DOCKER AND PYTHON

Making them play nicely and securely for Data Science and Machine Learning

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THESE SLIDES

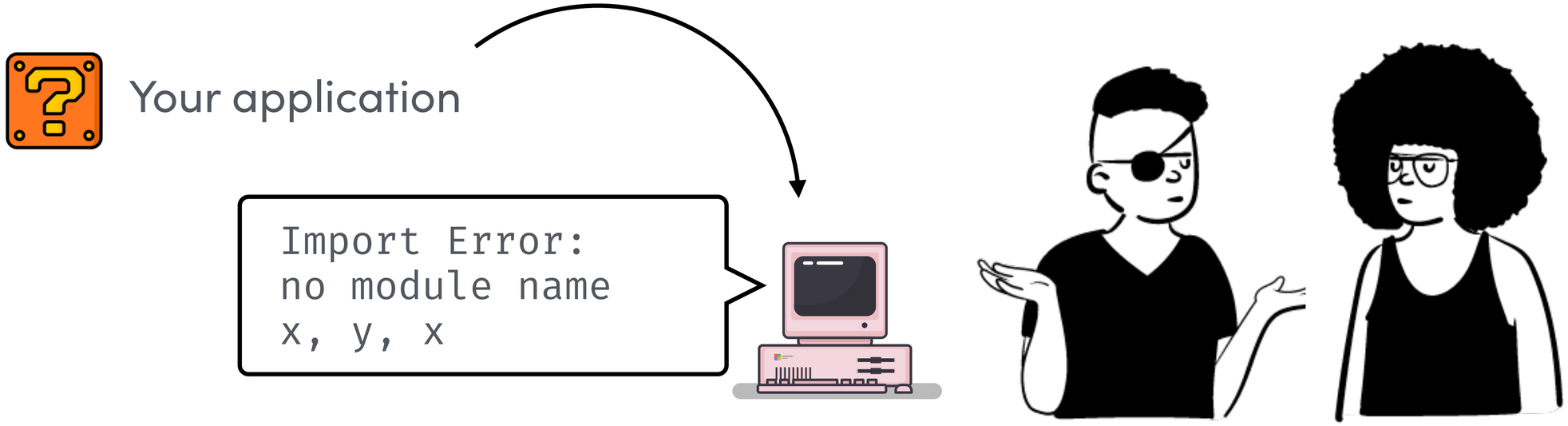
https://bit.ly/pycon2020-ml-docker

WHAT YOU'LL LEARN TODAY

- Why using Docker?
- Docker for Data Science and Machine Learning
- Security and performance
- Do not reinvent the wheel, automate
- Tips and trick to use Docker

WHY DOCKER?

DEV LIFE WITHOUT DOCKER OR CONTAINERS



How are your users or colleagues meant to know what dependencies they need?

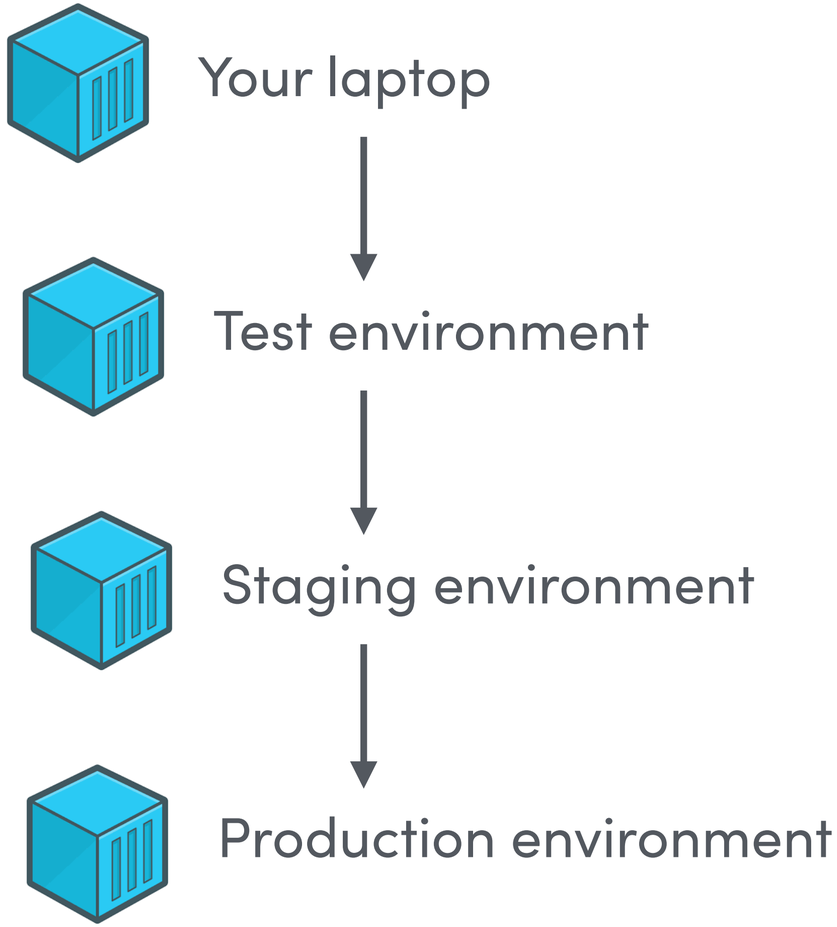
WHAT IS DOCKER?

A tool that helps you to create, deploy and run your applications or projects by using containers.

This is a container

HOW DO CONTAINERS HELP ME?

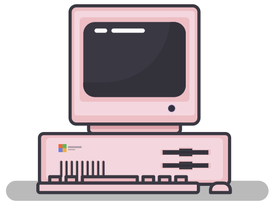
They provide a solution to the problem of how to get software to run reliably when moved from one computing environment to another



DEV LIFE WITH CONTAINERS

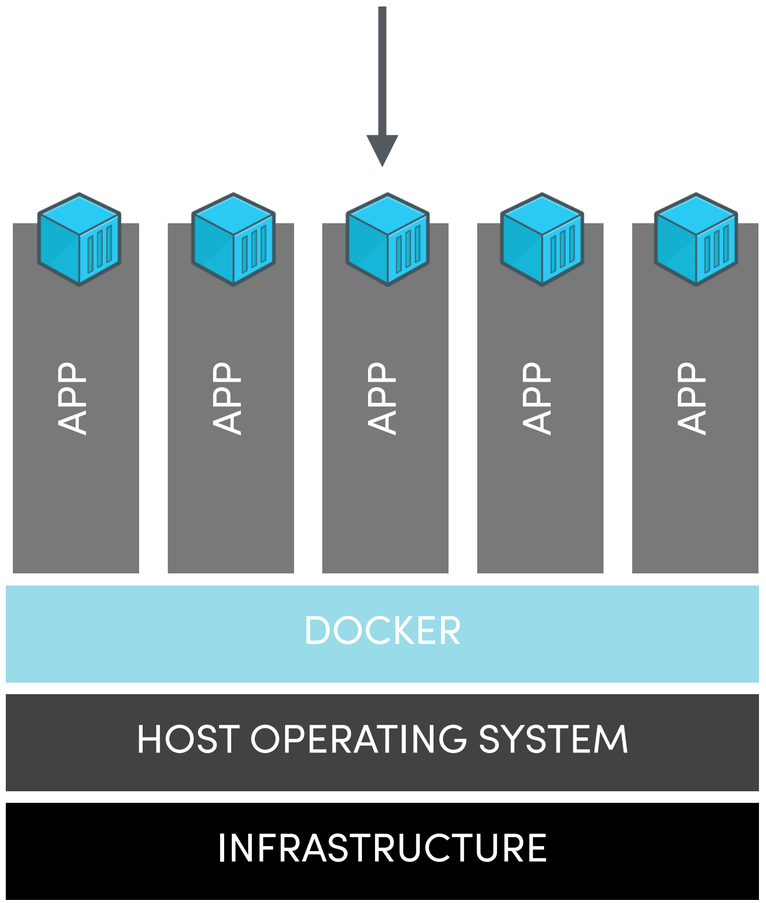
Your application

Libraries, dependencies,
runtime environment,
configuration files



THAT SOUNDS A LOT LIKE A VIRTUAL MACHINE

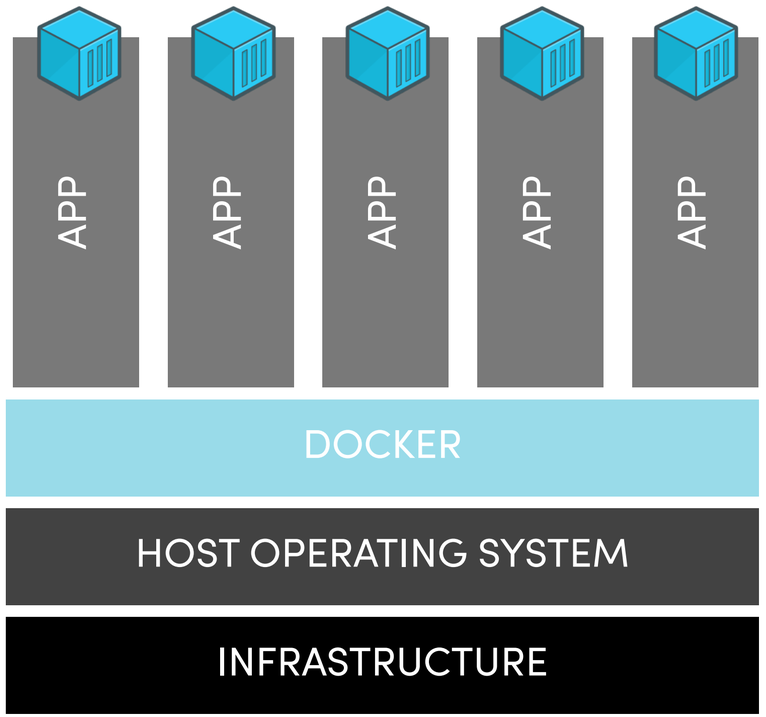
Each app is containerised



At the app level:
Each runs as an isolated process

THAT SOUNDS A LOT LIKE A VIRTUAL MACHINE

CONTAINERS



Full OS + app + binaries + libraries

VIRTUAL MACHINE

At the hardware level

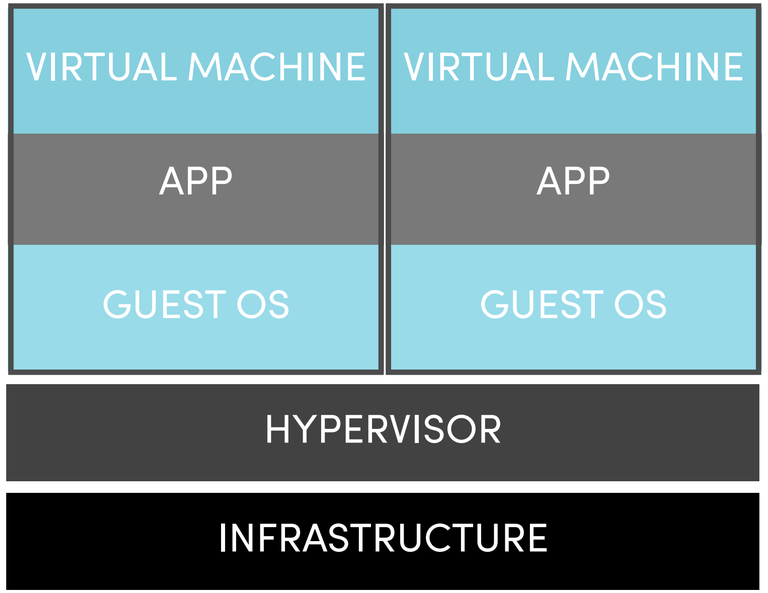
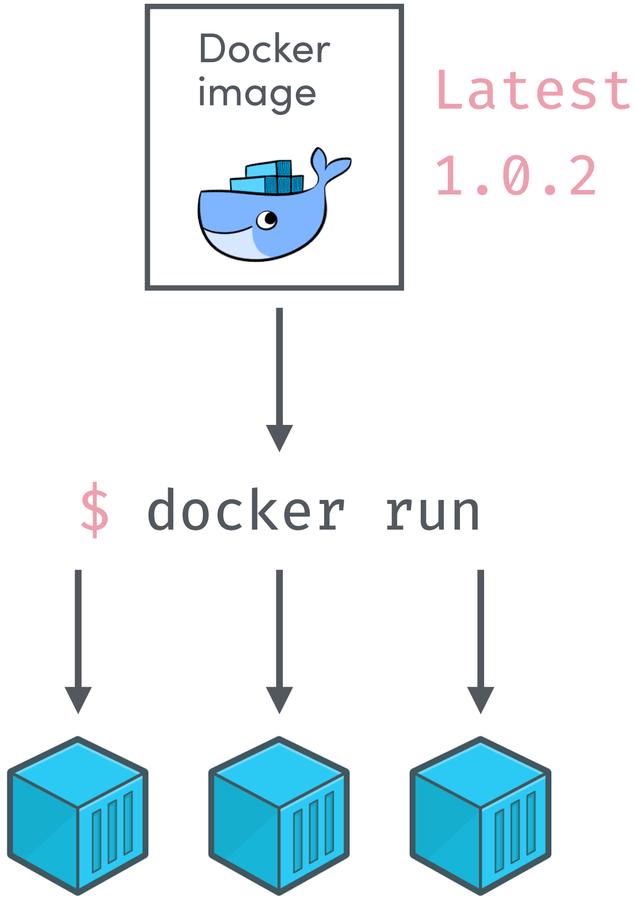


IMAGE VS CONTAINER

- Image: archive with all the data needed to run the app
- When you run an image it creates a container



COMMON PAIN POINTS IN DS AND ML

- Complex setups / dependencies
- Reliance on data / databases
- Fast evolving projects (iterative R&D process)
- Docker is complex and can take a lot of time to upskill
- Are containers secure enough for my data / model /algorithm?

DOCKER FOR DATA SCIENCE AND MACHINE LEARNING

HOW IS IT DIFFERENT FROM WEB APPS FOR EXAMPLE?

Drawing a line to the scope of Python packaging

Packaging

Tzu-ping Chung uranusjr — Feb '19

Another topic in the Big Picture thread I found interesting 🙂

twitter.com

Sylvain Corlay (SylvainCorlay)

@dstufft @pwang @WillingCarol @brettsky @vorpalsmith @zooba @uranusjr @acanthamoeba @ncoghlan_dev @kushaldas Although there is a continuum of things between "we need BLAS", and "we need R". Where is the limit?

It feels to me that with language-specific packaging tools, you soon find a cliff somewhere between those two usecases.

6:46 PM - 11 Feb 2019

https://twitter.com/dstufft/status/1095164069802397696

HOW IS IT DIFFERENT FROM WEB APPS FOR EXAMPLE?

- Not every deliverable is an app
- Not every deliverable is a model either
- Heavily relies on data
- Mixture of wheels and compiled packages
- Security access levels - for data and software
- Mixture of stakeholders: data scientists, software engineers, ML engineers

BUILDING DOCKER IMAGES

Dockerfiles are used to create Docker images by providing a set of instructions to install software, configure your image or copy files

docker-ds - Dockerfile

```
# word of caution - this is a bad example
FROM python:3

COPY yourscript.py /

RUN pip install flask

CMD [ "python", "./yourscript.py" ]
```

DISSECTING DOCKER IMAGES

Base image

Main instructions

Entry command

docker-ds - Dockerfile

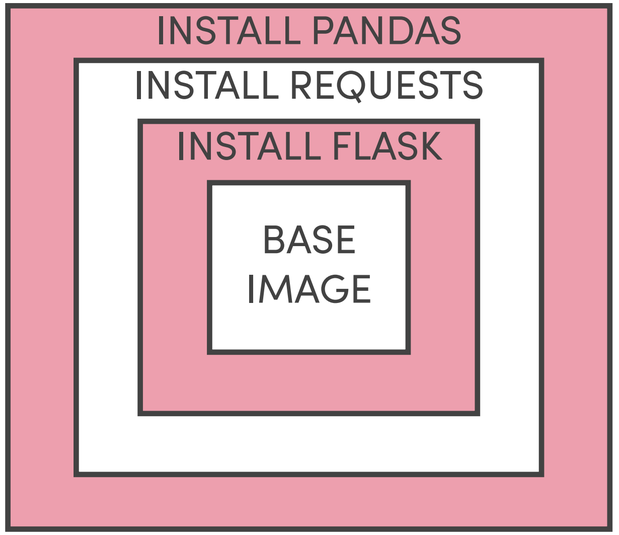
```
# word of caution - this is a bad example
FROM python:3

COPY yourscript.py /

RUN pip install flask

CMD [ "python", "./yourscript.py" ]
```

DISSECTING DOCKER IMAGES



docker-ds - Dockerfile

```
# word of caution - this is a bad example
FROM python:3

COPY yourscript.py /

RUN pip install flask
RUN pip install requests
RUN pip install pandas

CMD [ "python", "./yourscript.py" ]
```

Each instruction creates
A layer
(like an onion)

CHOOSING THE BEST BASE IMAGE

If building from scratch use the

official Python images

REPOSITORY	TAG	SIZE
python	3.7.7-alpine	96MB
python	3.7.7-slim-stretch	155MB
python	3.7.7-stretch	942MB
python	3.7.7-slim-buster	179MB
python	3.7.7-buster	919MB
python	3.8.2-slim-buster	194MB
python	3.8.2-buster	934MB

https://hub.docker.com/_/python

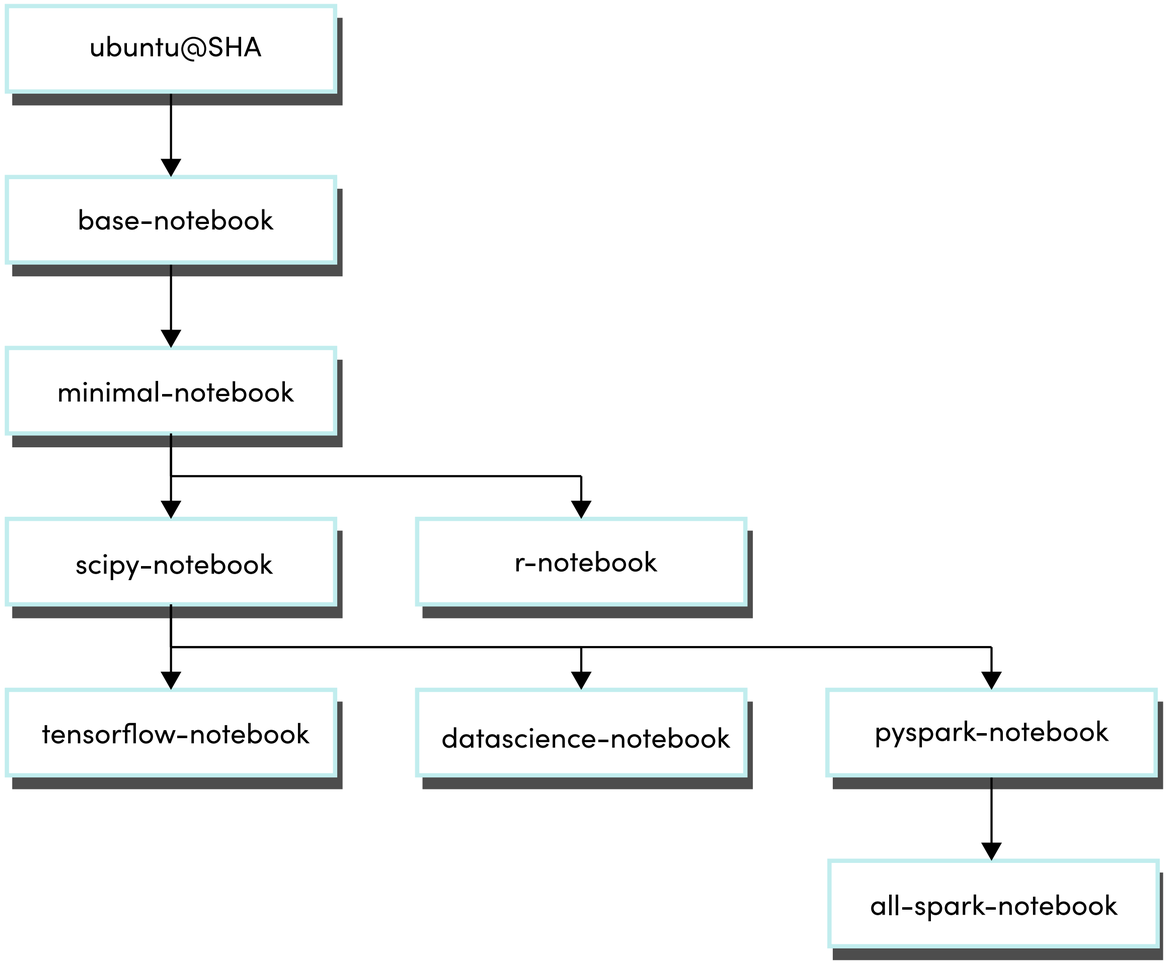
https://github.com/docker-library/docs/tree/master/python

THE JUPYTER DOCKER STACK

Need Conda, notebooks and scientific Python ecosystem?

Try Jupyter Docker stacks

https://jupyter-docker-stacks.readthedocs.io/



BEST PRACTICES

- Always know what you are expecting
- Provide context with LABELS
- Split complex RUN statements and sort them
- Prefer COPY to add files

docker-ds - Dockerfile

```
# Always use a concrete tag (avoid LATEST)
FROM jupyter/base-notebook:6.0.3

# Add metadata
LABEL maintainer="Tania Allard"
LABEL securitytxt="https://www.example.com/.well-known/security.txt"

# Use pinned versions always
RUN conda install --quiet --yes \
    'pandas==1.0.3' \
    'dask==2.14.*' \
    && \
    # do not forget to clean - reduce image
    conda clean --all -f -y

# separate instructions per scope
RUN mkdir data-sci-demo

COPY ./your-project data-sci-demo/
```

https://docs.docker.com/develop/develop-images/dockerfile_best-practices/

SPEED UP YOUR BUILD

- Leverage build cache
- Install only necessary packages

docker-ds - requirements.txt

```
pandas==1.0.3
dask==2.14.*
```

docker-ds - Dockerfile

```
# Always use a concrete tag (avoid LATEST)
FROM jupyter/base-notebook:6.0.3

# Add metadata
LABEL maintainer="Tania Allard"
LABEL securitytxt="https://www.example.com/.well-known/security.txt"

# Leveraging build cache
COPY ./requirements.txt /tmp/

RUN conda install --quiet --yes --file /tmp/requirements.txt &&\
    # do not forget to clean - reduce image
    conda clean --all -f -y

# Separate instructions per scope
RUN mkdir data-sci-demo

COPY ./your-project data-sci-demo/
```

https://docs.docker.com/develop/develop-images/dockerfile_best-practices/

SPEED UP YOUR BUILD AND PROOF

- Leverage build cache
- Install only necessary packages
- Explicitly ignore files

docker-ds - .dockerignore

```
# Documentation
Readme.md

# Never add data
./yourproject/data/

# Secrets
appsettings.json
.env
supersecretkeys.json
```

docker-ds - Dockerfile

```
# Always use a concrete tag (avoid LATEST)
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RUN mkdir data-sci-demo

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https://docs.docker.com/develop/develop-images/dockerfile_best-practices/

MOUNT VOLUMES TO ACCESS DATA

- You can use bind mounts to directories (unless you are using a database)
- Avoid issues by creating a non-root user

docker-ds - workflow.yml

```
# mount directory
docker run --volume /home/user/yourproject:/yourproject mycontainer
# mount directory as read-only
docker run --volume /home/user/yourproject:/yourproject:ro mycontainer
# mount multple directories, one with write access relative to current path (Linux)

docker run --volume /homse/user/article-x-supplement/data:/data:ro \
--volume $(pwd)/outputs:/output-data:rw mycontainer
```

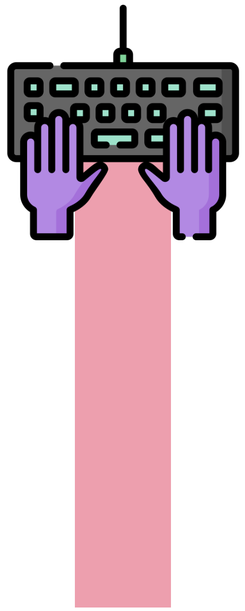
https://docs.docker.com/develop/develop-images/dockerfile_best-practices/

SECURITY AND PERFORMANCE

MINIMISE PRIVILEGE - FAVOUR LESS PRIVILEGED USER

Lock down your container:

- Run as non-root user (Docker runs as root by default)
- Minimise capabilities



docker-ds - Dockerfile

```
FROM python:3.8.2-slim-buster
RUN useradd --create-home jovyan
WORKDIR /home/jovyan
USER jovyan
```

DON'T LEAK SENSITIVE INFORMATION

Remember Docker images are like onions. If you copy keys in an intermediate layer they are cached.

Keep them out of your Dockerfile.

USE MULTI STAGE BUILDS

- Fetch and manage secrets in an intermediate layer
- Not all your dependencies will have been packed as wheels so you might need a compiler - build a compile and a runtime image
- Smaller images overall

docker-ds - Dockerfile

```
# Always use a concrete tag (avoid LATEST)
FROM python:3.8.2-slim-buster as compile-image

# Add metadata
LABEL maintainer="Tania Allard"
LABEL securitytxt=
"https://www.example.com/.well-known/security.txt"

RUN apt-get update
RUN
 apt-get install -y --no-install-recommends gcc build-essen
tial gcc gfortran


RUN python -m venv /opt/venv

# Ensure we use the virtualenv
ENV PATH="/opt/venv/bin:$PATH"

COPY requirements.txt /tmp/

RUN CFLAGS=
"-g0 -Wl,--strip-all -I/usr/include:/usr/local/include -L/u
sr/lib:/usr/local/lib"
 \
    pip install \
    --no-cache-dir \
    --compile \
    --global-option=build_ext \
    --global-option="-j 4" \
    -r /tmp/requirements.txt

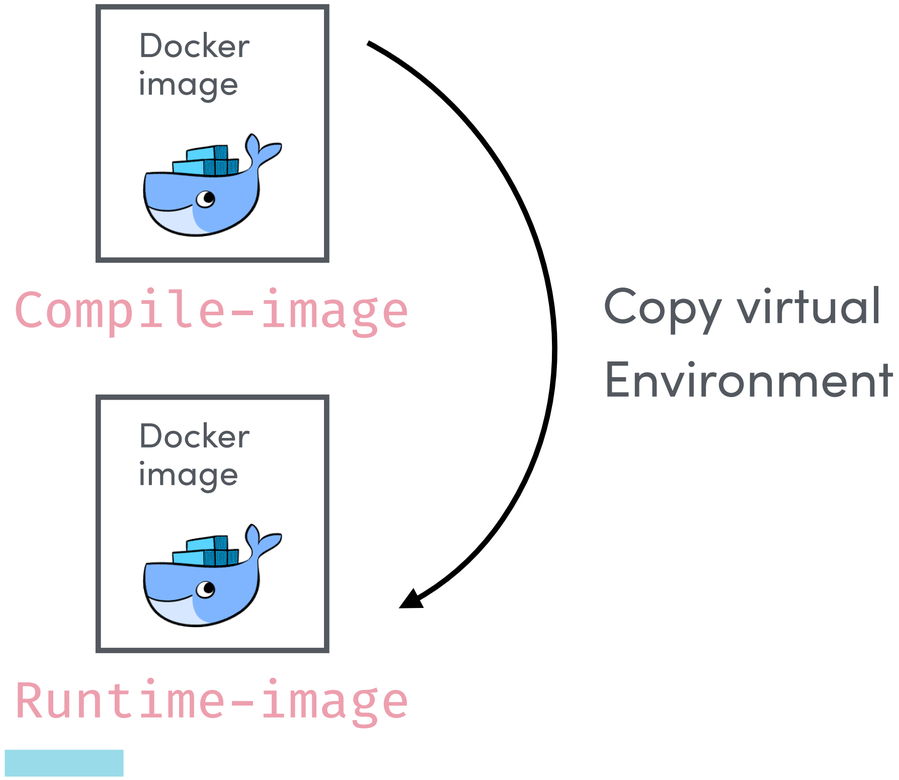
# -------------------------------------------------------
#  This is the second image that copies the compiled librar
y


FROM python:3.8.2-slim-buster as runtime-image

COPY --from=compile-image /opt/venv /opt/venv
# Ensure we use the virtualenv
ENV PATH="/opt/venv/bin:$PATH"
```

USE MULTI STAGE BUILDS

```
$ docker build --pull --rm -f “Dockerfile"\
 -t trallard:data-scratch-1.0 "."
```



docker-ds - Dockerfile

```
# Always use a concrete tag (avoid LATEST)
FROM python:3.8.2-slim-buster as compile-image

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COPY requirements.txt /tmp/

RUN CFLAGS=
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 \
    pip install \
    --no-cache-dir \
    --compile \
    --global-option=build_ext \
    --global-option="-j 4" \
    -r /tmp/requirements.txt

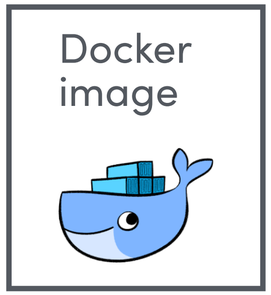
# -------------------------------------------------------
#  This is the second image that copies the compiled librar
y


FROM python:3.8.2-slim-buster as runtime-image

COPY --from=compile-image /opt/venv /opt/venv
# Ensure we use the virtualenv
ENV PATH="/opt/venv/bin:$PATH"
```

USE MULTI STAGE BUILDS

FINAL IMAGE



Runtime-image

trallard:data-scratch-1.0

docker-ds - Dockerfile

```
# Always use a concrete tag (avoid LATEST)
FROM python:3.8.2-slim-buster as compile-image

# Add metadata
LABEL maintainer="Tania Allard"
LABEL securitytxt=
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# Ensure we use the virtualenv
ENV PATH="/opt/venv/bin:$PATH"

COPY requirements.txt /tmp/

RUN CFLAGS=
"-g0 -Wl,--strip-all -I/usr/include:/usr/local/include -L/u
sr/lib:/usr/local/lib"
 \
    pip install \
    --no-cache-dir \
    --compile \
    --global-option=build_ext \
    --global-option="-j 4" \
    -r /tmp/requirements.txt

# -------------------------------------------------------
#  This is the second image that copies the compiled librar
y


FROM python:3.8.2-slim-buster as runtime-image

COPY --from=compile-image /opt/venv /opt/venv
# Ensure we use the virtualenv
ENV PATH="/opt/venv/bin:$PATH"
```

AUTOMATE

PROJECT TEMPLATES

Need a standard project template?

Use `cookie cutter data science`

Or `cookie cutter docker science`

docker-ds - workflow.yml

```
├── Makefile                      ← Makefile contains many targets such as create docker container or
│                                   get input files.
├── config                        ← This directory contains configuration files used in scripts
│   │                               or Jupyter Notebook.
│   └── jupyter_config.py
├── data                          ← data directory contains the input resources.
├── docker                        ← docker directory contains Dockerfile.
│   └── Dockerfile                ← Dockerfile have the container settings. Users modify Dockerfile
│                                   if additional library is needed for experiments.
├── model                         ← model directory store the model files created in the experiments.
├── my_data_science_project       ← cookie-cutter-docker-science creates the directory whose name is same
│   │                               as project name. In this directory users puts python files used in scripts
│   │                               or Jupyter Notebook.
│   └── __init__.py
├── notebook                      ← This directory stores the ipynb files saved in Jupyter Notebook.
├── requirements.txt              ← Libraries needed to run experiments. The library listed in this file
│                                   are installed in the Docker container.
└── scripts                       ← Users add the script files to generate model files or run evaluation.
```

https://github.com/docker-science/cookiecutter-docker-science

https://drivendata.github.io/cookiecutter-data-science/

```
$ conda install jupyter repo2docker
$ jupyter-repo2docker “.”
```

https://repo2docker.readthedocs.io/en/latest

DO NOT REINVENT THE WHEEL

Leverage the existence and usage of tools like `repo2docker`.

Already configured and optimised for Data Science / Scientific computing.

DO NOT REINVENT THE WHEEL

- Configuration Files
  - `environment.yml` - Install a Python environment
  - `Pipfile` and/or `Pipfile.lock` - Install a Python environment
  - `requirements.txt` - Install a Python environment
  - `setup.py` - Install Python packages
  - `Project.toml` - Install a Julia environment
  - `REQUIRE` - Install a Julia environment (legacy)
  - `install.R` - Install an R/RStudio environment
  - `apt.txt` - Install packages with apt-get
  - `DESCRIPTION` - Install an R package
  - `manifest.xml` - Install Stencila
  - `postBuild` - Run code after installing the environment
  - `start` - Run code before the user sessions starts
  - `runtime.txt` - Specifying runtimes
  - `default.nix` - the nix package manager
  - `Dockerfile` - Advanced environments

Leverage the existence and usage of tools like `repo2docker`. Already configured and optimised for Data Science / Scientific computing.

https://repo2docker.readthedocs.io/en/latest

docker-ds - workflow.yml

```yaml
name: Publish to Registry
on:
  release:
    types: [published]
  schedule:
    # Build your images frequently
    - cron: "0 2 * * 0" # Weekly on Sundays at 02:00
jobs:
  update:
    runs-on: ubuntu-latest
    steps:
      - uses: actions/checkout@master
      - name: Get release version
        id: get_version
        run: echo ::set-env name=RELEASE_VERSION::$(echo ${GITHUB_REF:10})
      - name: Build and publish
        uses: docker/build-push-action@v1
        with:
          username: ${{ secrets.DOCKER_USERNAME }}
          password: ${{ secrets.DOCKER_PASSWORD }}
          repository: myorg/myrepository
          tag_with_ref: true
          tag_with_sha: true
```

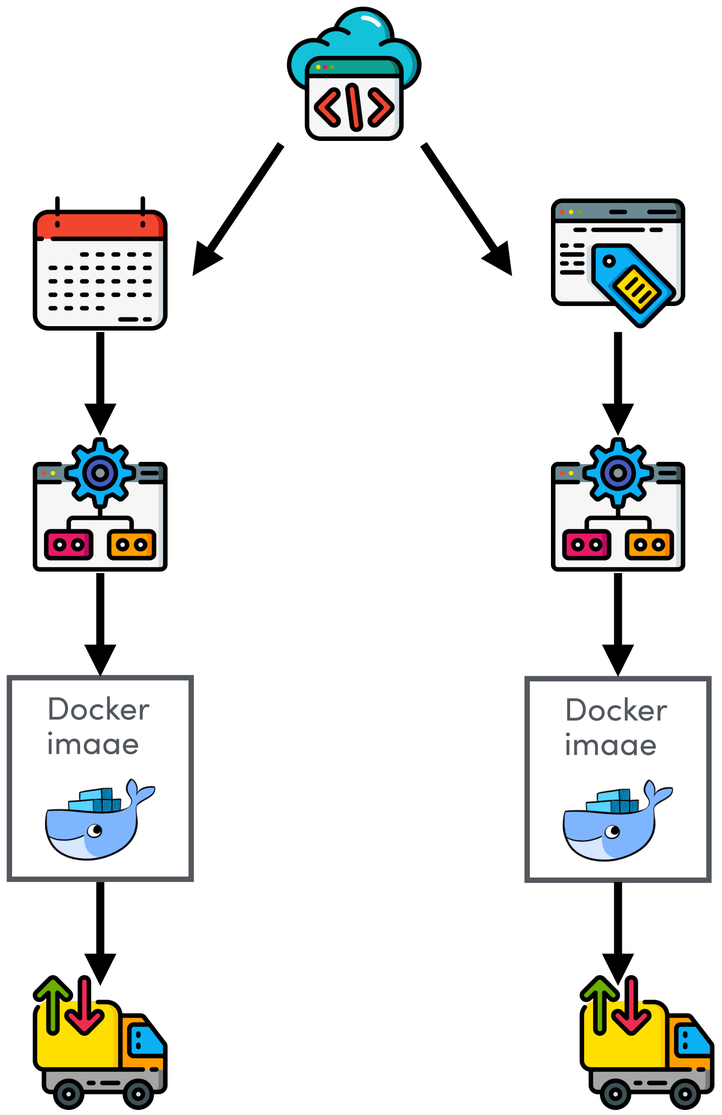
DELEGATE TO YOUR CONTINUOUS INTEGRATION TOOL

Set Continuous integration (Travis, GitHub Actions, whatever you prefer).

And delegate your build - also build often.

https://repo2docker.readthedocs.io/en/latest

THIS WORKFLOW



- Code in version control
- Trigger on tag / Also scheduled trigger
- Build image
- Push image

TOP TIPS

TOP TIPS

1. Rebuild your images frequently - get security updates for system packages
2. Never work as root / minimise the privileges
3. You do not want to use Alpine Linux (go for buster, stretch or the Jupyter stack)
4. Always know what you are expecting: pin / version EVERYTHING (use pip-tools, conda, poetry or pipenv)
5. Leverage build cache

TOP TIPS

6. Use one Dockerfile per project
7. Use multi-stage builds - need to compile code? Need to reduce your image size?
8. Make your images identifiable (test, production, R&D) - also be careful when accessing databases and using ENV variables / build variables
9. Do not reinvent the wheel! Use repo2docker
10. Automate - no need to build and push manually
11. Use a linter

THANK YOU

@ixek

@trallard

trallard.dev