# CONTAINERS

# OUTLINE

- The problem: dependencies
- Possible solutions
- Containers
  - What they are
  - Why use them
- Brief tutorial
- Additional advantages of containers
- Discussion

# THE PROBLEM: DEPENDENCIES

# A FIRST ATTEMPT AT REPRODUCIBILITY (C. 2018)

1. Create an R package for the method
2. Create an R package for data and helper routines
3. Create scripts to run the analyses
4. Put everything on github

# THEN TIME PASSES…

- When revising the paper, we updated our code, re-ran the analysis, and…
  got very different results for a method we had compared against
- After a great deal of debugging, we discovered a dependency of a dependency of a dependency had changed
- Moral: Saving your code is not enough. You need to save the entire computational environment

# EXAMPLE: `lme4`

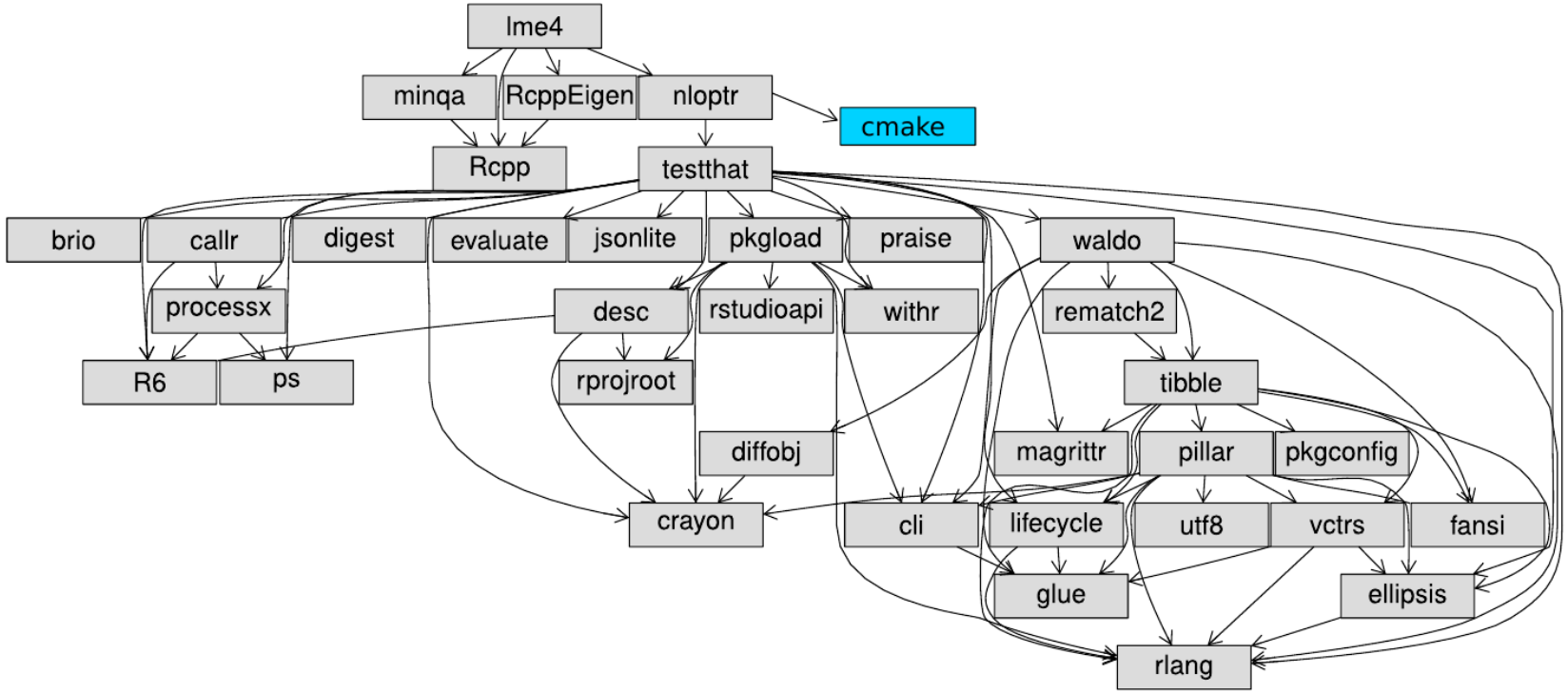



Figure 1: Dependency graph for the R package **lme4**. Grey boxes are R add-on packages. Arrows indicate dependency. The blue box indicates the system-level dependency of the package for Linux OS Ubuntu ver. 20.04.

# ANOTHER EXAMPLE (C. 2020) – NOT EVEN A "DEPENDENCY"!

- Writing a paper with a student that analyzed social media data (Tweets)
- The student created a full analysis pipeline and shared on github
- Fairly simple pipeline, so waited to containerize until final revisions complete

# ANOTHER EXAMPLE (C. 2020) – NOT EVEN A "DEPENDENCY"!

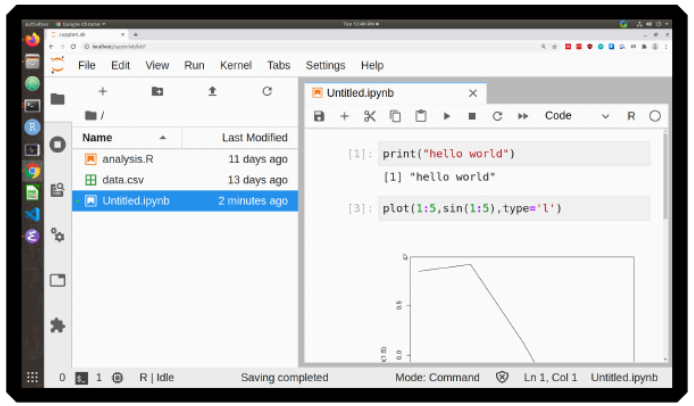
- Time passes… paper accepted, time to containerize
- One figure in the paper: Randomly selected example tweets
- They changed! (And one was now very offensive)
- The method of random number generation for the `sample` command had changed. See: link

# CONTAINERS

# WHAT ARE CONTAINERS

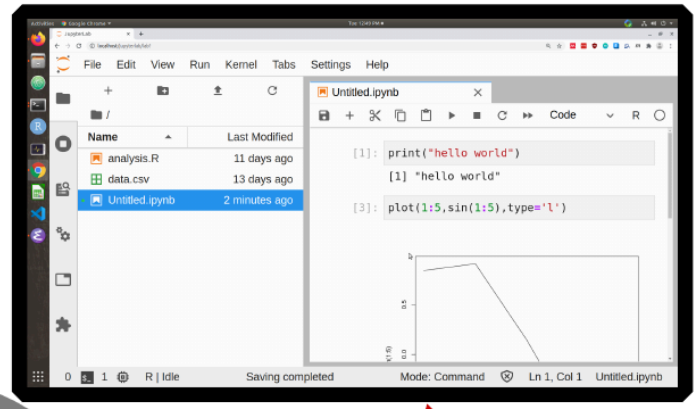
## Original Analysis

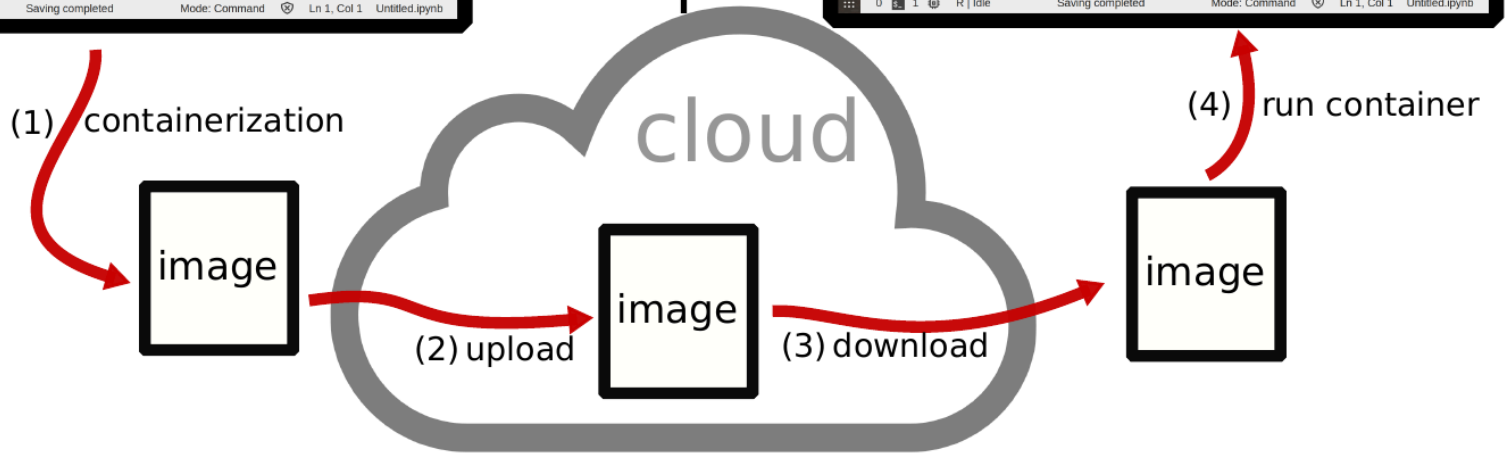
Original Computing Environment




## Third Party

container
(Copy of Computing Environment)



# WHAT ARE CONTAINERS

- Package up a computing environment in a share-able format.
- Essentially: a very light-weight version of virtualization.
- Very fast – almost native speed
- Potentially some issues with different hardware (AMD64 vs M1/2/3 vs ARM etc.)

# WHY USE THEM

- Save (nearly) the **entire computing environment**
  - System libraries and utilities
  - Python, R, etc.
  - Packages
- Fast
- Easy to share
  - Single file
  - Cross platform (Linux, Mac, Windows)

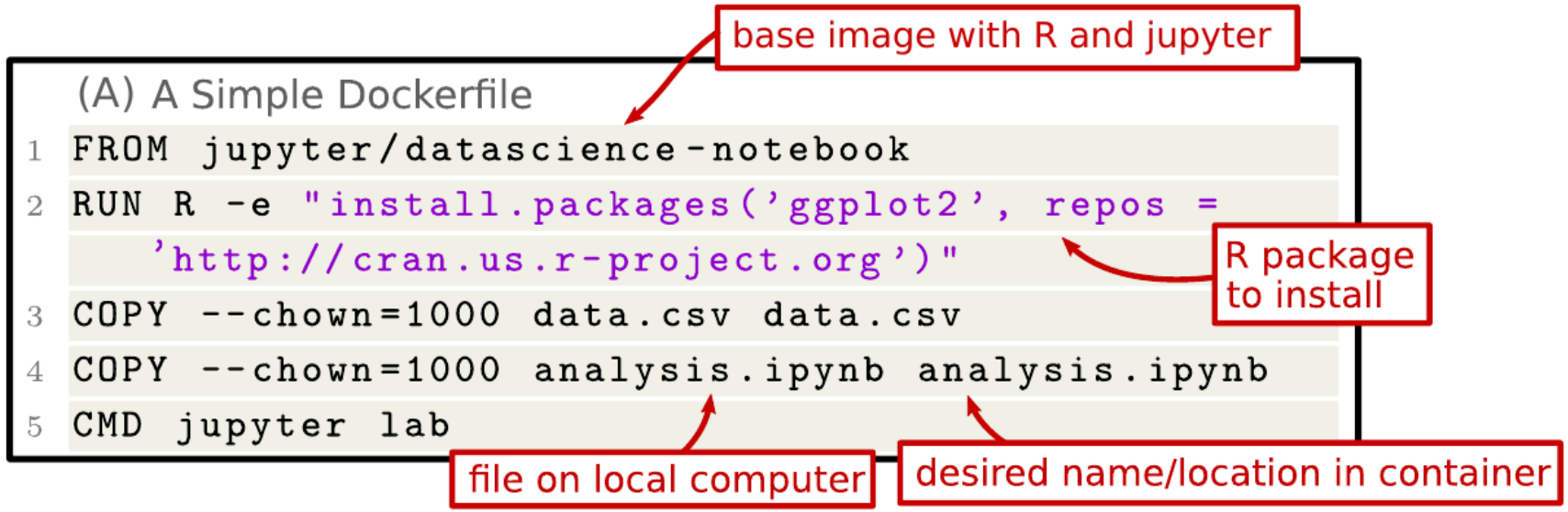
# KEY INGREDIENTS

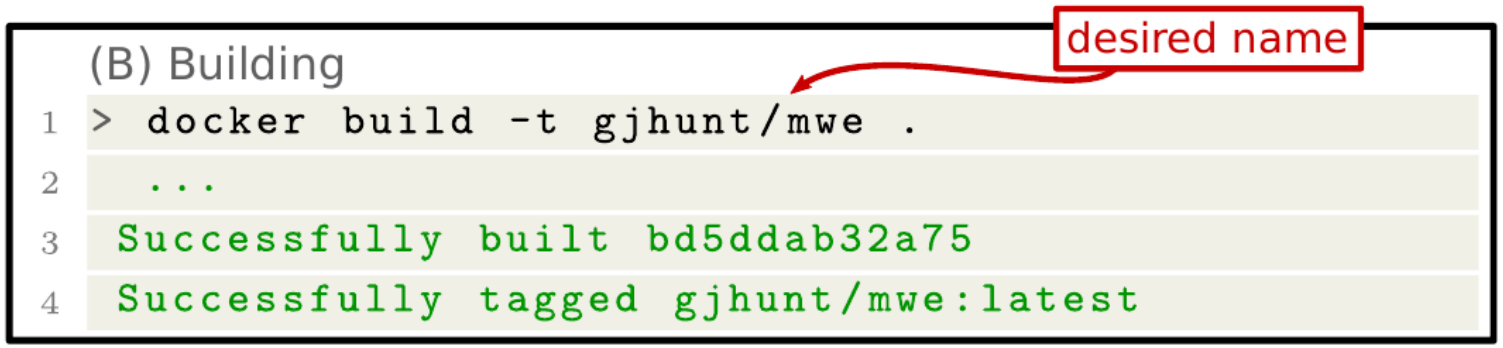
- Base image
- Configuration file (called either a Dockerfile or Containerfile)
- Your existing analysis

# BASE IMAGE

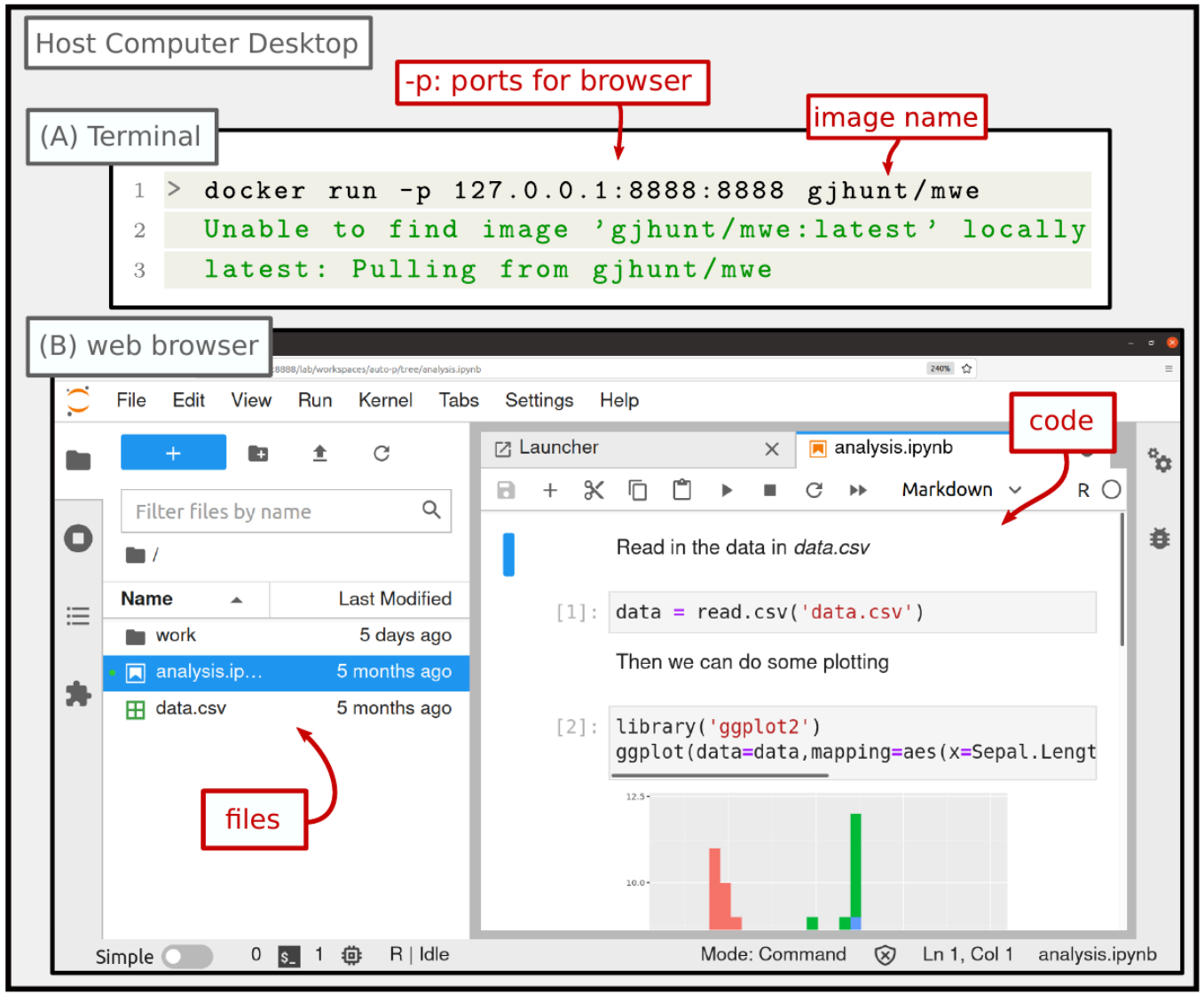
- Minimal Ubuntu
- R (Rocker)
- Jupyter
- Many, many more

# DOCKERFILE


base image with R and jupyter
(A) A Simple Dockerfile
1 FROM jupyter/datascience-notebook
2 RUN R -e "install.packages('ggplot2', repos =
'http://cran.us.r-project.org')"
3 COPY --chown=1000 data.csv data.csv
4 COPY --chown=1000 analysis.ipynb analysis.ipynb
5 CMD jupyter lab
R package to install
file on local computer
desired name/location in container


desired name
(B) Building
1 > docker build -t gjhunt/mwe .
2 ...
3 Successfully built bd5ddab32a75
4 Successfully tagged gjhunt/mwe:latest

# RUNNING


Host Computer Desktop
-p: ports for browser
image name
(A) Terminal
1 > docker run -p 127.0.0.1:8888:8888 gjhunt/mwe
2 Unable to find image 'gjhunt/mwe:latest' locally
3 latest: Pulling from gjhunt/mwe
(B) web browser
File Edit View Run Kernel Tabs Settings Help
code
Launcher
analysis.ipynb
Markdown
R
Filter files by name
/
Name
Last Modified
work 5 days ago
analysis.ip... 5 months ago
data.csv 5 months ago
files
Read in the data in data.csv
[1]: data = read.csv('data.csv')
Then we can do some plotting
[2]: library('ggplot2')
ggplot(data=data,mapping=aes(x=Sepal.Lengt
Simple 0 1 R | Idle
Mode: Command
Ln 1, Col 1
analysis.ipynb

# MINIMAL TUTORIAL

- Many great tutorials online
- Our paper:
  https://jdssv.org/index.php/jdssv/article/view/53

# MINIMAL TUTORIAL

## Using `podman`, a light-weight impl. of `docker`

## Containerfile:

```
FROM quay.io/jupyter/datascience-notebook
RUN R -e "install.packages('ggplot2', repos='http://cran.us.r-project.org')"
COPY --chown=1000 data.csv data.csv
COPY --chown=1000 analysis.ipynb analysis.ipynb
CMD jupyter lab
```

## build

```
podman build --format docker -t ex_image .
```

## run

```
podman run -it --rm -p 8888:8888 ex_image
```

# MINIMAL TUTORIAL

## saving

```
podman save ex_image -o ex.tar
```

## loading

```
podman load -i ex.tar
```

# COMMENTS AND DISCUSSION

# ADDITIONAL ADVANTAGES OF CONTAINERS

Our goals:

1. Exactly reproducible
2. User friendly
3. Transparent
4. Reusable
5. Archived
6. Version controlled

# USER FRIENDLY

- Code easy to access and inspect, ideally even without downloading
- Should require minimal effort for a user to install and run
- Should cause minimal disruption to a user’s resources (e.g., not install unwanted software on their system)
- etc.
- Minimize the user’s security concerns

# DISCUSSION

- How do you deal with dependency issues for your code?
- How do you share your code and analyses? Internally? Externally? What tools?

# EXERCISE

Follow our minimal tutorial but now containerize your EDA.