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republic

Docker for Data Scientists

Packaging your models & best practices

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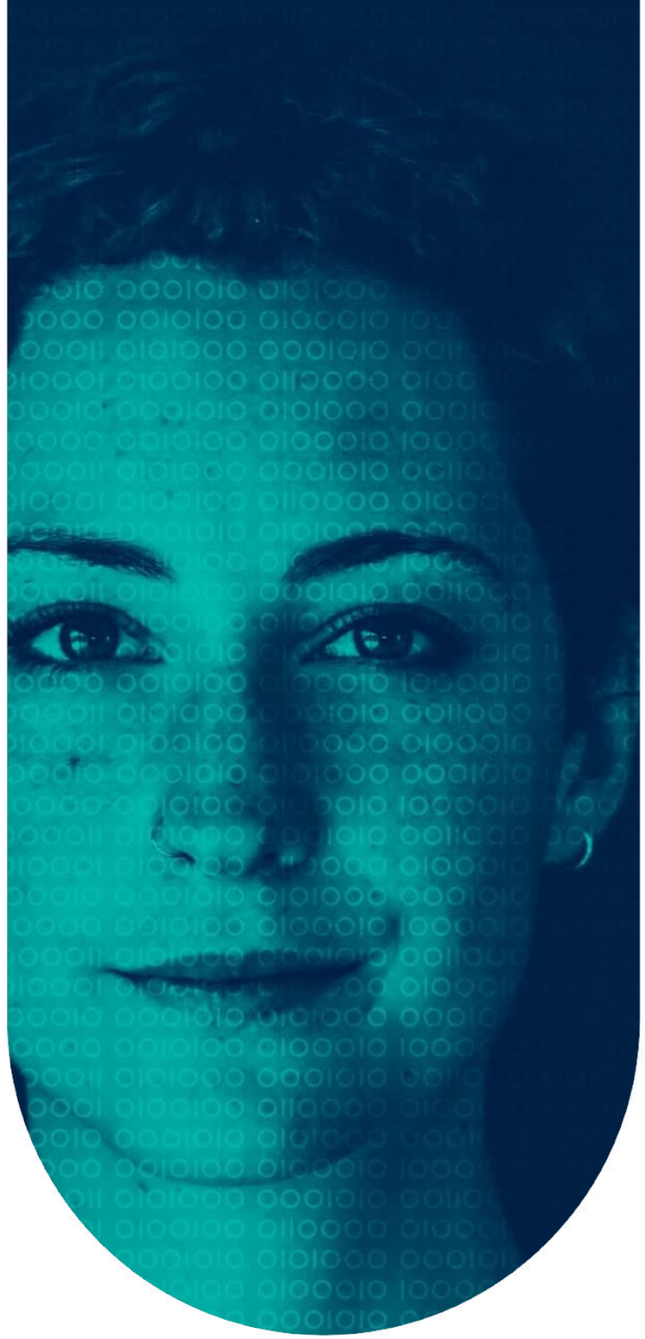

After this webinar, you will know...

Why you need Docker

How Docker works

How to use Docker in your workflow

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Data Scientists

Data Engineers

Presenters and contributors

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Data Scientist

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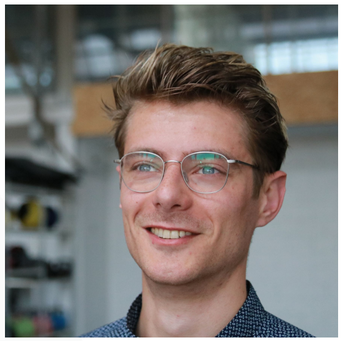

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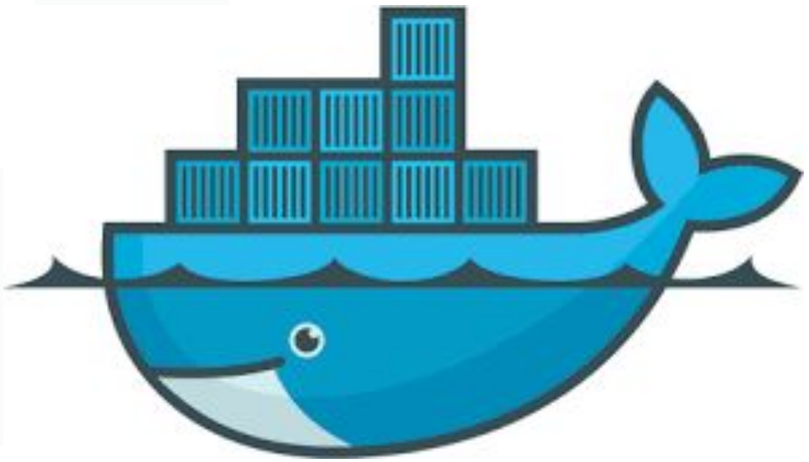
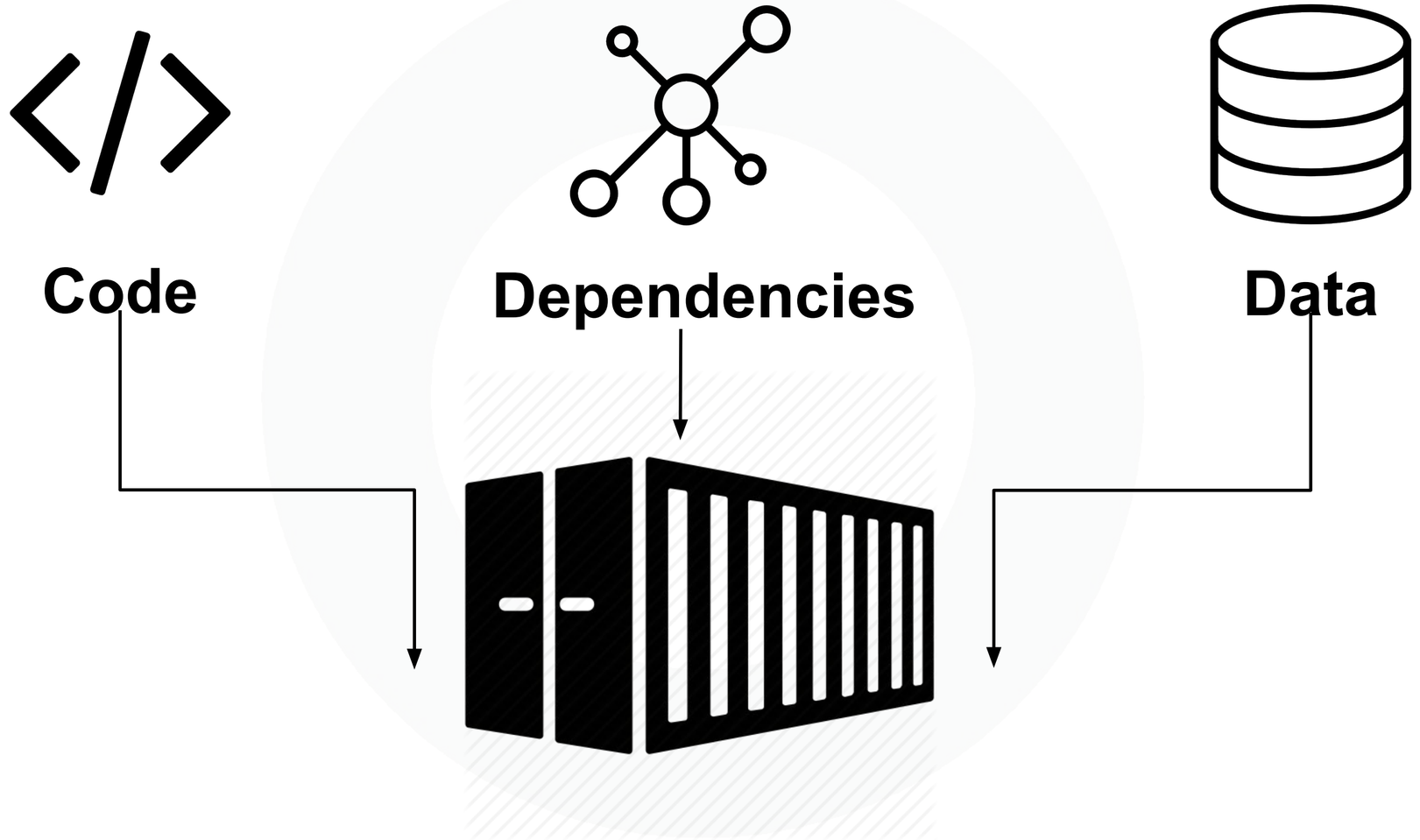
What does Docker do?

Docker allows us to package and run applications in an isolated environment



Docker Containers



Problems Docker solves

Reproducing models/environments:

Did I need this library in this branch of my code?

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What environment variables did I have to set when I started this project?

Reproducing models/environments:

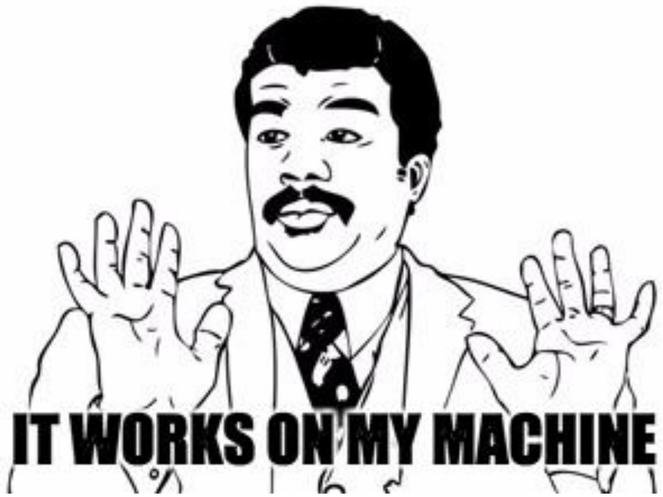
Did I need this library in this branch of my code?

What environment variables did I have to set when I started this project?

Did I use that confidential data when training this model?

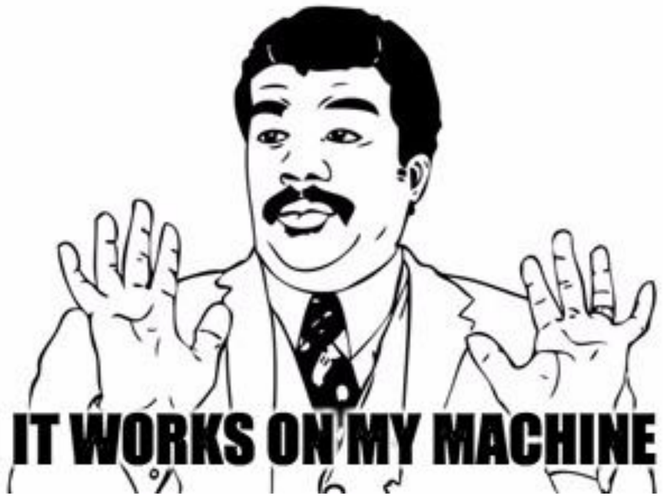
Sharing your work

- *Import error: no module named XXXX*



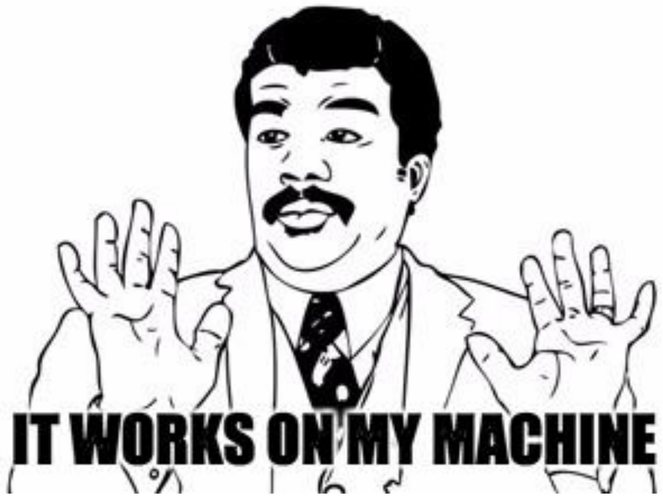
Sharing your work

- *Import error: no module named XXXX*
- *“Oh no all my devices only run Arch Linux...”*



Sharing your work

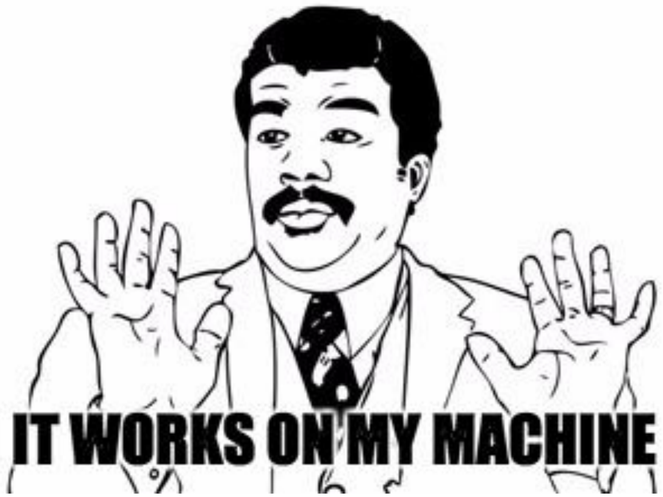
- *Import error: no module named XXXX*
- *“Oh no all my devices only run Arch Linux...”*
- *“Here is the Git repo, now you have to install X, Y, and Z. Oh right I forgot about W. Why don’t you have an up to date COBOL compiler?!”*



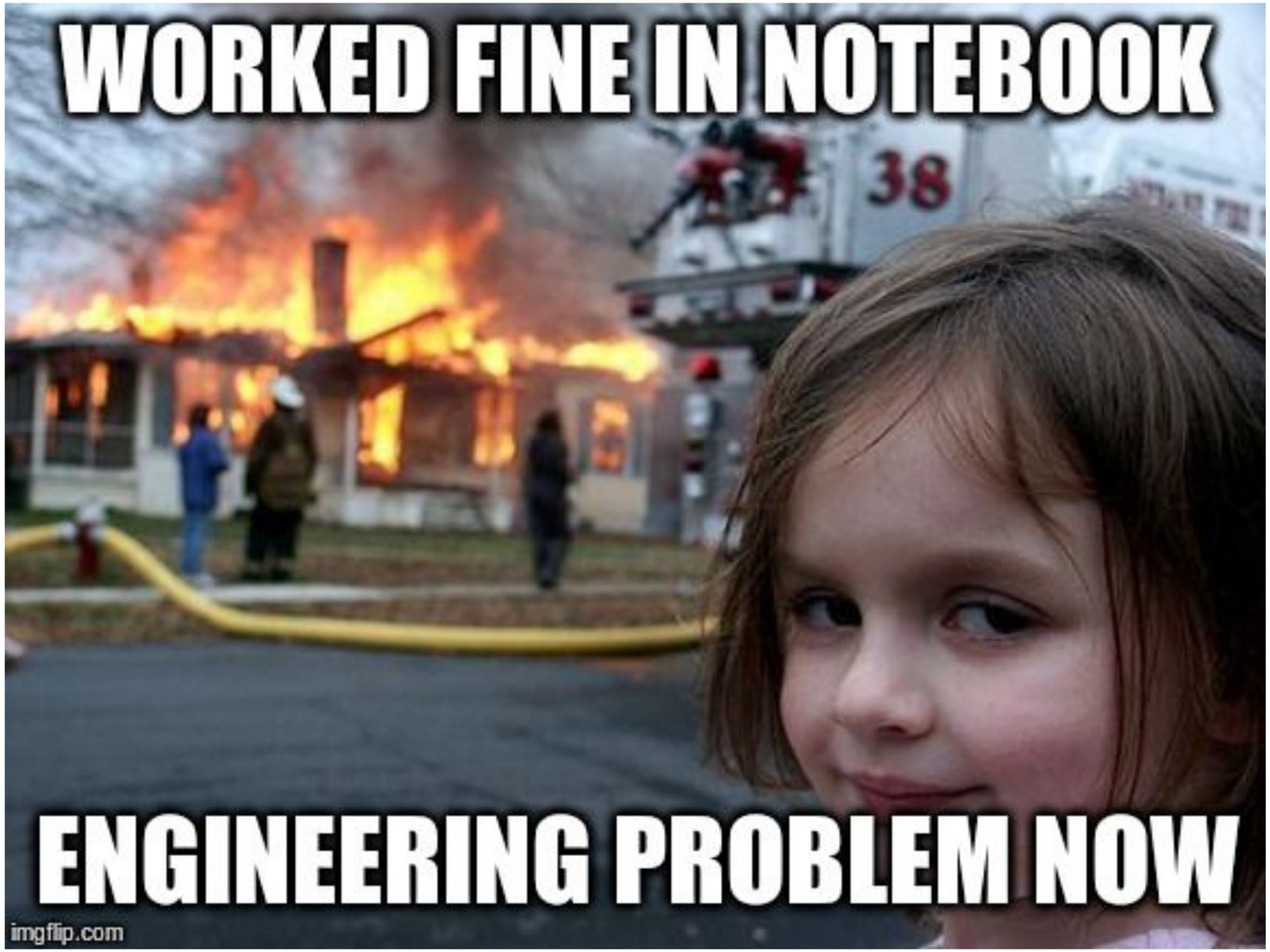
Sharing your work

- *Import error: no module named XXXX*
- *“Oh no all my devices only run Arch Linux...”*
- *“Here is the Git repo, now you have to install X, Y, and Z. Oh right I forgot about W. Why don’t you have an up to date COBOL compiler?!”*

→ Share code repo with a small text file (Dockerfile) and be done

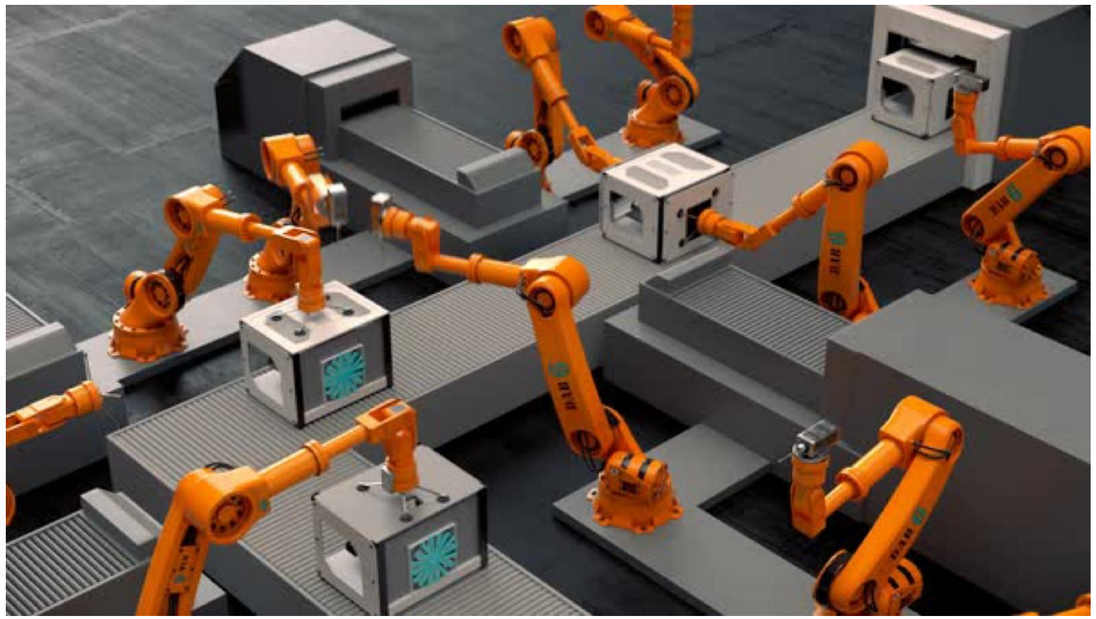


Deployment


WORKED FINE IN NOTEBOOK
38
ENGINEERING PROBLEM NOW
imgflip.com

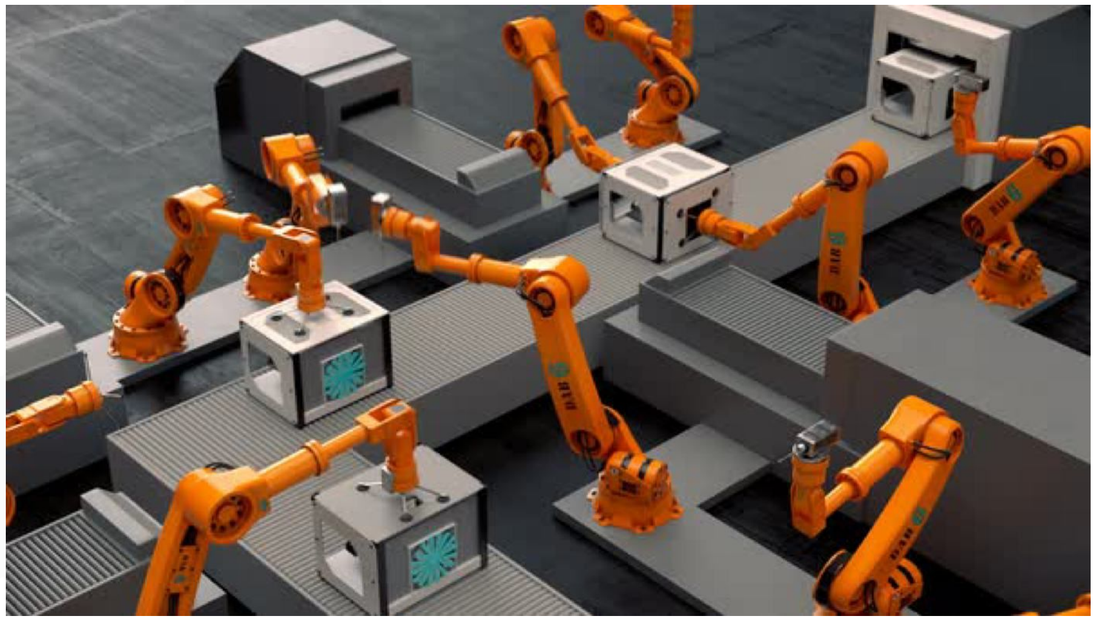
Deployment

- Independent of underlying hardware



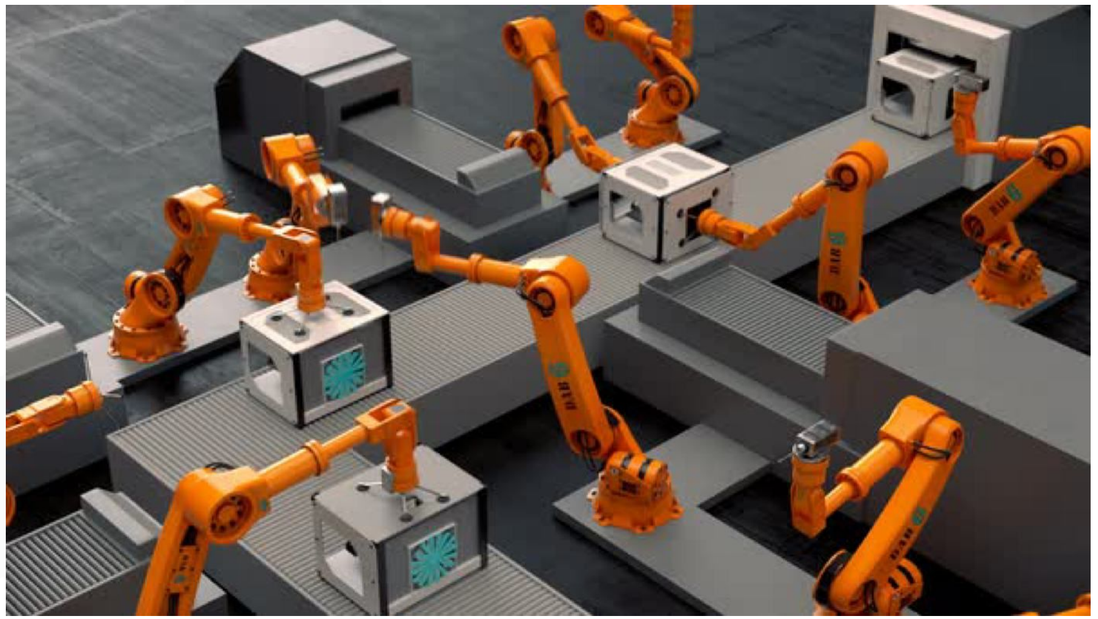
Deployment

- Independent of underlying hardware
- Easy to put anywhere, in any cloud environment



Deployment

- Independent of underlying hardware
- Easy to put anywhere, in any cloud environment
- Can be used in a cluster



How does Docker work

Definitions

Container

Image

Dockerfile

Volume

Definitions

Container: “Lightweight, standalone, executable software package;
includes everything: code, runtime, system tools, system libraries and settings.”

Image

Dockerfile

Volume

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Image: A frozen snapshot of a container.

Dockerfile

Volume

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Container: “Lightweight, standalone, executable software package;
includes everything: code, runtime, system tools, system libraries and settings.”

Image: A frozen snapshot of a container.

Dockerfile: An (often) short text-file detailing how to make an image from another image.

Volume

Definitions

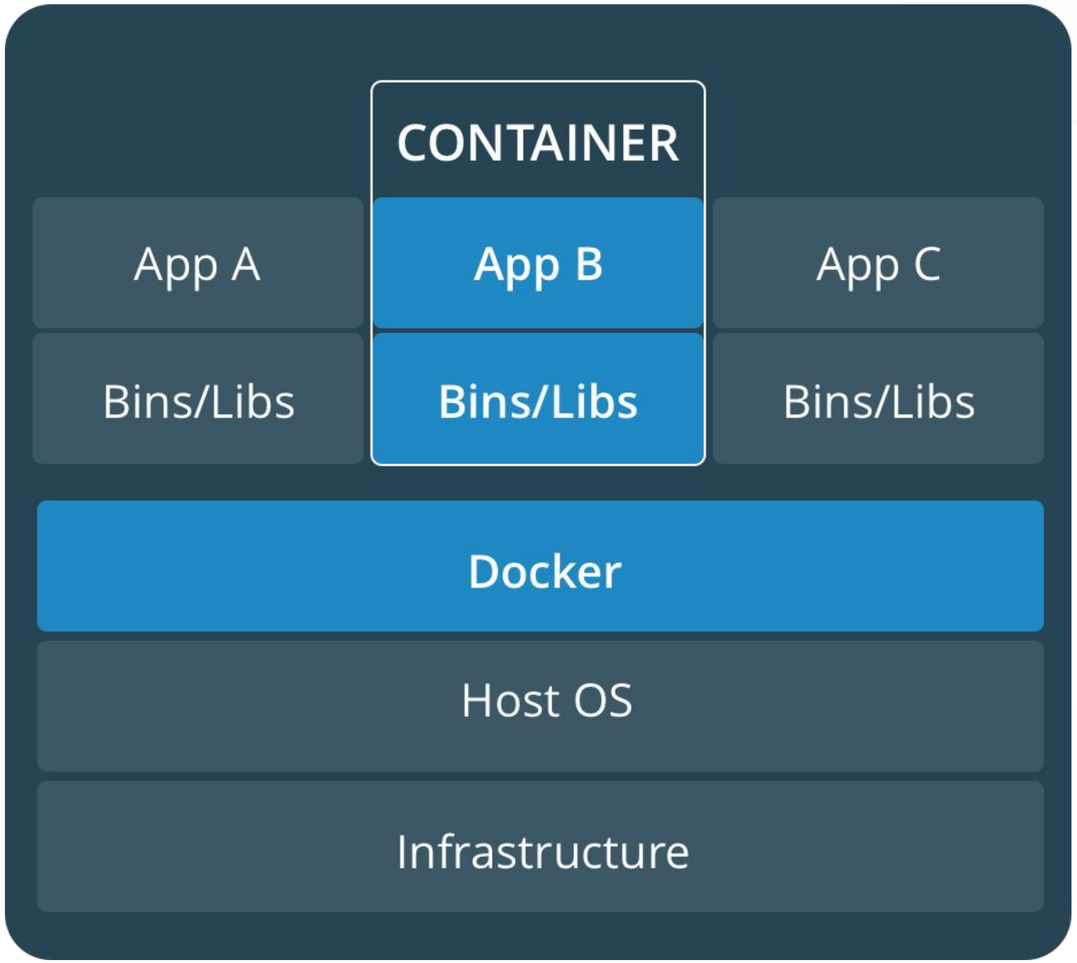
Container: “Lightweight, standalone, executable software package;
includes everything: code, runtime, system tools, system libraries and settings.”

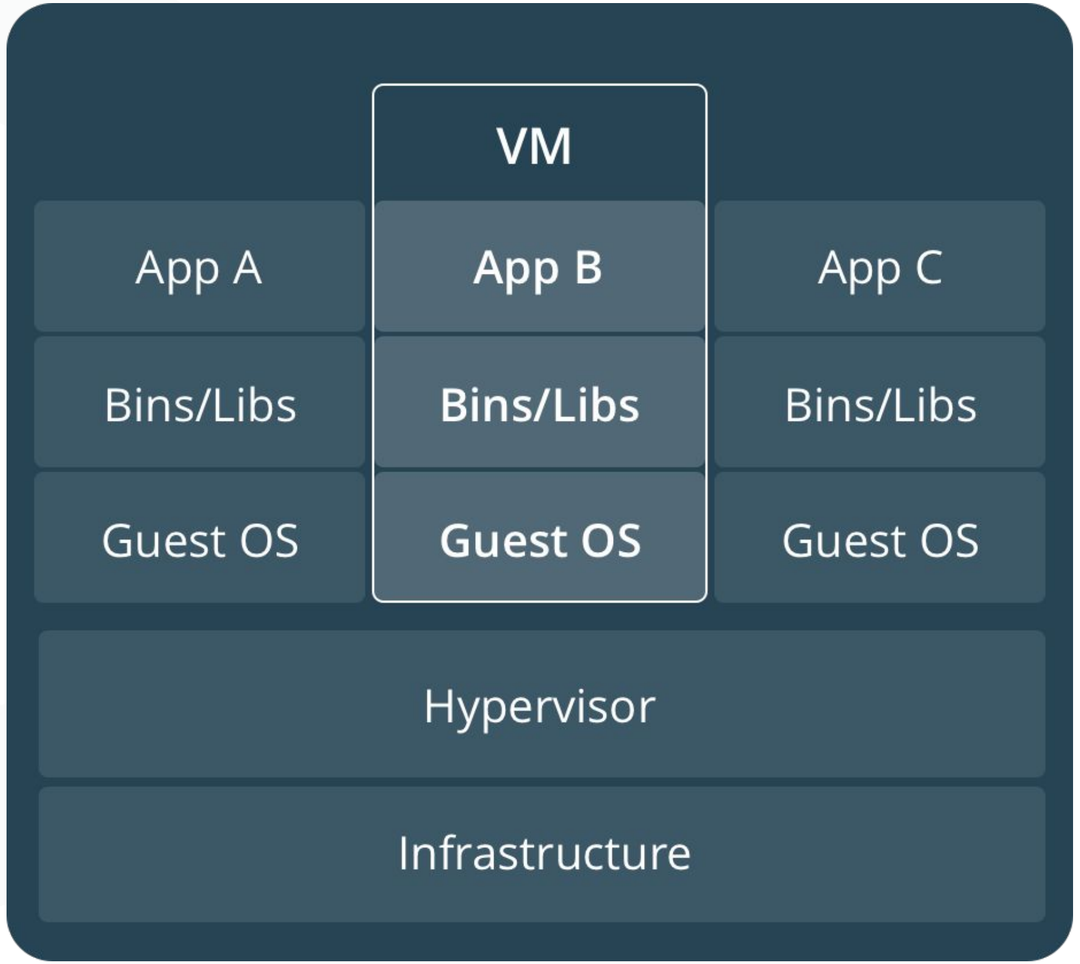
Image: A frozen snapshot of a container.

Dockerfile: An (often) short text-file detailing how to make an image from another image.

Volume: A chunk of filesystem (“folder”) that can be accessed by both containers as well as the host computer, and can persist.

Definitions: Containers vs Virtual Machines





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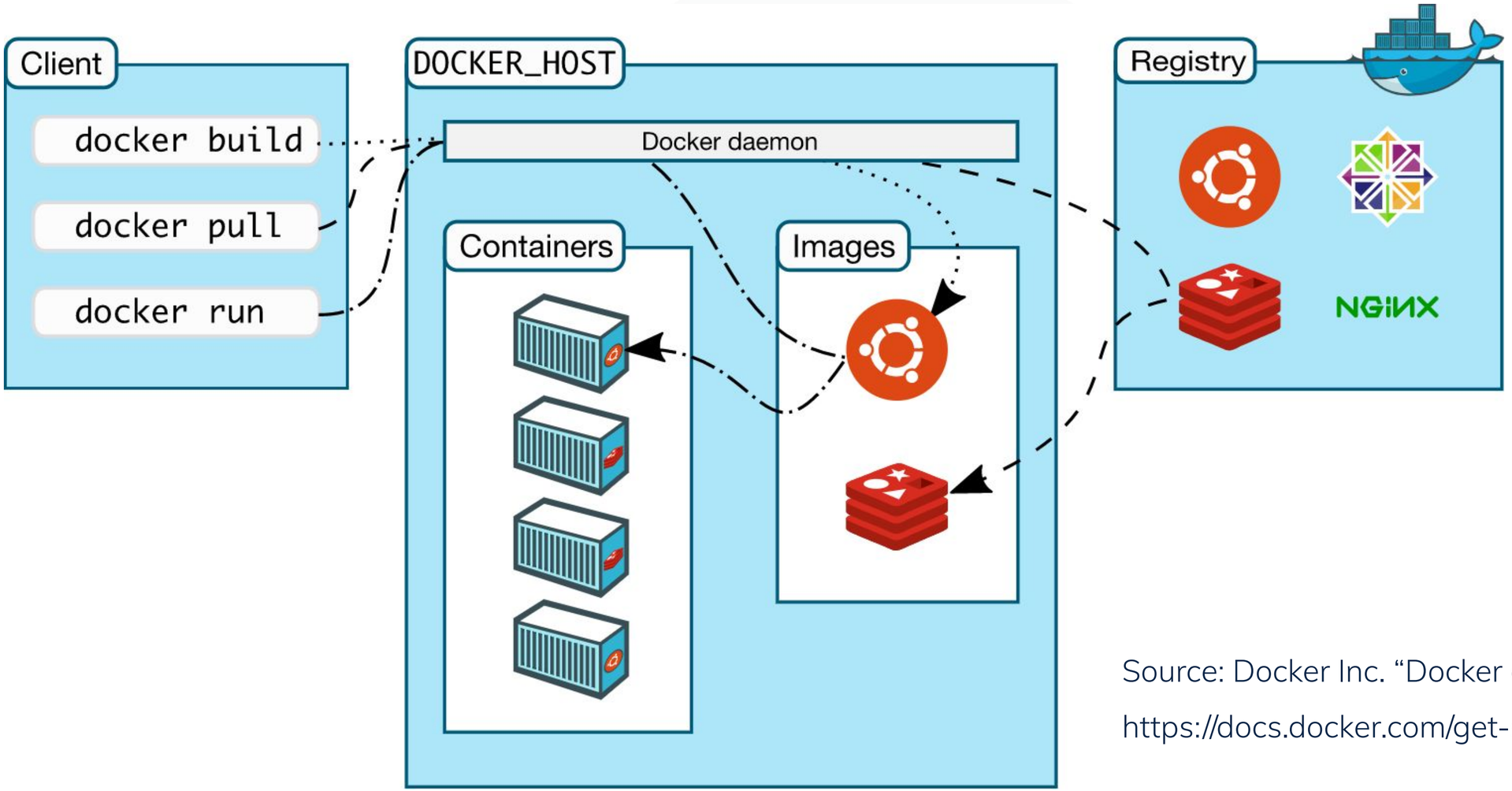
How it actually works



Source: Docker Inc. “Docker overview” located at https://docs.docker.com/get-started/overview/

Search

OFFICIAL REPOSITORY

python ☆

Last pushed: 5 hours ago

Repo Info | Tags

Short Description

Python is an interpreted, interactive, object-oriented, open-source programming language.

Full Description

Supported tags and respective `Dockerfile` links

Simple Tags

- `3.7.0b3-stretch`, `3.7-rc-stretch`, `rc-stretch` *(3.7-rc/stretch/Dockerfile)*
- `3.7.0b3-slim-stretch`, `3.7-rc-slim-stretch`, `rc-slim-stretch`, `3.7.0b3-slim`, `3.7-rc-slim`, `rc-slim` *(3.7-rc/stretch/slim/Dockerfile)*
- `3.7.0b3-alpine3.7`, `3.7-rc-alpine3.7`, `rc-alpine3.7`, `3.7.0b3-alpine`, `3.7-rc-alpine`, `rc-alpine` *(3.7-rc/alpine3.7/Dockerfile)*

Building our first container

Using Docker

Dockerfile basics

```
1  FROM ubuntu:18.04
2  RUN apt-get update && apt-get install -y python python-pip
3  RUN pip install numpy
4  COPY ./calculate_pi.py /
5  ENTRYPOINT [ "python", "/calculate_pi.py" ]
6  CMD ["1000"]
7
```

https://github.com/BigDataRepublic/docker_webinar

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Dockerfile basics

- Constructed as layers
- Each instruction ~ 1 layer
- Start with base image - FROM
- Copy files to image - COPY or ADD
- Execute shell commands - RUN
- Run model - ENTRYPOINT with CMD

Image layers

- Each layer read-only
- Layer stores changes from previous layer

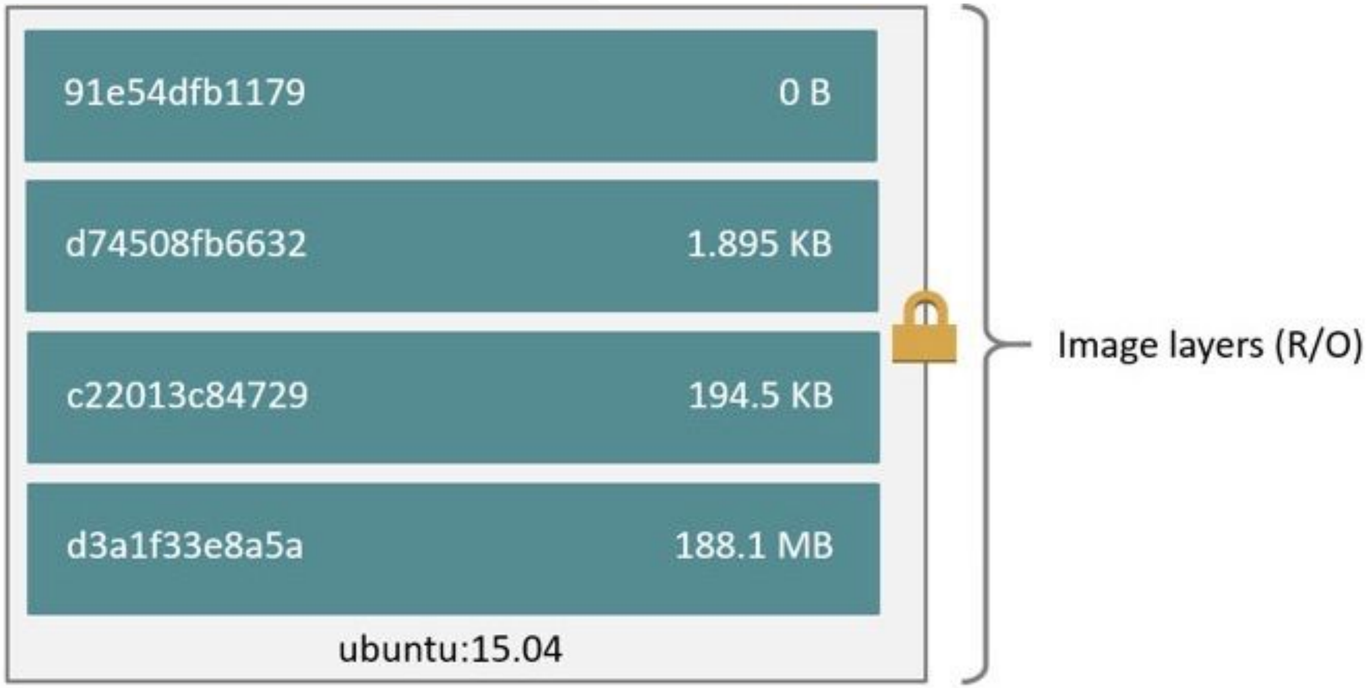
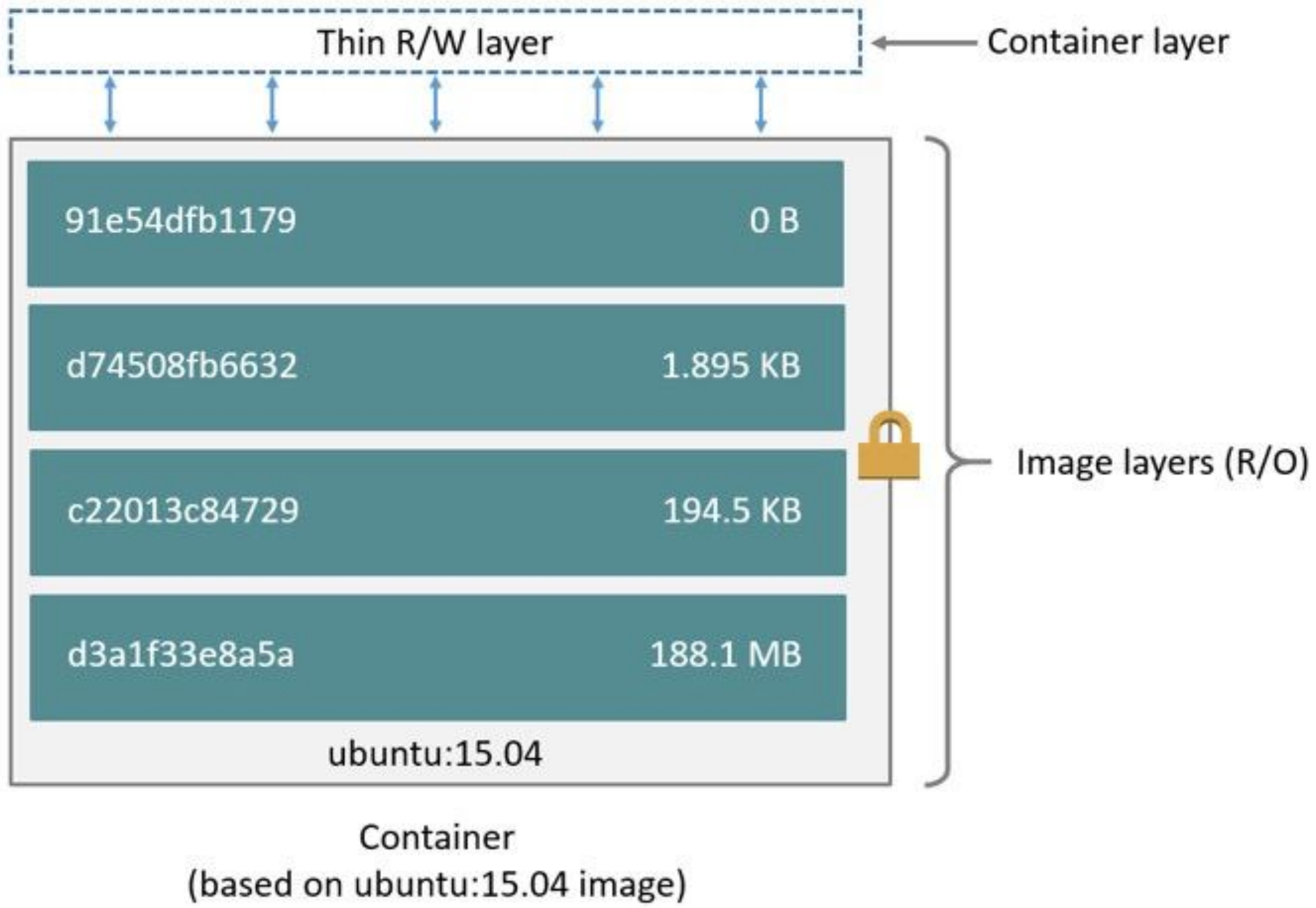


Image layers → container

- Each layer read-only
- Layer stores changes from previous layer
- Container > adds writeable layer on last image layer



Running it all

- docker build -t approx_pi -f Dockerfile_first .
- docker run approx_pi:latest

```
docker build -t approx_pi -f Dockerfile_first .
Sending build context to Docker daemon  587.8kB
Step 1/6 : FROM ubuntu:18.04
 ---> 4e5021d210f6
Step 2/6 : RUN apt-get update && apt-get install -y python python-pip
 ---> Using cache
 ---> 19ccdd3989ae
Step 3/6 : RUN pip install numpy
 ---> Using cache
 ---> 4551ccf0b8a2
Step 4/6 : COPY ./calculate_pi.py /
 ---> Using cache
 ---> 5c5d4bb4a615
Step 5/6 : ENTRYPOINT [ "python", "/calculate_pi.py" ]
 ---> Using cache
 ---> 2ef60e6036a5
Step 6/6 : CMD ["1000"]
 ---> Using cache
 ---> 523087ef7bd6
Successfully built 523087ef7bd6
```

Training a model with Docker

Using Docker for Data Science

Thursday, April 30, 2020

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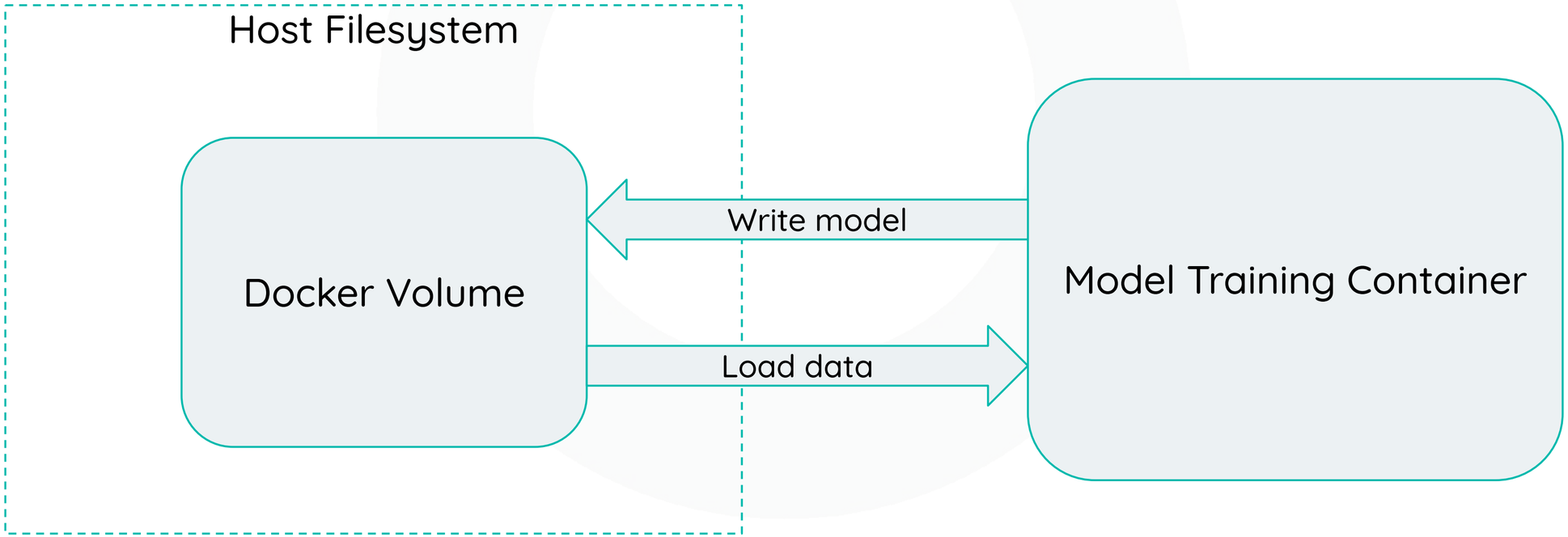
Training & saving models

- Python model training in container
- Need to retrieve our model after training
- Docker volumes: sharing storage



Training & saving models

- To initialize with local filesystem folder:
  docker run -v /foo/data:/app/data my_container

- docker build -t iris_trainer -f Dockerfile_training .
- docker run -v /full/path/to/model:/app/model iris_trainer

Training & saving models continued

Dockerfile_training

```
FROM ubuntu:18.04

LABEL version="1.0"
LABEL description="This container trains a random forest on the iris dataset."
LABEL maintainer="joris.bukala@bigdatarepublic.nl,jacobus.herman@bigdatarepublic.nl"

COPY --chown=root:root ./security/add_user_group.sh ./training_app/requirements.txt /app/
RUN apt-get update -y && \
    apt-get install -y python-pip python-dev && \
    pip install -r /app/requirements.txt && \
    chmod 550 /app/add_user_group.sh && \
    /app/add_user_group.sh && \
    rm /app/add_user_group.sh && \
    rm -rf /var/lib/apt/lists/* && \
    mkdir -p /app/model && \
    chown -R dockerapp:dockerapp /app/model

USER dockerapp

COPY --chown=dockerapp:dockerapp ./training_app /app

VOLUME [ "/app/model" ]
ENTRYPOINT [ "python" ]
CMD [ "/app/train.py" ]
```

Serving predictions

Using Docker for Data Science

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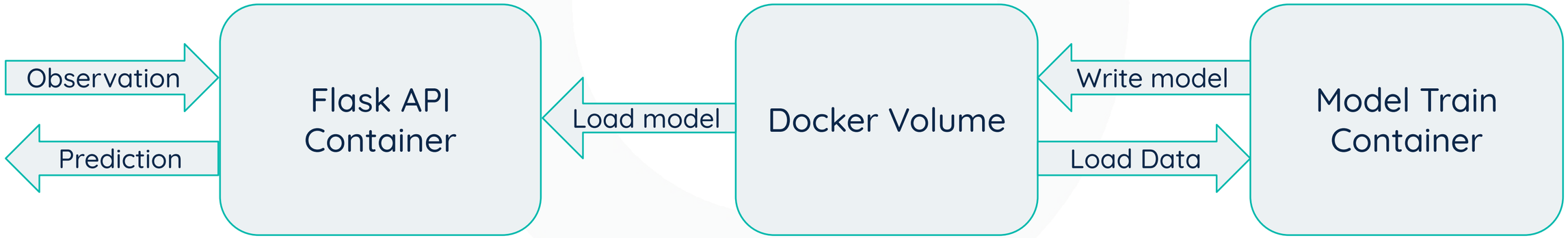
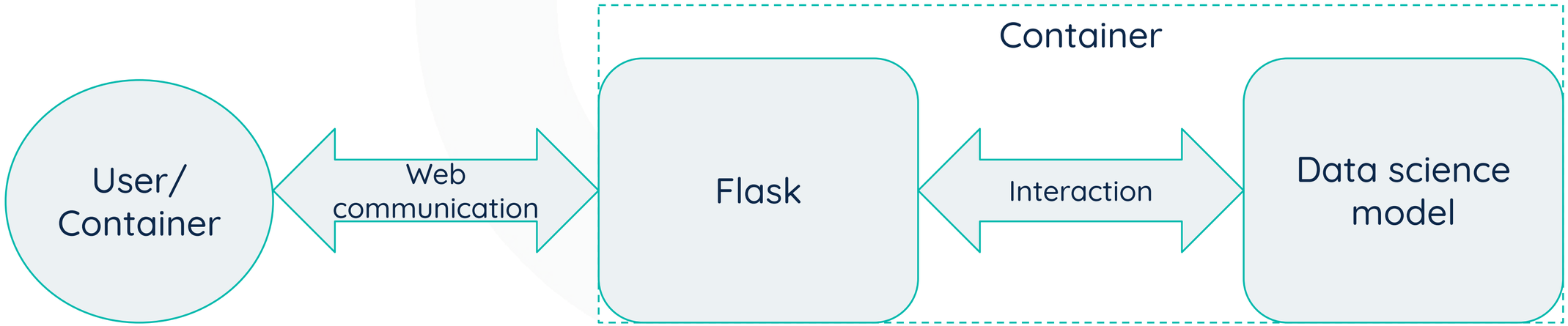
Serving models

- Use trained model with Flask API
- Share same volume
- Receives array with 2 numbers & returns number



What is Flask?

- Micro framework for building web applications
- Allows creation of interface to something through web communication
- Similar to website: user interacts with content
- End result (web) Application Programming Interface (API)



Flask source: https://palletsprojects.com/p/flask/

Serving models

- docker build -t iris_predictor -f Dockerfile_prediction .
- docker run -p 5000:5000 -v ~/model_volume:/app/model iris_predictor

- -p maps host port to container port
- Communication to 5000 on host goes to 5000 on container (like a mirror)
- Ports can be different, e.g. -p 80:5000

Serving models image

Dockerfile_prediction

```
FROM ubuntu:18.04

LABEL version="1.0"
LABEL description="This container exposes a fitted random forest model with Flask on the Iris dataset."
LABEL maintainer="joris.bukala@bigdatarepublic.nl,jacobus.herman@bigdatarepublic.nl"

COPY --chown=root:root ./security/add_user_group.sh ./prediction_app/requirements.txt /app/
RUN apt-get update -y && \
    apt-get install -y python-pip python-dev && \
    pip install -r /app/requirements.txt && \
    chmod 550 /app/add_user_group.sh && \
    /app/add_user_group.sh && \
    rm /app/add_user_group.sh && \
    rm -rf /var/lib/apt/lists/* && \
    mkdir -p /app/model && \
    chown -R dockerapp:dockerapp /app/model

USER dockerapp

COPY --chown=dockerapp:dockerapp ./prediction_app /app

ENV FLASK_APP=/app/main.py

VOLUME [ "/app/model" ]
EXPOSE 5000
ENTRYPOINT [ "flask" ]
CMD [ "run", "--host=0.0.0.0" ]
```

Making a front-end

Using Docker for Data Science

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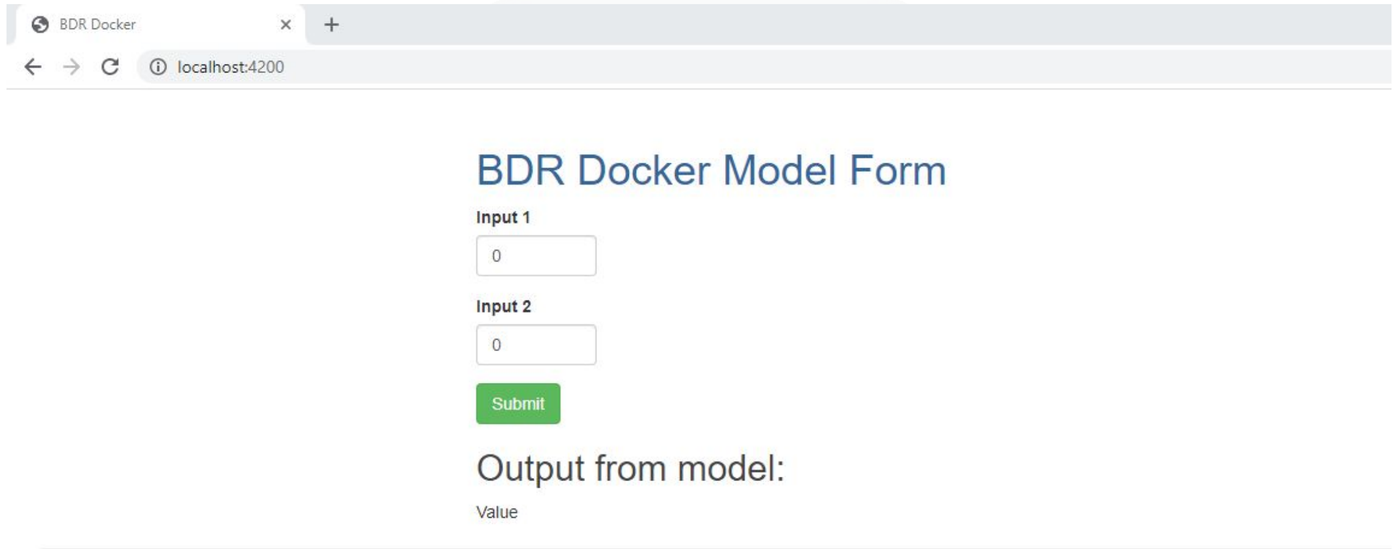
Add web UI

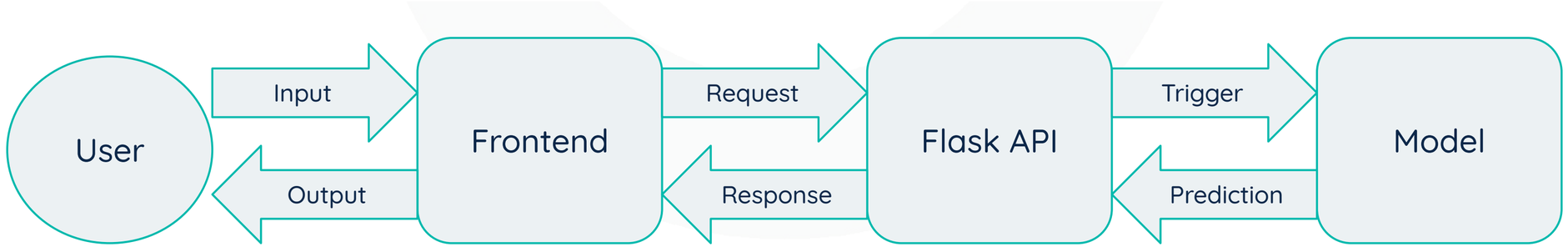
- AngularJS web application for access to production model
- Frontend container interacts with prediction container

<u>To run:</u>

- docker build -t iris_frontend -f Dockerfile_frontend .
- docker run -d -p 4200:4200 iris_frontend

Web UI flow


BDR Docker
localhost:4200
BDR Docker Model Form
Input 1
0
Input 2
0
Submit
Output from model:
Value


User
Input
Output
Frontend
Request
Response
Flask API
Trigger
Prediction
Model

Web UI image

Dockerfile_frontend

```
FROM node:12.16.2

LABEL version="1.0"
LABEL description="This container runs an Angular JS app that connects to a REST API on localhost:5000."
LABEL maintainer="joris.bukala@bigdatarepublic.nl,jacobus.herman@bigdatarepublic.nl"

WORKDIR /app

ENV PATH /app/node_modules/.bin:$PATH

COPY --chown=root:root ./security/add_user_group.sh ./frontend/model-display/package.json /app/
RUN npm install && \
    chmod 550 /app/add_user_group.sh && \
    /app/add_user_group.sh && \
    rm /app/add_user_group.sh

USER dockerapp

COPY --chown=dockerapp:dockerapp ./frontend/model-display /app/

EXPOSE 4200
ENTRYPOINT [ "ng", "serve" ]
CMD [ "--host", "0.0.0.0", "--disableHostCheck", "true" ]
```

Best practices

For writing Dockerfiles

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Docker-compose

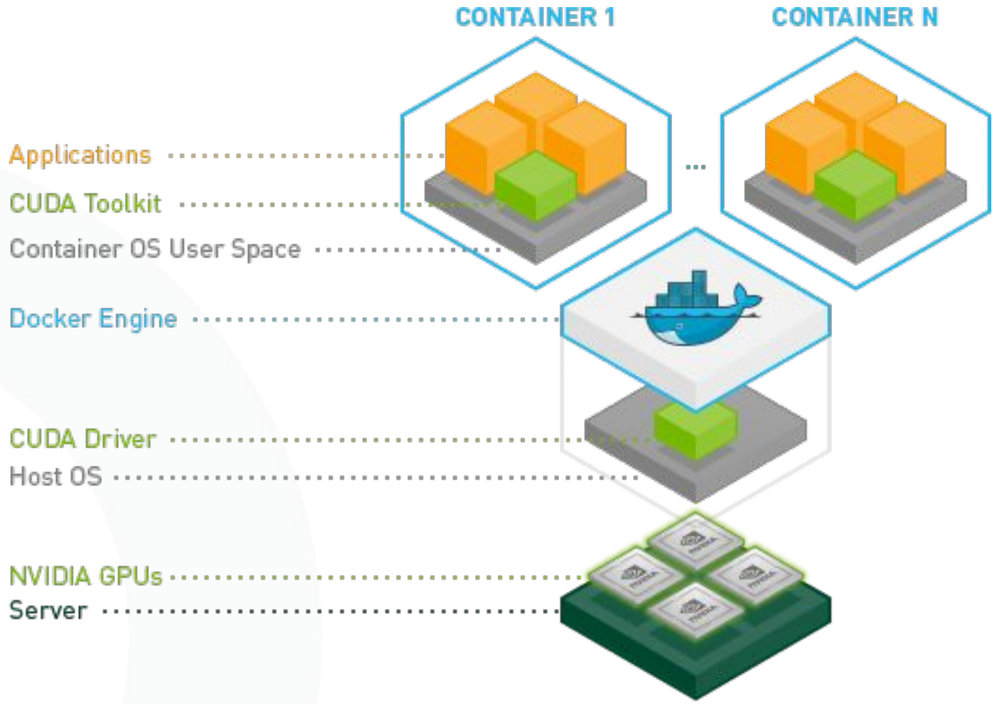
- All containers with arguments in one config file
- docker-compose up -d
- docker-compose down

```yaml
version: "3.4"
services:
    iris_frontend:
        build:
            context: .
            dockerfile: Dockerfile_frontend
        ports:
            - "4200:4200"
        depends_on:
            - iris_prediction
        networks:
            default:
                aliases:
                    - frontend
    iris_prediction:
        build:
            context: .
            dockerfile: Dockerfile_prediction
        ports:
            - "5000:5000"
        depends_on:
            - iris_training
        volumes:
            - "iris_model_vol:/app/model"
        networks:
            default:
                aliases:
                    - rest-api
    iris_training:
        build:
            context: .
            dockerfile: Dockerfile_training
        volumes:
            - "iris_model_vol:/app/model"
volumes:
    iris_model_vol:
networks:
    default:
```

Using a GPU with NVIDIA-Docker

- Training/ preparing DL model on your (Linux) laptop

- Quick deployment to Cloud service when necessary




```
#### Test nvidia-smi with the latest official CUDA image
docker run --gpus all nvidia/cuda:10.0-base nvidia-smi
```

Dockerfile writing

- Use .dockerignore: avoids unnecessary files, speeds up build process

```
**/.env
**/.idea
**/.vscode
**/.git
**/.cache
**/docker-compose.yml
**/*.md
**/node_modules
```

- Create stateless images: able to restart without data loss

- Single purpose: decoupling interacting parts for simple containers

- Multi-stage builds: single image file to build and deploy app

```
FROM golang:1.7.3
WORKDIR /go/src/github.com/alexellis/href-counter/
RUN go get -d -v golang.org/x/net/html
COPY app.go .
RUN CGO_ENABLED=0 GOOS=linux go build -a -installsuffix cgo -o app .

FROM alpine:latest
RUN apk --no-cache add ca-certificates
WORKDIR /root/
COPY --from=0 /go/src/github.com/alexellis/href-counter/app .
CMD ["./app"]
```

Dockerfile writing continued

- Minimize layers: combine RUN statements
- Frequently changing commands bottom of Dockerfile
- Reduce container size:
  - Use Alpine Linux base image for smallest size
  - Add rm -rf /var/lib/apt/lists/* to apt-get install
  - Try --no-install-recommends flag in apt-get install
- Use trusted official base images
- Specify image versions

```
$ docker build -t mynewimage .
Sending build context to Docker daemon  3.072kB
Step 1/3 : FROM python:3.8-slim-buster
 ---> 3d8f801fc3db
Step 2/3 : COPY build.sh .
 ---> 541b65a7b417
Step 3/3 : RUN ./build.sh
 ---> Running in 9917e3865f96
Building...
```

Summary & next steps

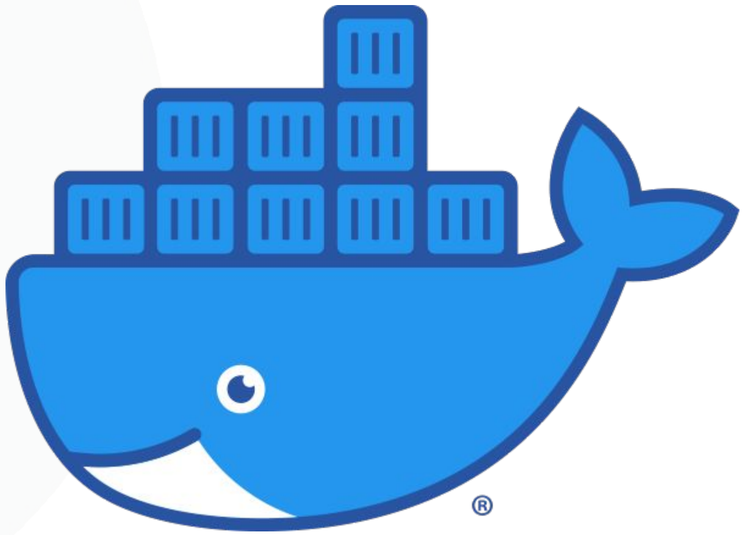
Docker usage

Summary

- Docker decouples project from environment → reproducibility
- Eases sharing of models → better collaboration
- Improves deployability → greater impact

- Be aware of security and optimizations

Next steps: Docker-swarm & Kubernetes



https://github.com/BigDataRepublic/docker_webinar

Presenters and contributors

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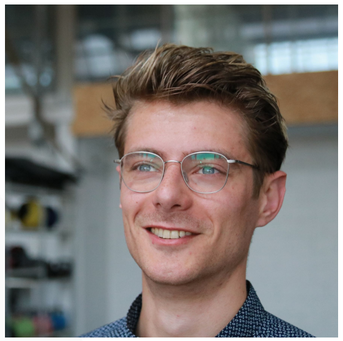
Data Scientist

/in/tomderuijter/



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