Docker training

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Challenges

Struggles with sharing software:

- It works on my laptop!
- Oh, you use Windows? I use MacOS.
- Are you using the "correct" version of Python?
- Are we using the same version of pandas, numpy, etc.?

More formally, we desire:

- Environment consistency
  - Ability to recreate the same environment
- Dependency management
  - Better than relying on documentation only
- Isolation
  - The packaged app is not affected by the rest of the system
  - Think of permissions in Android and iOS

What is Docker?

Docker is a software for packaging and running your application in an isolated environment.

The result can be easily shared with others.

Docker comes with a command line tool.

Advantages

Docker is widely used in bioinformatics and software development because it addresses several challenges that are common in these fields:

- Reproducibility
- Portability
- Software dependencies management
- Scalability
- Collaboration
- Version control of environments
- Integration with other bioinformatics tools (e.g. Nextflow)

The only solution?

Virtual machines (images, snapshots of)

- The hardware must support emulation:
  - CPU and IO, including GPU, storage, networking, etc. (VT-x, AMD-V, VT-d, AMD-Vi)
- They emulate an entire operating system
  - and not just your application: more memory is required

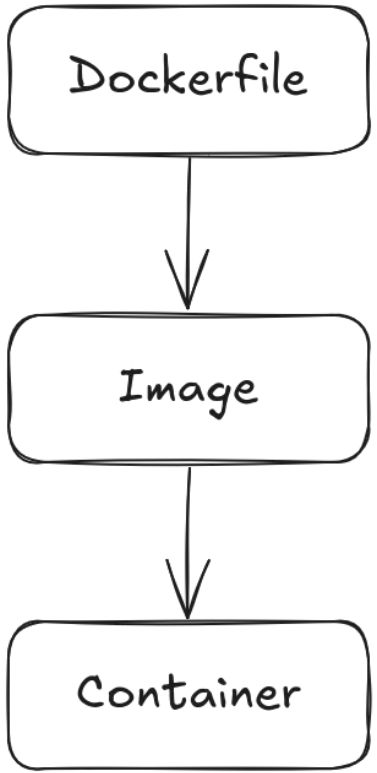
Docker containers

- They share the host's operating system
  - more memory available to your app
- Easier to package and share your work
- Faster to create, destroy, start, stop, etc.

Both solutions provide a consistent and isolated environment for your application.

Docker terminology

- Dockerfile
  - A text file that describes how to package and run your app
- Image
  - A package of your code and its dependencies
  - Is immutable: ideal for sharing with others
  - ~~package~~ image
  - Created from a Dockerfile
- Container
  - A running copy of an image
  - Is mutable
  - Best if ephemeral, stateless
  - Created from an image

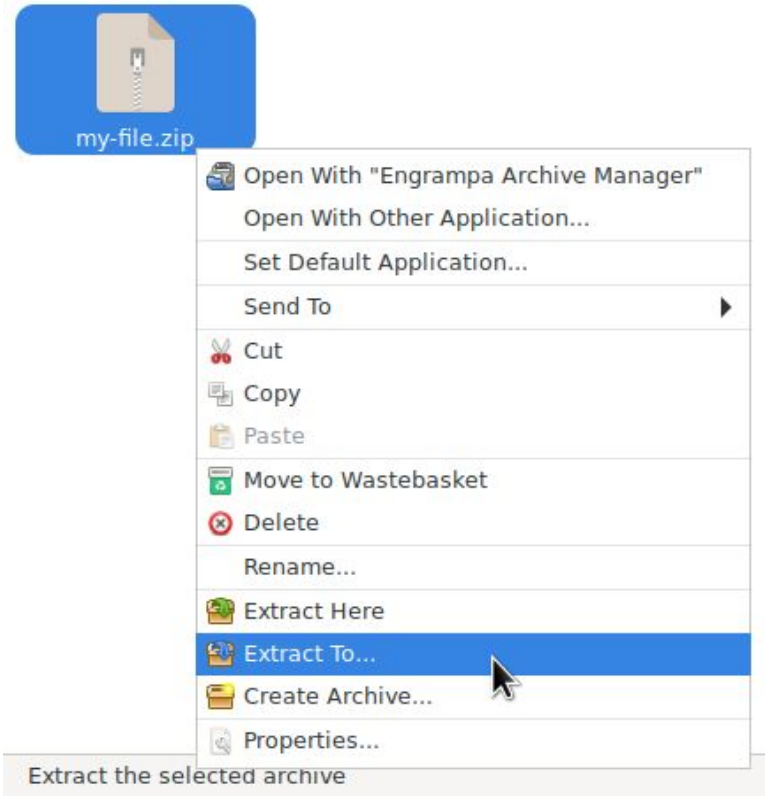


Think of it like…

- Docker images as .zip files
- Docker containers as the extracted content

Point being: a .zip file can be extracted multiple times, to different destination folders. The content of those folders is the same.

People do not work directly on a .zip file. They work on the extracted content.



Dockerfiles

It is a text file. It describes how to package and run your application.

```
FROM python:3.13
COPY app.py /home/app.py
CMD ["python", "/home/app.py"]
```

Find base images on Docker Hub:

- https://hub.docker.com/_/debian
- https://hub.docker.com/_/python
- https://hub.docker.com/_/ubuntu

No dependencies in this app.

More instructions for Dockerfiles

- ADD - Add local or remote files and directories
- ENTRYPOINT - Specify default executable
- ENV - Set environment variables
- RUN - Execute build commands
- WORKDIR - Change working directory

All instructions: https://docs.docker.com/reference/dockerfile/

Images and containers

Given a Dockerfile, create an image:

```
docker build -t name[:tag] .
```

Given an image, create a container and start it:

```
docker run name[:tag]
```

Exploring a container

```
docker pull debian:12
docker run --rm -it debian:12 bash
```

```
0 ~ docker pull debian:12
12: Pulling from library/debian
Digest: sha256:4abf773f2a570e6873259c4e3ba16
Status: Image is up to date for debian:12
docker.io/library/debian:12
```

```
0 ~ docker run --rm -it debian:12 bash
root@993b9e728972:/# whoami
root
root@993b9e728972:/# id
uid=0(root) gid=0(root) groups=0(root)
root@993b9e728972:/# ls /home
root@993b9e728972:/#
```

Enter `exit` to get out of the container. And it'll be removed because of `--rm`.

Running some commands…

… on the host:

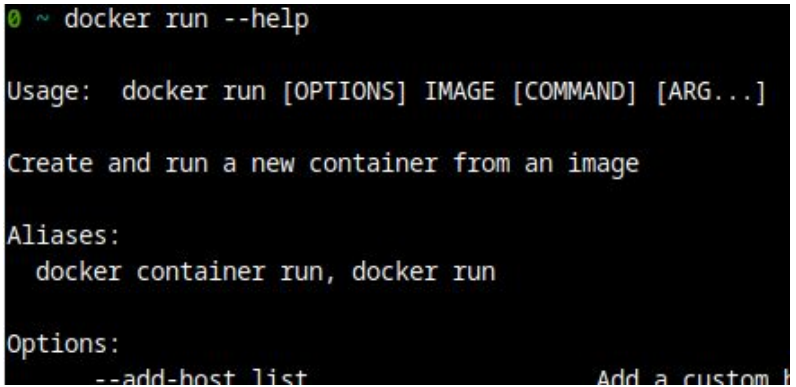
```
+ hostname
work-laptop

+ ls -ahl /home
total 12K
drwxr-xr-x  3 root root 4.0K Nov 26  2023 .
drwxr-xr-x 19 root root 4.0K Feb  8 22:46 ..
drwx------ 42 user user 4.0K Feb 17 15:09 user

+ ip -o link show
lo
eth0
docker0
br-123dfb4a82c1
```

… within the container:

```
+ hostname
06dbdcf97766

+ ls -ahl /home
total 8.0K
drwxr-xr-x 2 root root 4.0K Dec 31 10:25 .
drwxr-xr-x 1 root root 4.0K Feb 17 14:14 ..


+ ip -o link show
ip: command not found
```

Ask for help

```
docker build --help

docker run --help

docker ps --help
```



Each help page provides a list of Aliases and Options.

Reproducibility 1/4

Tracking the versions of your dependencies is very important.

- requirements.txt
  - basic reproducibility: it tracks direct dependencies versions
- lock file (environment.lock, Pipfile.lock, poetry.lock)
  - good reproducibility: it tracks direct and indirects dependencies versions

Try them out:

- https://docs.conda.io/projects/conda/en/latest/commands/index.html
- https://pipenv.pypa.io/en/latest/commands.html
- https://python-poetry.org/docs/cli/

Reproducibility 2/4

```
conda create --name app-with-conda python=3.12
conda activate app-with-conda
conda install conda-lock numpy
conda env export > environment.yml
conda-lock -f environment.yml -p linux-64
# To recreate the environment:
conda-lock install -n another-env -f conda-lock.yml
```

https://www.anaconda.com/blog/8-levels-of-reproducibility

Reproducibility 3/4

```
pyenv local 3.13
python -m venv venv
source venv/bin/activate
pip install pipenv
pipenv install numpy
# It generated two files: Pipfile and
Pipfile.lock
```

```
FROM python:3.13
WORKDIR /app
COPY Pipfile.lock ./
RUN pip install pipenv && pipenv sync
COPY app.py ./
ENTRYPOINT ["pipenv", "run", "python", "app.py"]
```

- pyenv: https://github.com/pyenv/pyenv
  - Tool for installing and selecting versions of Python
- venv: https://docs.python.org/3/library/venv.html
  - Module from the standard library for creating virtual environments

Reproducibility 4/4

- Remember to track the lock file in git
- Keep your dependencies fresh
  - Once in a while (e.g. every 6 months) try upgrading your dependencies
    - If all works as expected, update the lock file in git
  - Avoid surprises due to breaking changes
    - Changelogs: https://pandas.pydata.org/pandas-docs/stable/whatsnew/index.html
    - Update guides: https://angular.dev/update-guide
- docker build --pull --no-cache

Exposing data to/from a container

- Via bind mounts
  - https://docs.docker.com/engine/storage/bind-mounts/
  - Alternative: volumes https://docs.docker.com/engine/storage/volumes/

```
FROM debian:12-slim
CMD ["cat", "/data/info.txt"]
```

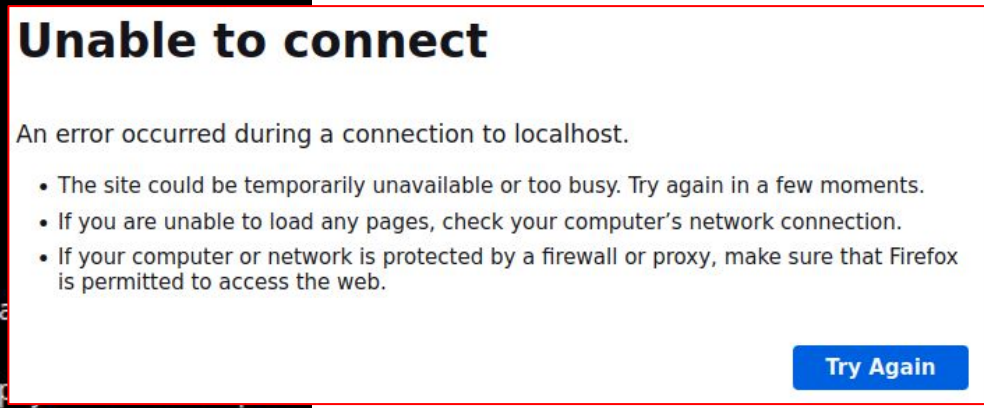
```
0 cat-text-data tree
.
├── Dockerfile
└── precious-data
    └── info.txt

2 directories, 2 files
0 cat-text-data docker build -q -t cat-text-data .
sha256:80b5adef402e8f178149dc77ed71b2dd74ec2b4d133cb48f65de7b9d43bdcf55
0 cat-text-data docker run cat-text-data
cat: /data/info.txt: No such file or directory
1 cat-text-data docker run -v $PWD/precious-data:/data:ro cat-text-data
I reside on the host's filesystem.
You can read me because the directory I reside
in is mounted to the container's filesystem.
0 cat-text-data
```

Network communication 1/3

- Communication between containers
  - enabled by default for containers in the same bridge network
- Communication host <-> container
  - blocked by default; ports must be published

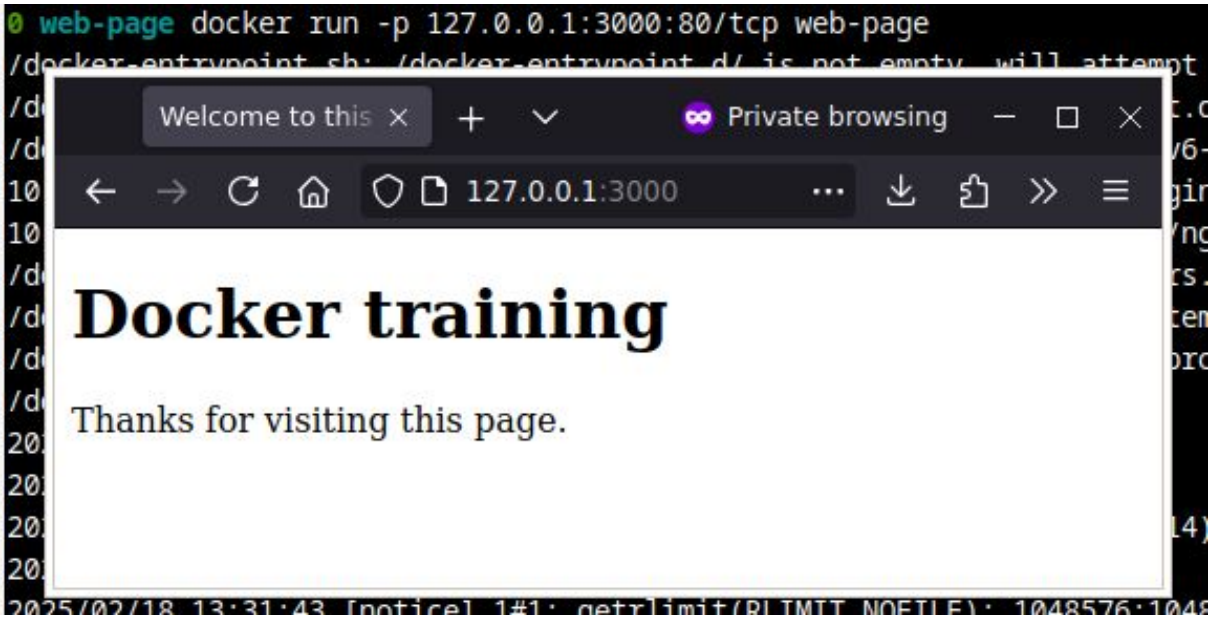
```
FROM nginx:stable
WORKDIR /usr/share/nginx/html
COPY content/index.html ./
```

```
0 web-page tree
.
├── content
│   └── index.html
└── Dockerfile

2 directories, 2 files
0 web-page docker build -q -t web-page .
sha256:82aef7d4ae23db3693563bde945a6681113066d63723759a
0 web-page docker run web-page
/docker-entrypoint.sh: /docker-entrypoint.d/ is not emp
/docker-entrypoint.sh: Looking for shell scripts in /docker-entrypoint.d/
```



Network communication 2/3

docker run -p host_ip:host_port:container_port/protocol



Challenge:
Can you achieve the same result, without copying index.html into the image?

https://docs.docker.com/reference/cli/docker/container/run/#publish

Network communication 3/3

Challenge:
Can you achieve the same result, without copying index.html into the image?

Solution:
We could bind mount the folder containing the index.html file into the container.

```
docker run \
    -v $PWD/content:/usr/share/nginx/html:ro \
    -p 127.0.0.1:3000:80 \
    nginx:stable
```

Bonus term: registry

A storage and distribution system of Docker images. Docker Hub is a registry.

Registry terms:

- repository: related images
- tag: labels identifying specific image versions

Example:

docker pull my-registry.com/image-name:some-tag

Share Docker images

- Create an account on https://hub.docker.com and sign in
- Navigate to *Repositories*, create one
  - https://hub.docker.com/repository/create
- In your terminal, remember to execute `*docker login*`

Pushing images

You can push a new image to this repository using the CLI:

```
docker tag local-image:tagname new-repo:tagname
docker push new-repo:tagname
```

Make sure to replace `tagname` with your desired image repository tag.

Multi-platform images

- Images can be built with support for multiple platforms
  - docker build --platform linux/amd64,linux/arm64 .
    - Provides support for the two most common architectures

https://docs.docker.com/build/building/multi-platform/

Authors might forget to build an image for your platform.

Solution: tell Docker which image to use!

```
docker run --platform linux/amd64 image-name:tag
```

```
0 ~ docker pull --help | grep platform
      --platform string         Set platform if server is multi-platform capable
0 ~ docker build --help | grep platform
      --platform stringArray          Set target platform for build
0 ~ docker run --help | grep platform
      --platform string                     Set platform if server is multi-platform capable
```

Install instructions and best practices

- How to install: https://docs.docker.com/engine/install/
- Building images: https://docs.docker.com/build/building/best-practices/
  - Very important paragraphs:
    - Choose the right base image
    - Rebuild your images often
    - Exclude with .dockerignore
    - Create ephemeral containers
    - Don't install unnecessary packages
    - Sort multi-line arguments
    - Dockerfile instructions
  - Reference: https://docs.docker.com/reference/dockerfile/
- Code samples: https://docs.docker.com/reference/samples/
- Compose: https://docs.docker.com/compose/how-tos/environment-variables/best-practices/
- WSL: https://docs.docker.com/desktop/features/wsl/best-practices/

Further support

For Docker and software engineering: pasdom@dtu.dk

You're welcome to:

- share feedback
- show off your Dockerfiles
- share your git repos
- ask for code reviews

Idea: software engineering hour, e.g. once a week, for topics such as git, programming languages, conventions, best practices, etc.