Winter Institute in Data Science and Big Data

Containers, Cloud Computing, and Code Reproducibility: Docker, Kubernetes, and Code Ocean

Le Bao

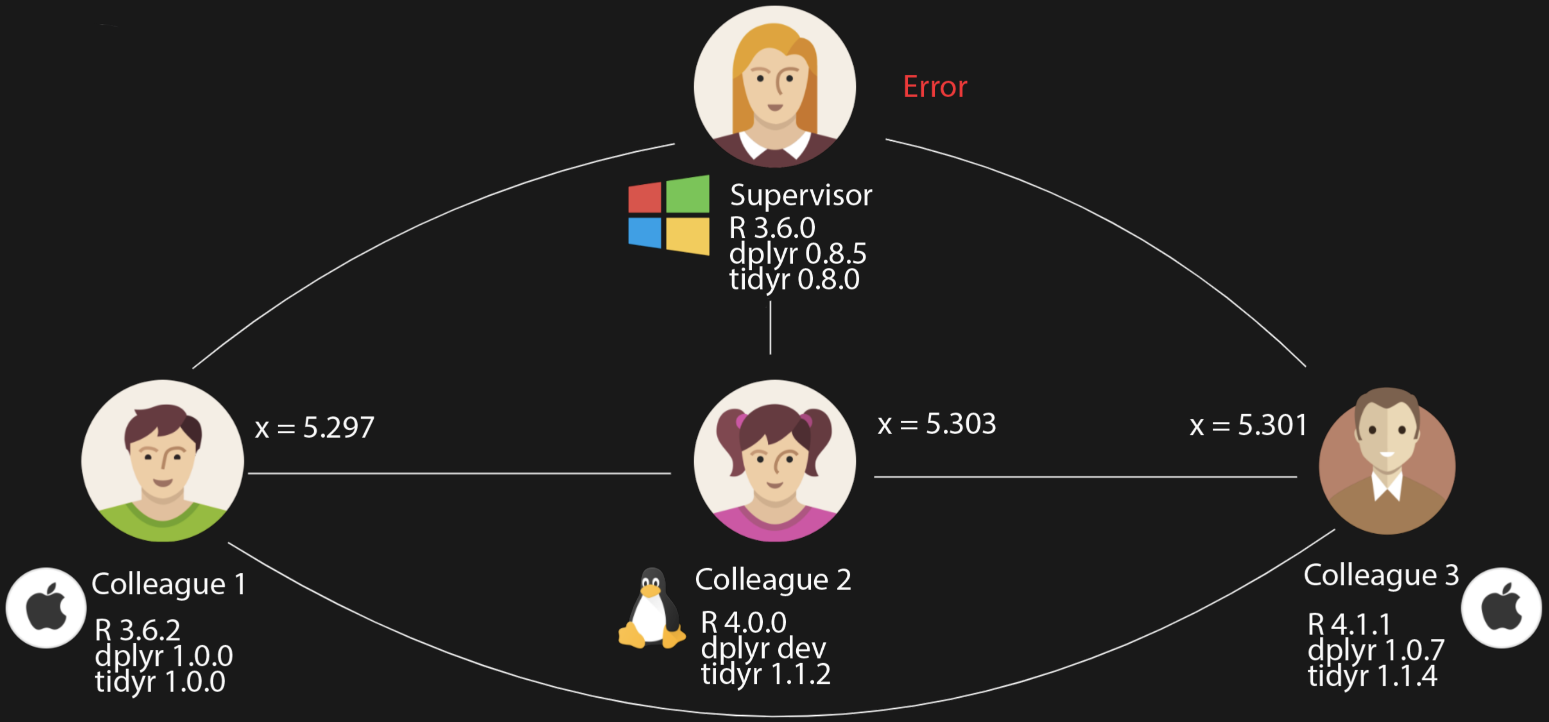
Massive Data Institute, Georgetown University

January 10th, 2023

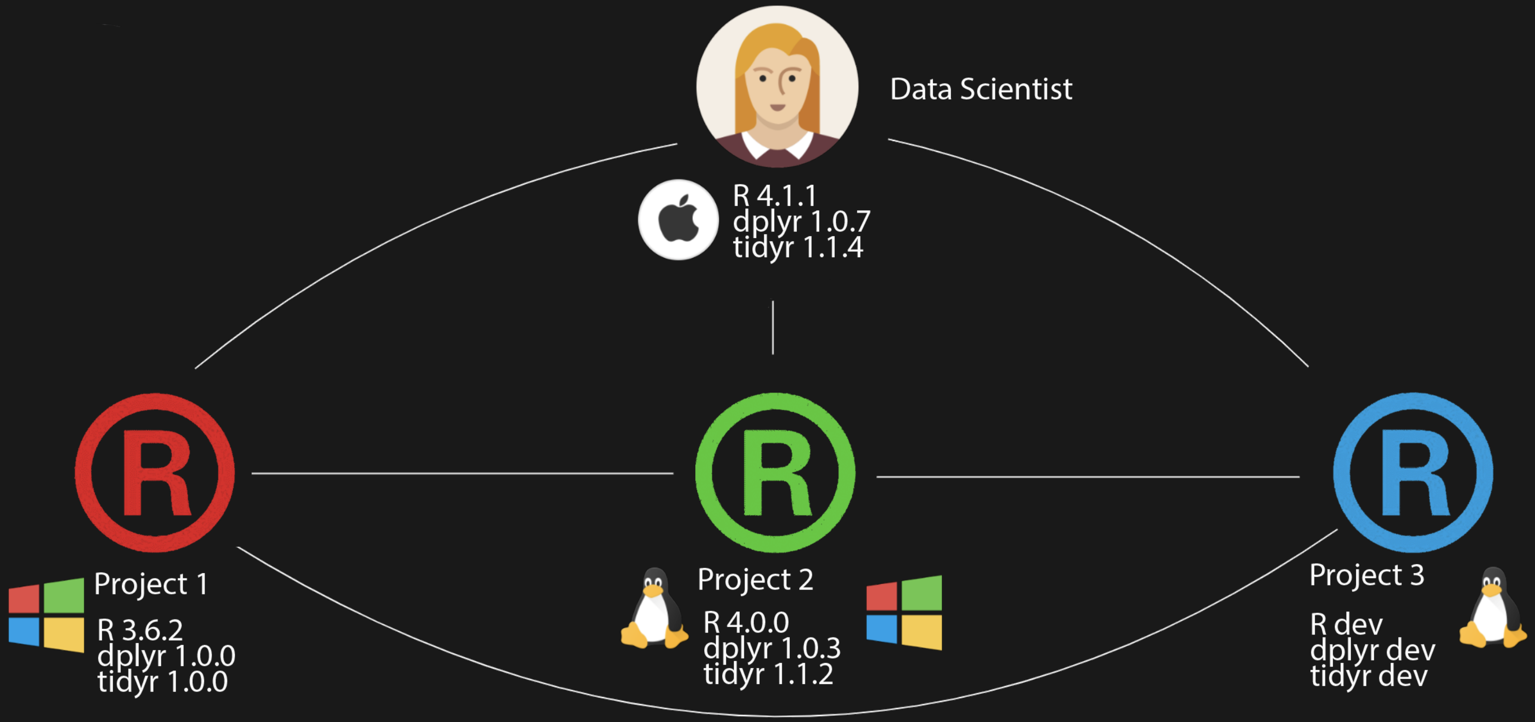
Why?

- Docker and Kubernetes are the cutting-edge tools for tech and tech-related industries and scientific research.
- "The share of jobs containing Docker as a skill on Indeed increased by 9,538% from 2014 to 2019."

The Problem of Reproducibility



The Problem of Reproducibility



The Problem of Reproducibility

- Our computing tools are increasingly powerful, diverse, cloud-based.
  - iPhone 6 is 32,600 times faster than the Apollo Guidance Computer (APC).
  - Supercomputer is now accessible to everyone through cloud computing.
- Our work is required to be more open, transparent, and collaborative.
  - Reproducible research, open-sourced projects, etc.
- Our data becomes bigger, higher dimensional, multimodal.
  - Big data, image/voice data, etc.
- Our analysis needs to be fast, instant, and real-time.
  - Real-time analytic, the pandemic, OpenTable & the State of the Industry
- …

- **Our computing environment is increasingly complex and convoluted.**

Computing Environment

- Computing environment:
  - Hardware
  - Software
    - Operating system
    - System dependencies
    - R/python: versions, packages/libraries (last time)

- Goals:
  - Control the whole computing environment.
  - Configure the environments as we want.
  - Make the environment reproducible.
  - Share the code (that may require specific environment).

Today

- Container
- Docker
  - Run `R`/`python` with Docker
- Kubernates
- Cloud computing and Code Ocean
  - Both front- and back-ends

What is a Container?

↓

What is a Container?

- A standard unit of software that packages up code and all its dependencies
    - Operating system: linux (most common), Windows, Mac OS, etc. and data center, cloud, serverless.
    - System-level dependencies
    - Software packages: R, python, TensorFlow, MySQL, etc.
    - Software dependencies: tidyverse, NumPy, PyTorch
    - Including everything needed to run code

Why Container?

- Lightweight
- Standalone and standard implementation
- Isolated from host system
- Portable and shareable
- Secure

- Container allows us to deploy, replicate, move, and back up a workload in one streamlined way

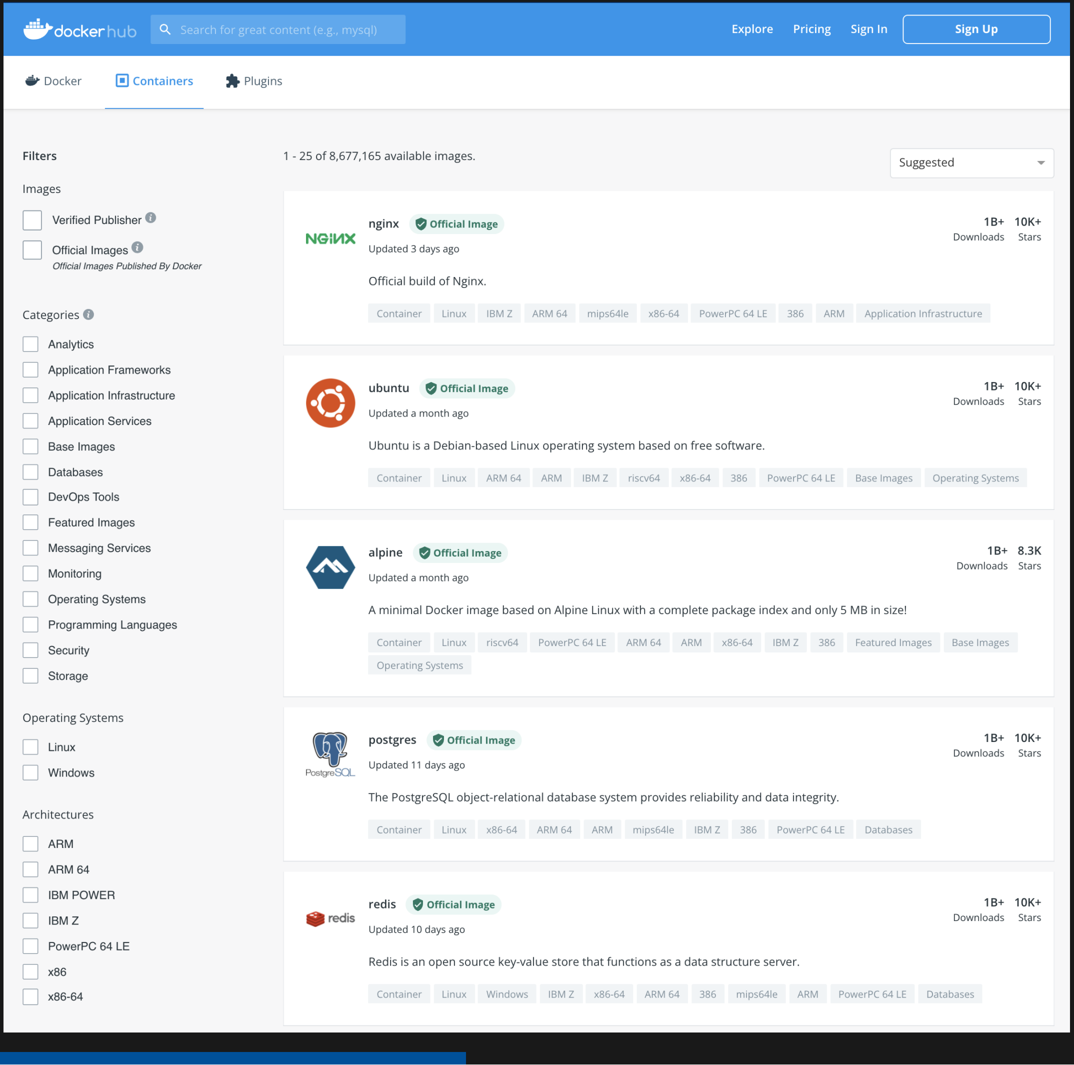
Docker

- Docker is a platform for building, configuring, and delivering containers
- Docker (2013-) is the *de facto* industry standard for containers (1970-)

- Features:
  - Improved and seamless portability from labtop to any desktop, data center and cloud environment.
    - Collaboration
    - HPC and cloud application
  - Isolated, transparent, and reproducible implementation
  - Open-sourced, and community optimized
    - Docker Hub
    - User-created images
  - Versioned
    - Almost all the versions of R, python, etc.
  - Layered
    - Each additional layer will built upon the existing ones

Docker Image

- A static, read-only template for creating containers.



Filters

Images

□ Verified Publisher

□ Official Images
Official Images Published By Docker

Categories

□ Analytics
□ Application Frameworks
□ Application Infrastructure
□ Application Services
□ Base Images
□ Databases
□ DevOps Tools
□ Featured Images
□ Messaging Services
□ Monitoring
□ Operating Systems
□ Programming Languages
□ Security
□ Storage

Operating Systems

□ Linux
□ Windows

Architectures

□ ARM
□ ARM 64
□ IBM POWER
□ IBM Z
□ PowerPC 64 LE
□ x86
□ x86-64

1 - 25 of 8,677,165 available images.

Suggested

nginx Official Image
Updated 3 days ago
1B+ Downloads · 10K+ Stars

Official build of Nginx.

Container · Linux · IBM Z · ARM 64 · mips64le · x86-64 · PowerPC 64 LE · 386 · ARM · Application Infrastructure

ubuntu Official Image
Updated a month ago
1B+ Downloads · 10K+ Stars

Ubuntu is a Debian-based Linux operating system based on free software.

Container · Linux · ARM 64 · ARM · IBM Z · riscv64 · x86-64 · 386 · PowerPC 64 LE · Base Images · Operating Systems

alpine Official Image
Updated a month ago
1B+ Downloads · 8.3K Stars

A minimal Docker image based on Alpine Linux with a complete package index and only 5 MB in size!

Container · Linux · riscv64 · PowerPC 64 LE · ARM 64 · ARM · x86-64 · IBM Z · 386 · Featured Images · Base Images · Operating Systems

postgres Official Image
Updated 11 days ago
1B+ Downloads · 10K+ Stars

The PostgreSQL object-relational database system provides reliability and data integrity.

Container · Linux · x86-64 · ARM 64 · ARM · mips64le · IBM Z · 386 · PowerPC 64 LE · Databases

redis Official Image
Updated 10 days ago
1B+ Downloads · 10K+ Stars

Redis is an open source key-value store that functions as a data structure server.

Container · Linux · Windows · IBM Z · x86-64 · ARM 64 · 386 · mips64le · ARM · PowerPC 64 LE · Databases

Use Docker to Run R

- Rocker project: https://www.rocker-project.org/

Image	Description
r-base	Current R version
r-devel	R-devel added side-by-side onto r-base
r-ver	Specify R version
rstudio	Adds rstudio
tidyverse	Adds tidyverse & devtools
verse	Adds tex & publishing-related packages
geospatial	Adds geospatial libraries

Run `R` Using Pre-built Images

- Command:

```
docker run -it --rm rocker/r-base
```

- `docker run`: run processes based on an image
- General form: `docker run [OPTIONS] IMAGE[:TAG|@DIGEST] [COMMAND] [ARG … ]`
- `-it`: interactive session
- `-rm`: automatically remove container once stopped
- `rocker/r-base`: pull latest r-base from rocker repository

Run `R` Using Pre-built Images

- Pull a specific version using `rocker/r-ver:4.0.1`

```
docker run -it --rm rocker/r-ver:4.0.1
```

- Run an RStudio server

```
docker run --rm -p 8888:8787 -e PASSWORD='mypassword' rocker/rstudio:4.0.5
```

- `-p`: publish a port
- `-e`: set environment variable

Using Docker to Run `python`

- Lots of images with different support and configurations

```
docker run -it --rm python
docker run -it --rm python:3.7.4
```

Build Your Own `R` Docker Image

`Dockerfile`: instructions for assembling and configuring an Docker image.

```
FROM rocker/r-ver:4.0.3

# System dependencies
RUN apt-get update && apt-get install -y curl libz-dev

# R packages
RUN Rscript -e 'install.packages("MASS")'
RUN install2.r readr dplyr ggplot2 forcats

## Copy files
RUN mkdir docker-demo
COPY data docker-demo/data
COPY code docker-demo/code
RUN mkdir docker-demo/output
#ADD . docker-demo

## Set working directory
WORKDIR docker-demo
```

Build Your Own `R` Docker Image

- Build image

```
docker build -t demo:r .
```

- `-t`: name tag for the image
- `.`: root directory (where the Dockerfile is)

- Run a container using the image

```
docker run -i -t demo:r /bin/bash
```

- `-i`: interactive
- `-t`: name tag of the image
- `/bin/bash`: start a bash session

Build Your Own `python` Docker Image

```
FROM python:3.8

# python libraries
RUN pip install -U bs4

## Copy files
RUN mkdir docker-demo
RUN mkdir docker-demo/data
ADD . docker-demo

## Set working directory
WORKDIR docker-demo
```

- Build image

```
docker build -t demo:python .
```

- Run a container using the image

```
docker run -i -t demo:python /bin/bash
```

Managing Docker Container

- List and commit current containers

```
docker ps -l
docker commit [CONTAINER ID] [NAME]
```

- Build a Docker image

```
docker images
docker create [IMAGE ID]
```

- Extract files

```
docker cp [ID]:[Container PATH] [Local PATH]
```

- Remove containers and images

```
docker rm -f [Container ID]
docker image rm [Image ID]
docker system prune -all
```

Exercise

- Verify Docker Installation
  - Open Terminal (Mac/Linux) or Command Prompt/PowerShell (Windows)
  - Run `docker run hello-world`
- Run an R or python container with a specific version using `docker run`.
- Run R and python container using Dockerfile.
  - Go to `/docker-demo-python` and build a `demo-python` container using the provided Dockerfile.
  - *Feel free to use your own project.
  - Run the container and test the code script in `/docker-demo-python/code`
  - Extract the output file using `docker cp`
  - Follow the same procedure for `/docker-demo-r`

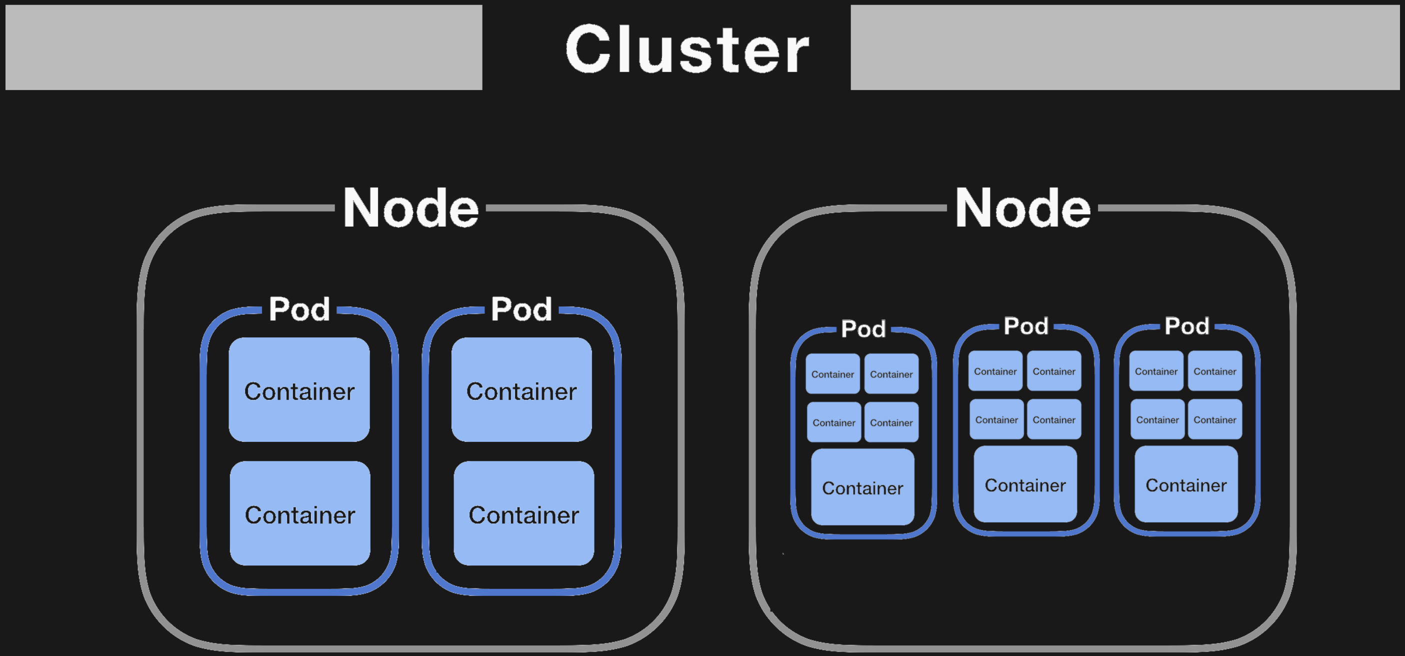
Kubernates

- What is Kubernates (aka. K8s)

↓

What is Kubernates (aka. K8s)

- Container management
  - Deployment, scaling, scheduling, etc.
- Works with Docker, Containerd, and CRI-O, etc.



Code Ocean

- An integrative, collaborative platform for computational research
  - Develop, collaborate, share, and publish code using a web browser (without the need for much specialized knowledge)
  - Similar tools: Digital Ocean, Vultr, Kamatera, Google Cloud/Amazon Web Service, etc.

- Both:
  - a *product* of Docker and K8s *and*
  - an *application* of cloud computing

- **Capsule**
  - Container (using images supplied by CO)
  - Cloud computing + environment + code + (optional) data

- The backend of Code Ocean
  - AWS computing instance: 16 cores, 120 GB of memory
  - Docker for configuring computing environment (user-accessible)
  - K8s for allocating and scheduling resources (not user-accessible)

Exercise

- *You can use the example code or create your own capsule for your project.*
- Create a Code Ocean account at https://codeocean.com
  - `.edu` account comes with 10 hours computing time
- Create a new capsule
- Add `R` (4.1.0) as the base environment
- Install `python` support by adding `python3-pip:latest` to `apt-get`
- Install system dependency using `apt-get`: `libudunits2-dev`, `libgdal-dev`, `libgeos-dev`, `libproj-dev`, `libfontconfig1-dev`.
- Add packages/libraries along with their specific versions
  - Install `beautifulsoup4:4.11.1`, `requests:latest` via `pip3`
  - Install `dplyr:1.0.9`, `tidyr:1.2.0`, `ggplot2:3.4.0`, `sf:latest` via R (CRAN) and `fiftystater` via Github (`wmurphyrd/fiftystater`)
- Upload files
  - Upload code scripts to `/code`
  - Upload data to `/data`
  - The only runtime writable folder is `/results`

(continued on next page …)

Exercise (cont'd)

- Create a `run` script for running the code and set as file to run

```
#!/usr/bin/env bash
set -ex
mkdir -p ../results/data # make a dir for saving scraped data
mkdir -p ../results/output # make a dir for saxing output figs
python3 -u election-2020.py "$@" # running python script
Rscript election-map-2020.R "$@" # running R script for analysis
```

- Edit metadata and readme
- Commit the changes
- Execute a Reproducible Run