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`

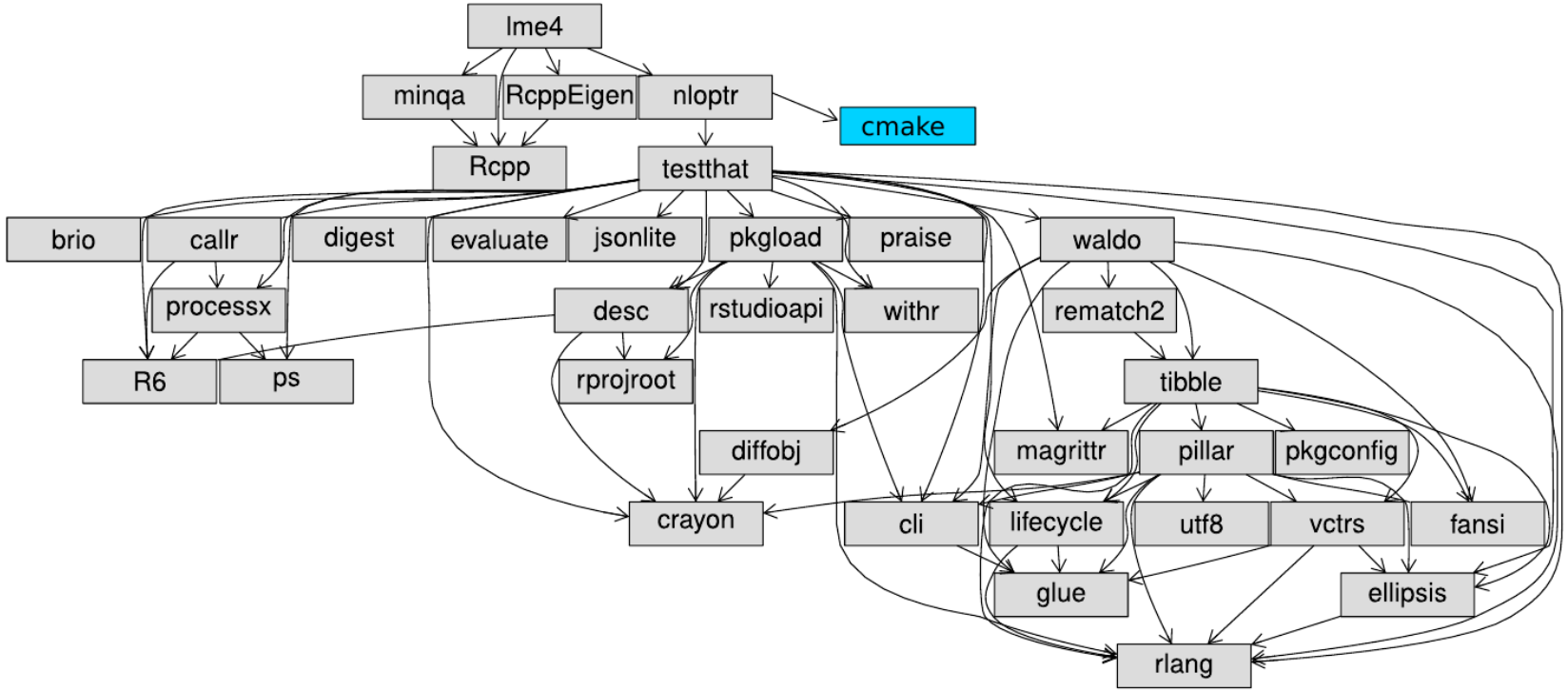


Figure 1: Dependency graph for the R package **lme4**. Grey boxes are R add-on packages. Arrows indicate dependency. The blue box indicates the system-level dependency of the package for Linux OS Ubuntu ver. 20.04.

POSSIBLE SOLUTIONS

- Python: `venv`
- R: `renv`
- Containers (e.g., Podman, Docker)
- Others?

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

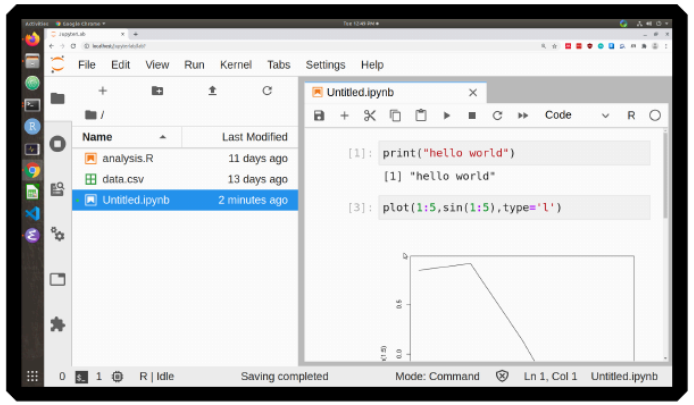
- Writing a paper with a student that analyzed social media data (Tweets)
- The student created a full analysis pipeline and shared on github
- Fairly simple pipeline, so waited to containerize until final revisions complete
- Time passes… paper accepted, time to containerize
- One figure in the paper: 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

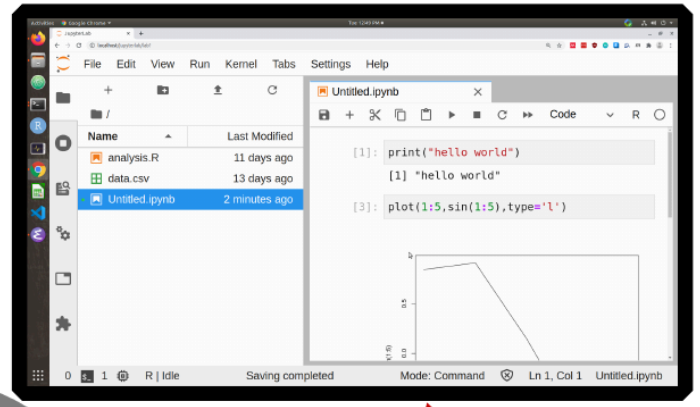
Original Analysis

Original Computing Environment



Third Party

container
(Copy of Computing Environment)



(1) containerization

image

cloud

image

(2) upload

(3) download

image

(4) run container

WHAT ARE CONTAINERS

- For a user, feels very similar to virtualization
- But technically, not quite – the kernel is shared
- Very fast – almost native speed
- Still need similar 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
- Dockerfile or Containerfile
- Your existing analysis

BASE IMAGE

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

DOCKERFILE

(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
```

base image with R and jupyter

R package to install

file on local computer

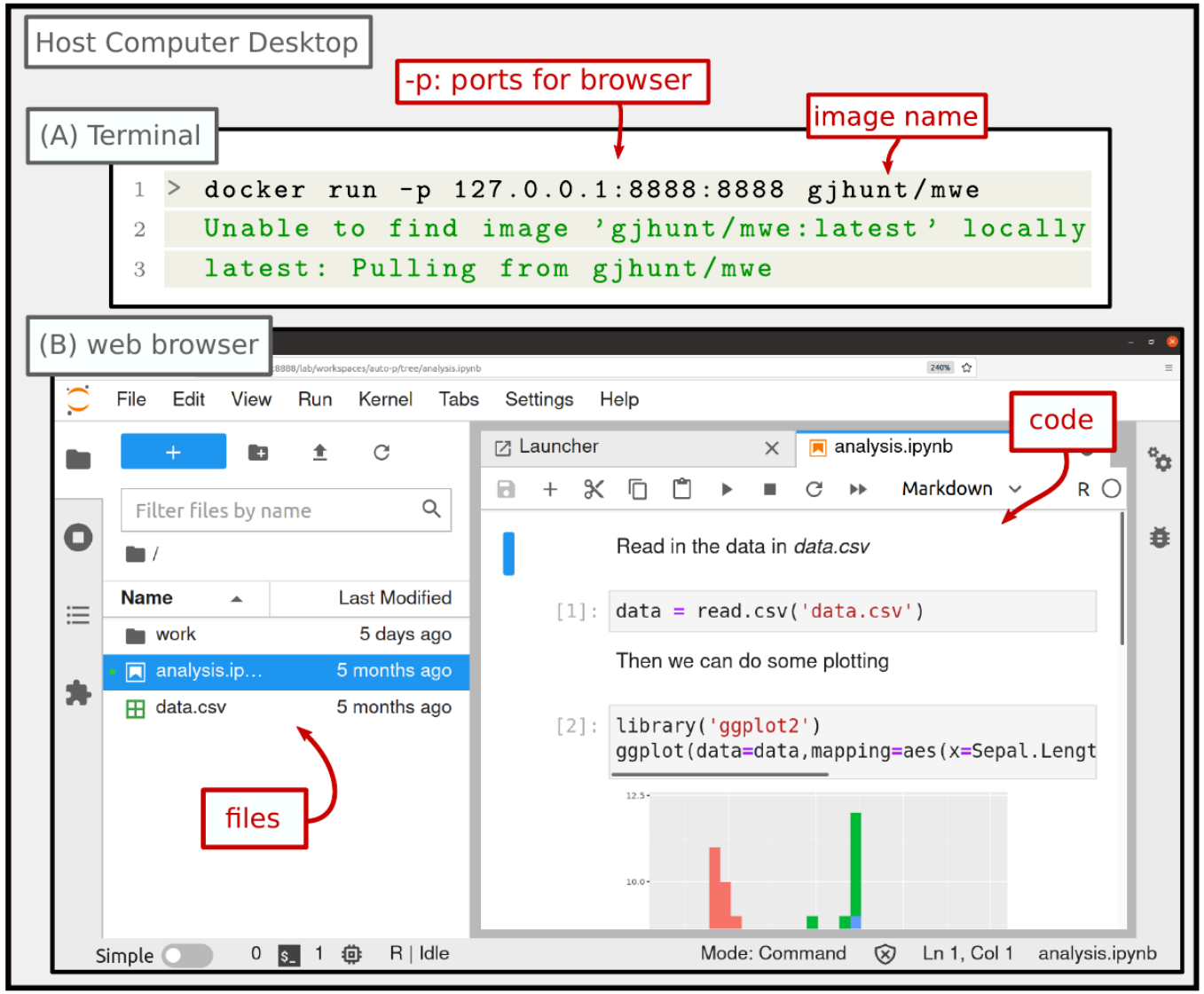
desired name/location in container

(B) Building

```
1 > docker build -t gjhunt/mwe .
2   ...
3  Successfully built bd5ddab32a75
4  Successfully tagged gjhunt/mwe:latest
```

desired name

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

ANOTHER EXAMPLE

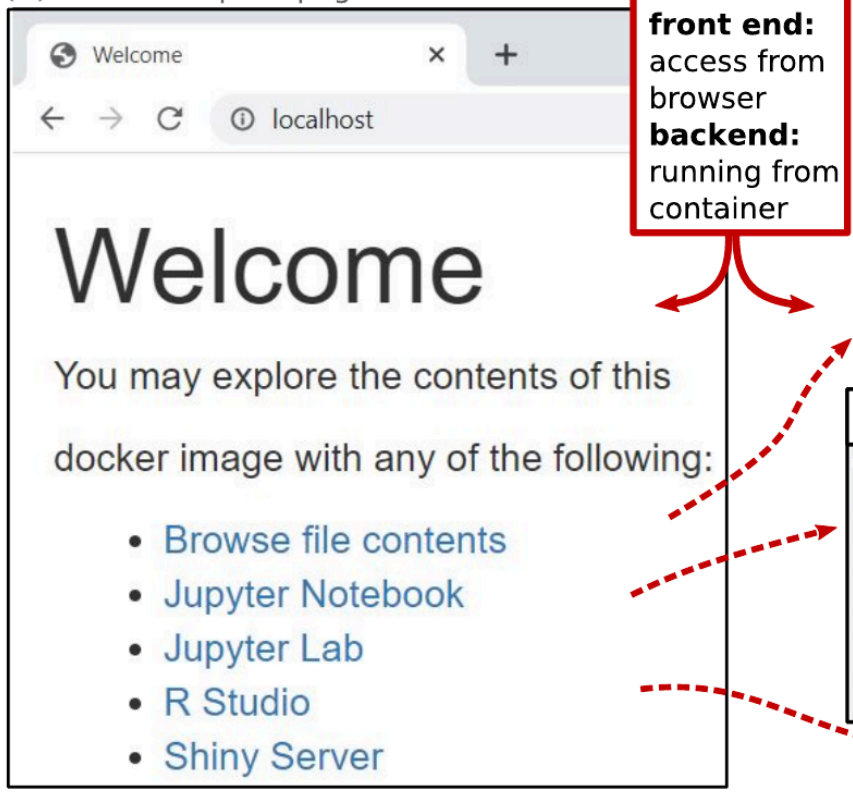
(A) Interactive Dockerfile

```
1 FROM johanngb/rep-int
2 WORKDIR /home/rep/
3 COPY data.csv data.csv
4 COPY analysis.ipynb analysis.ipynb
5 RUN jupytext --set-formats ipynb,rmarkdown,R
      analysis.ipynb
6 RUN jupyter nbconvert --to html analysis.ipynb
```

(B) Running an interactive Container

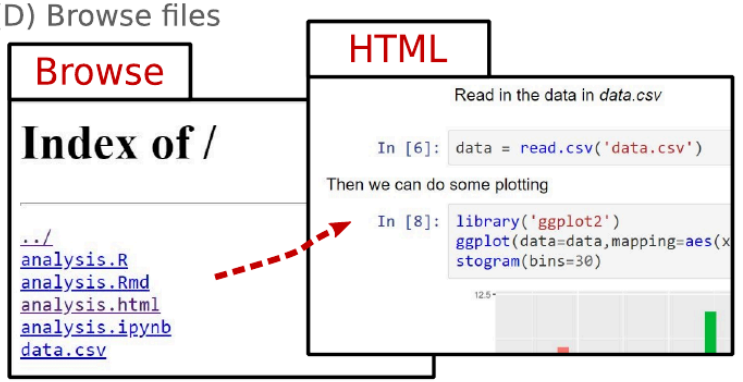
```
1 > docker run -it --name ex_container -p
      127.0.0.1:80:80 gjhunt/mwe:2
2   To get started, please enter the following
      URL into your web browswer:
3           http://localhost/
4   ...
```

(C) Welcome Splashpage

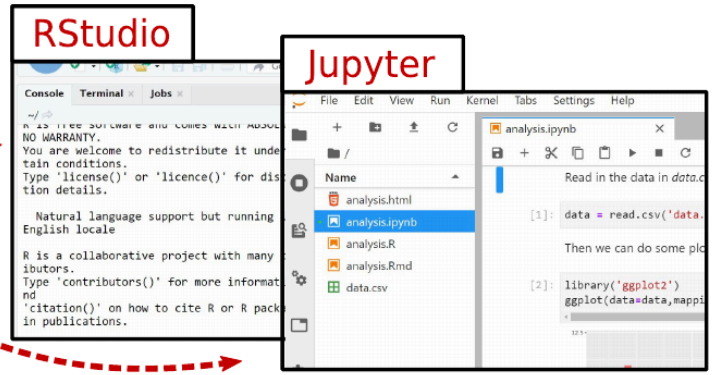


front end: access from browser
backend: running from container

(D) Browse files



(E) Interact with notebooks



BRIEF TUTORIAL

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

TUTORIAL

I'll be using `podman` which is a reimplementation of `docker`

Containerfile:

```
FROM 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 -t ex_image .
```

run

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

TUTORIAL

saving

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

loading

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

TUTORIAL

listing images

```
podman image ls -a
```

listing containers

```
podman container ls -a
```

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