybody is ignorant, only on different subjects."
- Will Rogers

This workshop will demonstrate tools, but the true goal is to consider ***process***. We cannot cover any one idea or tool comprehensively.

You will already know some things, but maybe not all the things. Don't be afraid to be wrong. Ask for help when you want it. Help others when you can (*if* they want you to!).

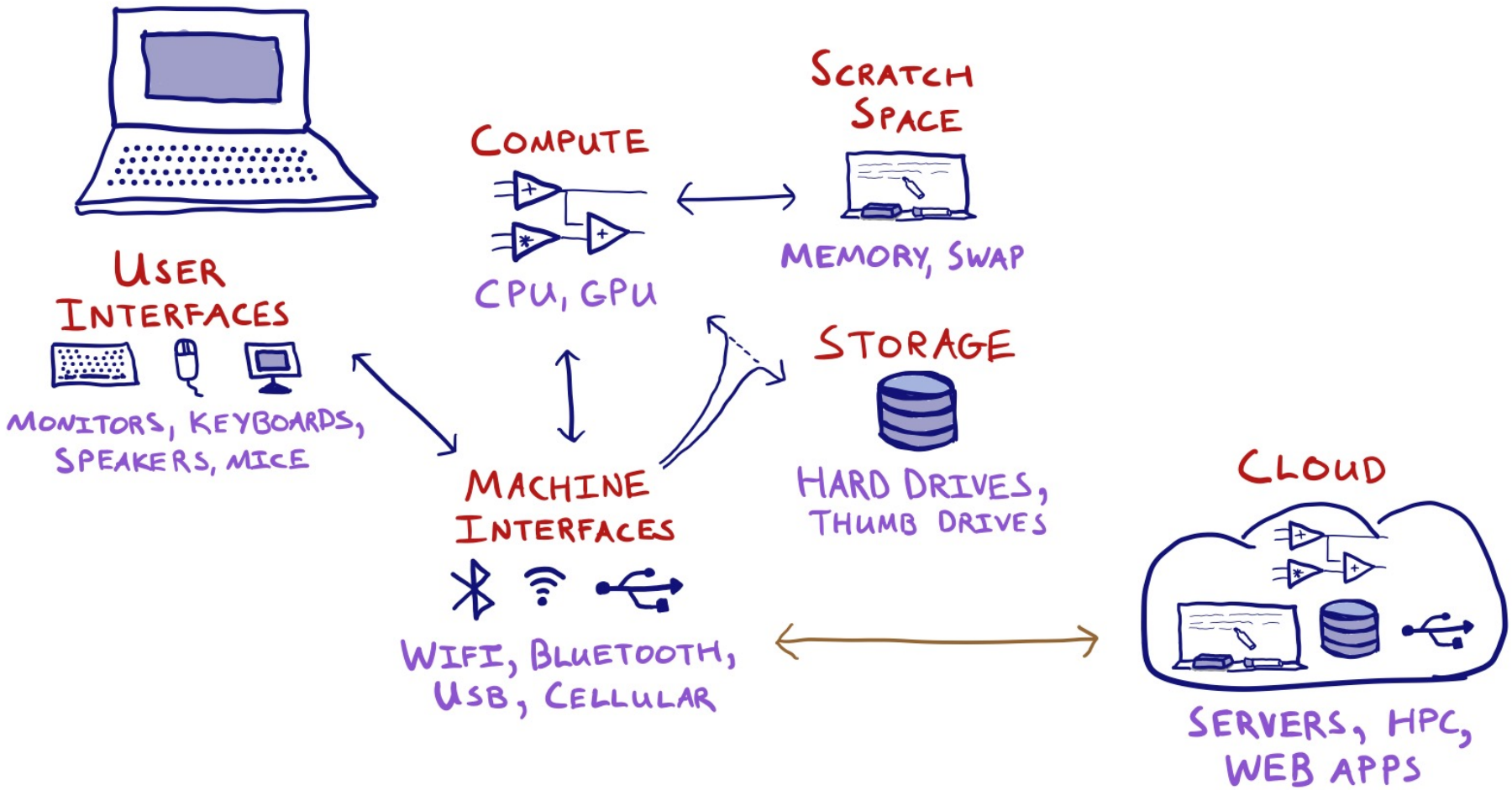
You will need to learn and do things your PIs and mentors do not, because the practice of science is changing faster than the people doing it.

I have my ways. Develop any process that works for you (and your colleagues…).

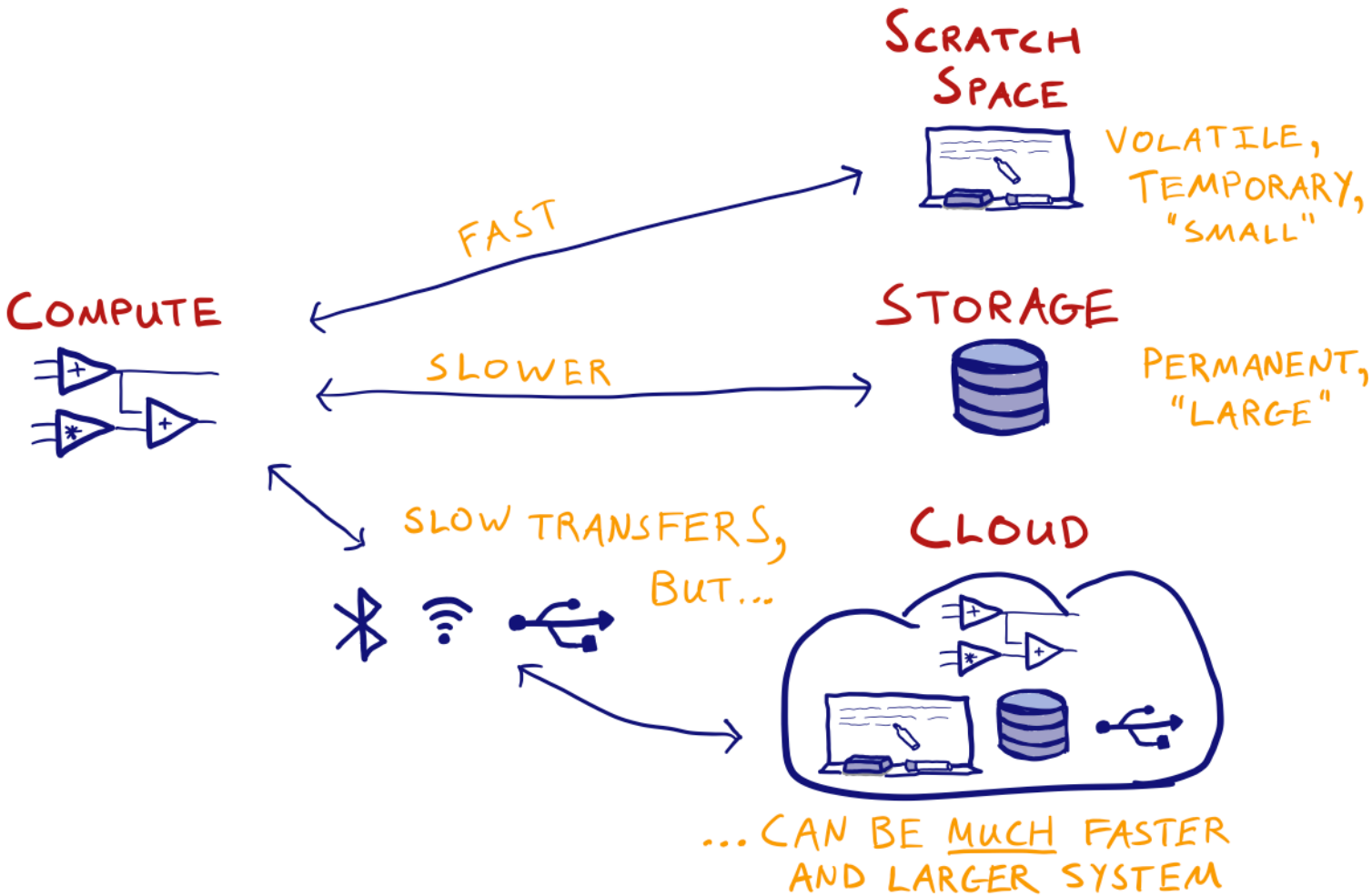
What is data analysis? What is statistics?

And why do we use computers?

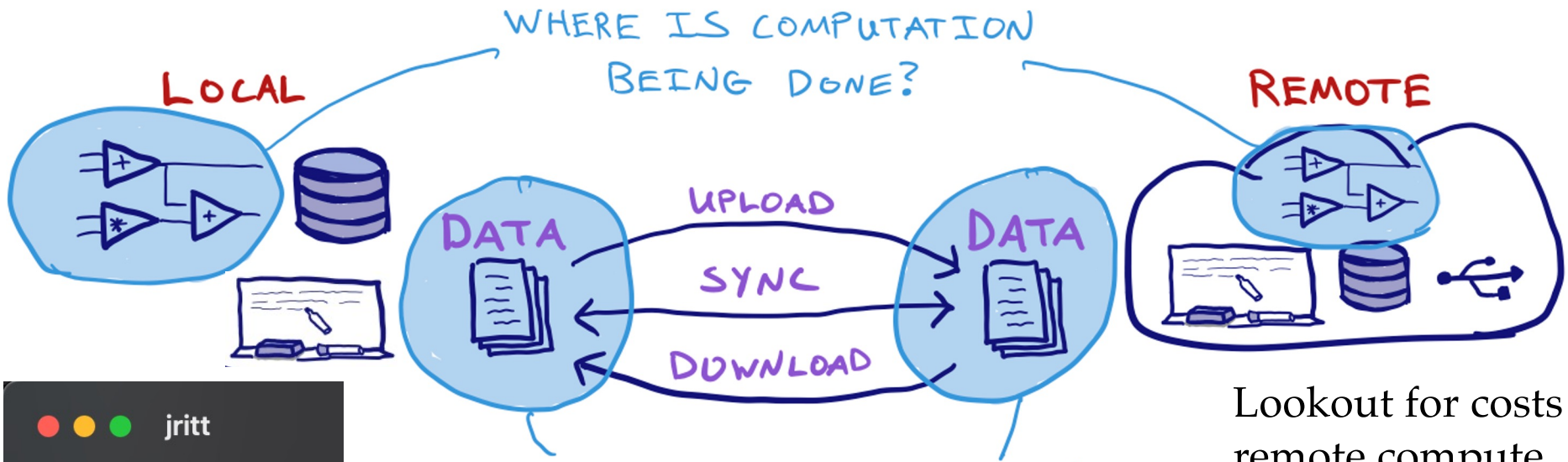
Back to basics: What is a computer?

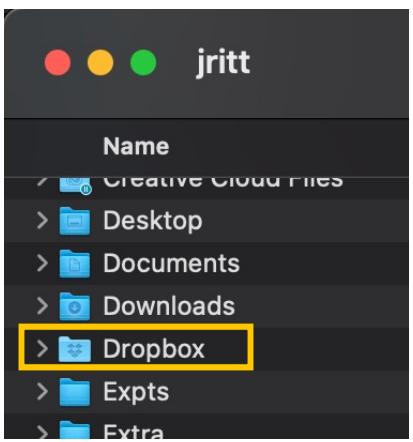


Varied choices of information capacity and transfer speeds



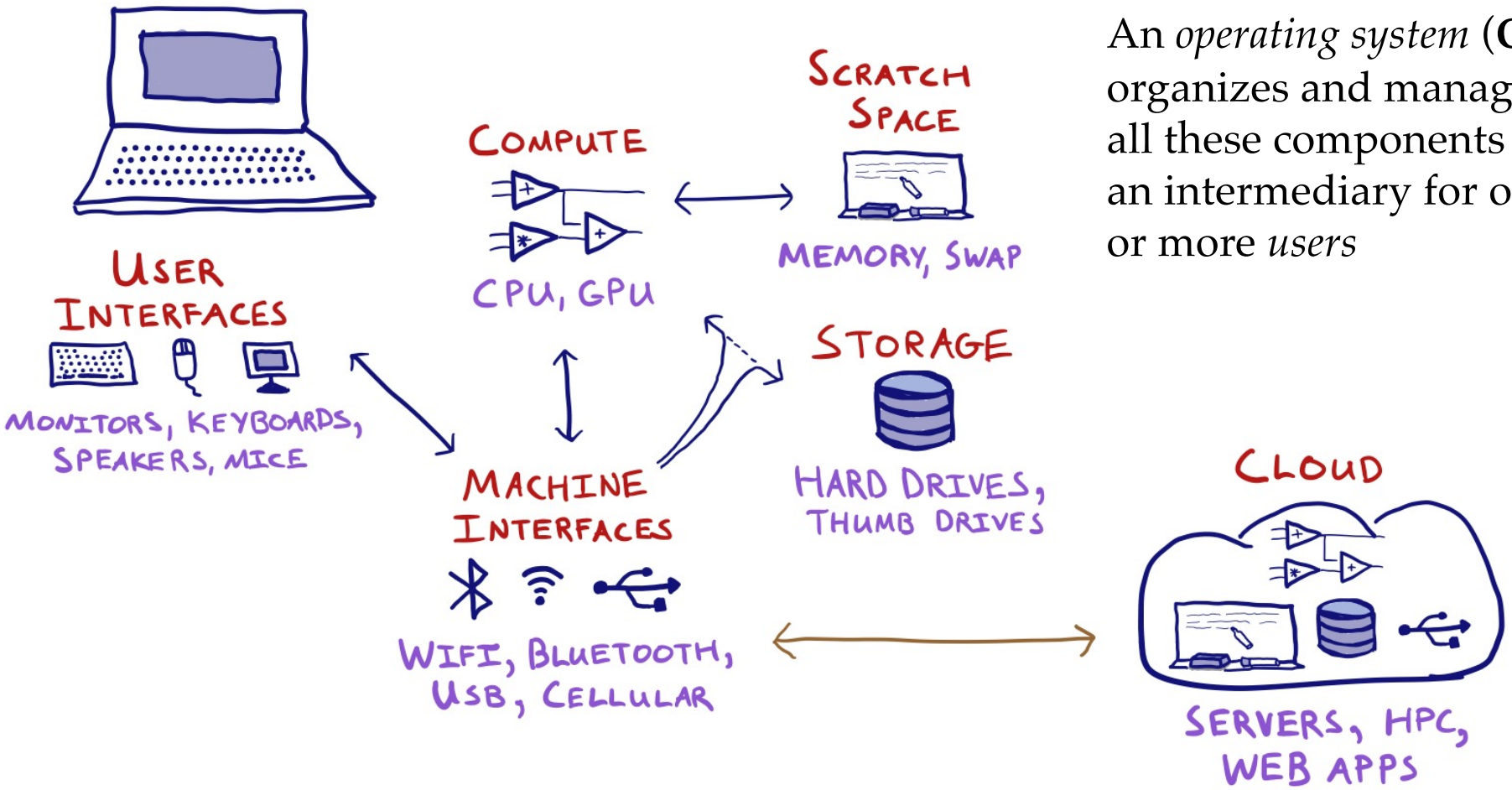
“Cloud” use: Keep your data close, and your compute closer





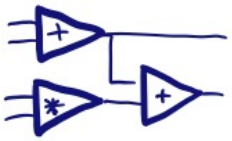
Lookout for costs for remote compute, transfer, and/or storage

The core (conceptual) components of computers

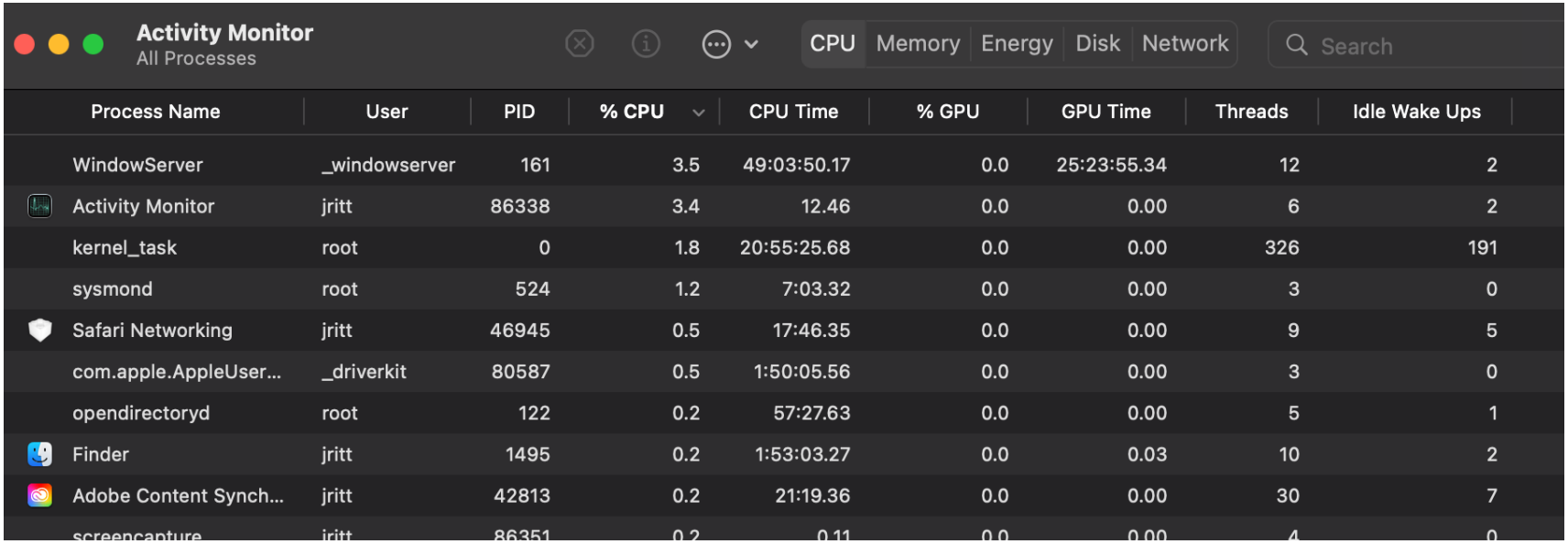


An *operating system* (**OS**) organizes and manages all these components as an intermediary for one or more *users*

How is Compute organized?



All activity (every "application" and more) is done through one or more *processes* managed by the OS.



Activity Monitor
All Processes

CPU | Memory | Energy | Disk | Network | Search

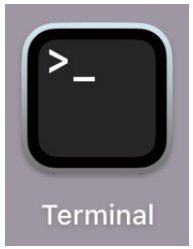
Process Name	User	PID	% CPU	CPU Time	% GPU	GPU Time	Threads	Idle Wake Ups
WindowServer	_windowserver	161	3.5	49:03:50.17	0.0	25:23:55.34	12	2
Activity Monitor	jritt	86338	3.4	12.46	0.0	0.00	6	2
kernel_task	root	0	1.8	20:55:25.68	0.0	0.00	326	191
sysmond	root	524	1.2	7:03.32	0.0	0.00	3	0
Safari Networking	jritt	46945	0.5	17:46.35	0.0	0.00	9	5
com.apple.AppleUser...	_driverkit	80587	0.5	1:50:05.56	0.0	0.00	3	0
opendirectoryd	root	122	0.2	57:27.63	0.0	0.00	5	1
Finder	jritt	1495	0.2	1:53:03.27	0.0	0.03	10	2
Adobe Content Synch...	jritt	42813	0.2	21:19.36	0.0	0.00	30	7
screencapture	jritt	86351	0.2	0.11	0.0	0.00	4	0

Every process has some key properties:

- Who am I? ***Accounts***
- What am I allowed to do? ***Permissions, Priority***
- Where am I? ***Working directory (path)***

User interfaces for the technically minded

A *command line interface* (**CLI**) executes commands given by text input. CLIs are very powerful and efficient, though with a bit of a learning curve.



Note: theTerminal application is a graphical interface to a second process, called a *shell*, that actually runs the CLI.

```
em-event-detection-demo — -bash — 69×17
jritt: ~ $ cd Code/EM_event_detection/GitLab/
jritt: GitLab $ ls
.DS_Store                          em-event-detection-demo/
jritt: GitLab $ cd em-event-detection-demo/
jritt: em-event-detection-demo $ ls
.DS_Store                          EM_algorithm_demo.pdf
.git/                              LICENSE
.gitignore                         README.md
.ipynb_checkpoints/                README.md~
EM_algorithm_demo.ipynb            environment.yml
jritt: em-event-detection-demo $ git status
On branch main
Your branch is up to date with 'origin/main'.

nothing to commit, working tree clean
jritt: em-event-detection-demo $
```

CLIs are a common example of a Read-Eval-Print Loop (REPL) interface.

User interfaces for the technically minded

A *text editor* manipulates arbitrary text-based files.

```
em-event-detection-demo — nano README.md — 83×17
  UW PICO 5.09                          File: README.md

# EM Event Detection Demo #

A demonstration of using expectation-maximization to find "spiking" events in calc$

**You will need a numpy data file** to run the notebook yourself (except for secti$

```python
A = np.load('F.npy')
df_data = A[0,:]
```

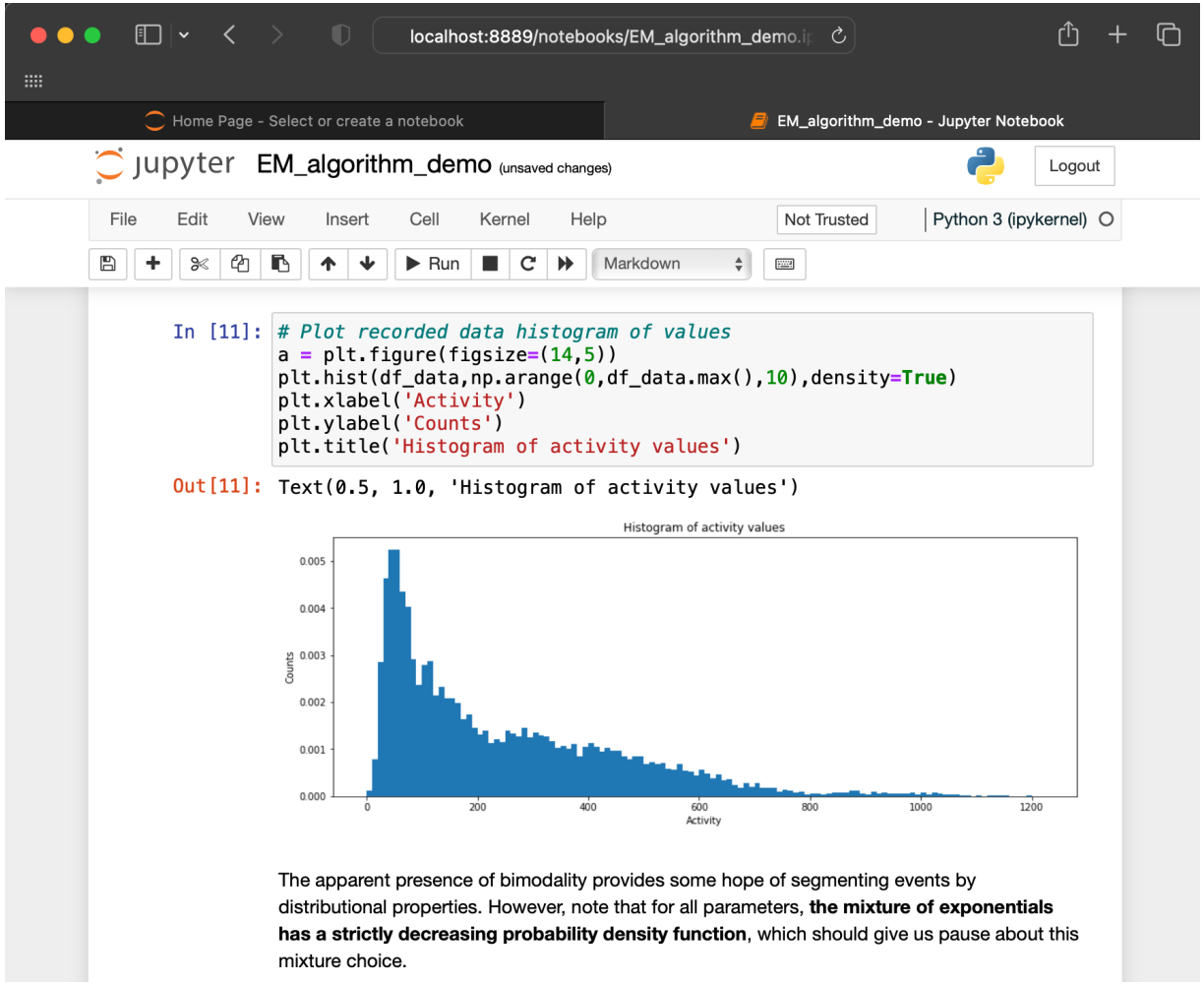
Only `data_df` is used from there on. Probably any such file will work, or you can$

^G Get Help   ^O WriteOut   ^R Read File ^Y Prev Pg   ^K Cut Text   ^C Cur Pos
^X Exit   ^J Justify   ^W Where is ^V Next Pg   ^U UnCut Text^T To Spell
```

Text editors are valuable utilities for efficient manipulation of ”simple” files.

User interfaces for the technically minded

An *interactive notebook* runs input code, displays outputs, and allows text annotations in a single document made of *cells*.

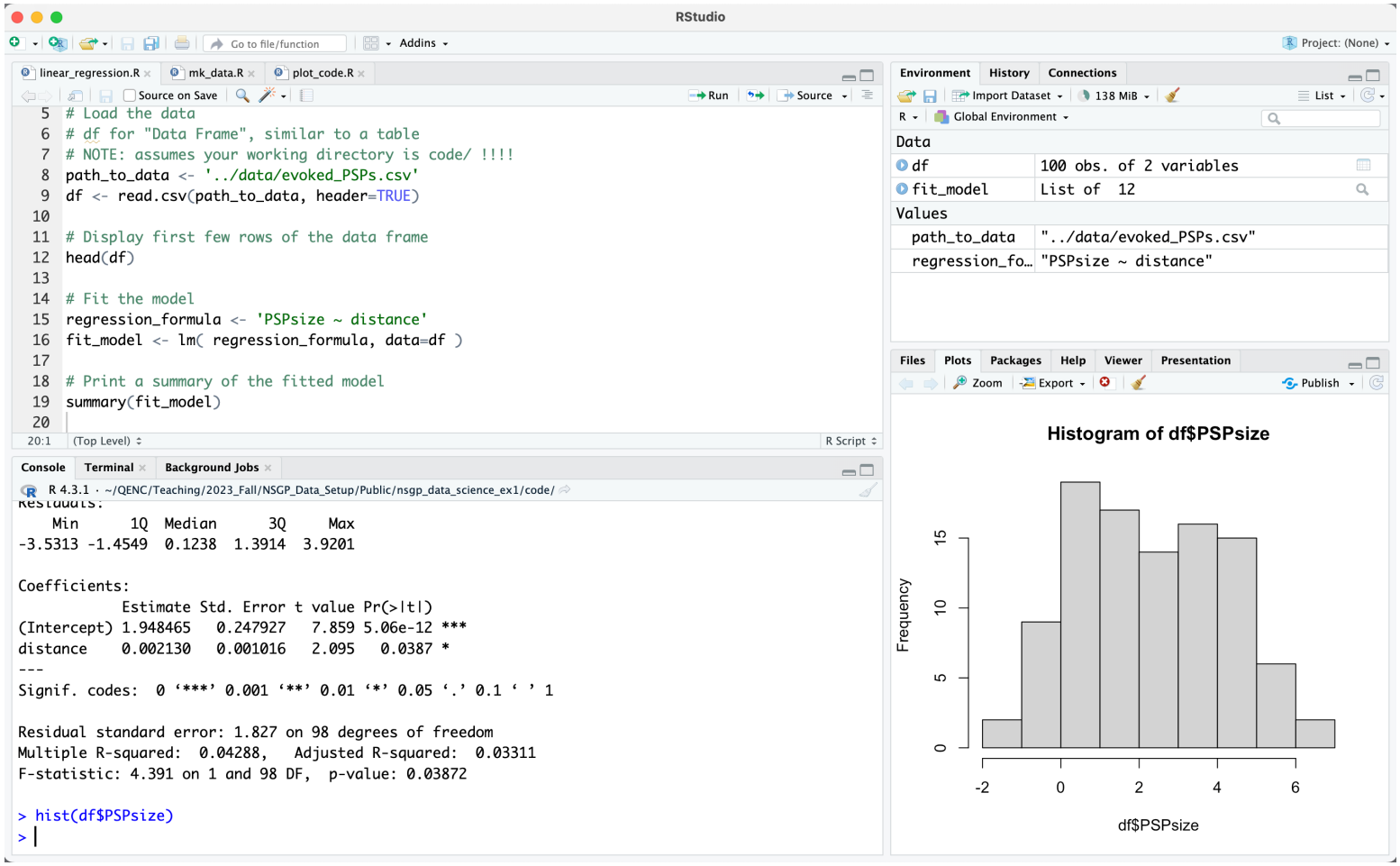


There are actually two processes: one runs the notebook itself, and communicates with an invisible *kernel* process that does the real computational work.

Beware: is a REPL that keeps its history, but can get "out of order"!

User interfaces for the technically minded

An *integrated development environment* (**IDE**) combines a "smart editor" (syntax highlights, error checks, code hints, etc), a (REPL) *console* for running interactive commands, and other coding and file handling utilities.



User interfaces for the technically minded

There are **many** other tools for computational projects, and everyone has their own preferred tool chain.

Common use cases:

- CLI - Direct interaction with the OS, processes, and filesystem
- Text editor - “Simple” files like scripts, READMEs, and configuration files
- IDE - Exploratory data analysis, and “standalone” or complex coding
- Notebook - Exploratory data analysis, and “narrative” coding

Do not use Excel:

nature

NEWS | 13 August 2021 | Correction 25 August 2021

Autocorrect errors in Excel still creating genomics headache

Despite geneticists being warned about spreadsheet problems, 30% of published papers contain mangled gene names in supplementary data.

https://www.nature.com/articles/d41586-021-02211-4

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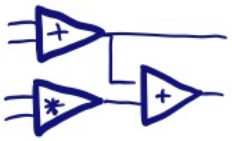

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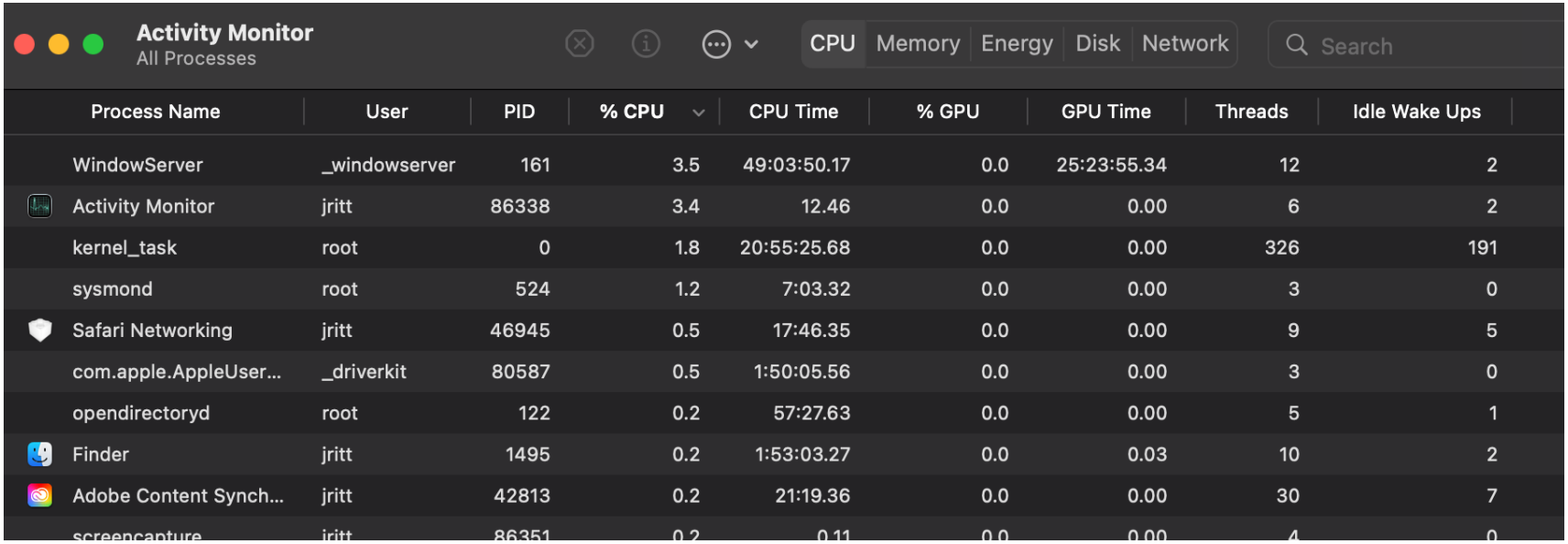

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Dude, where's my data? (and also my code, and my messages, and …)

Storage is organized by the OS: Information is kept in *files*. Every file is located in some *directory*, within a *tree* of other directories.

Locations are described by *paths*:

`/Users/jritt/Code/EM_event_detection/EM_algorithm_demo.ipynb`

root directory

subdirectories

filename

file type *extension*

Remote locations (URLs) include networking information:

`https://gitlab.com/fleischmann-lab/calcium-imaging/em-event-detection-demo/-/blob/master/EM_algorithm_demo.ipynb`

protocol

domain name (the "server")

Note: these are not always "real" files or directories on the remote OS

Absolute and relative paths each have their place

Every process runs in some *working directory*. A ***relative path*** starts from this working directory; an ***absolute path*** starts from the top of the filesystem tree.

An absolute path :

`/Users/jritt/Code/EM_event_detection/EM_algorithm_demo.ipynb`

From my *home directory* `jritt/` :

`Code/EM_event_detection/EM_algorithm_demo.ipynb`

From `EM_event_detection/` :

`./EM_algorithm_demo.ipynb` or just `EM_algorithm_demo.ipynb`

`./` means "this directory"

`../` means "go up one directory"

`~/` means "my home directory"