# **Dockerfiles & Vetiver**

Lecture 21

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### Dockerfile(s)

Docker can build images automatically by reading the instructions from a Dockerfile. A Dockerfile is a text document that contains all the commands a user could call on the command line to assemble an image.

command	Description
FROM	specify a base image
RUN	run commands (e.g. apt or yum), changes saved to image
COPY	copy a local file into the image
ENV	set environment variables for Dockerfile and image
USER	set user to use (affects subsequent RUN, CMD, ENDPOINT)
WORKDIR	set the working directory
<b>EXPOSE</b>	specify which ports will be used (not published automatically)
CMD	specify default command run when running the image
• • •	•••

### A basic example

ex1/Dockerfile

```
1 FROM ubuntu:24.04
2
3 ENV DEBIAN_FRONTEND=noninteractive
4
5 RUN apt update
6 RUN apt install -y r-base
7 RUN Rscript -e "install.packages('tibble')"
8
9 CMD ["R", "--vanilla"]
```

## Building

```
> docker build -t example .
[+] Building 105.1s (9/9) FINISHED
=> [internal] load build definition from Dockerfile
=> => transferring dockerfile: 227B
=> [internal] load metadata for docker.io/library/ubuntu:24.04
=> [auth] library/ubuntu:pull token for registry-1.docker.io
=> [internal] load .dockerignore
=> => transferring context: 2B
=> [1/4] FROM docker.io/library/ubuntu:24.04@sha256:72297848456d5d37d1262630108ab308d3e9ec7ed1c32
=> => resolve docker.io/library/ubuntu:24.04@sha256:72297848456d5d37d1262630108ab308d3e9ec7ed1c32
=> sha256:72297848456d5d37d1262630108ab308d3e9ec7ed1c3286a32fe09856619a782 6.69kB / 6.69kB
=> => sha256:a3f23b6e99cee41b8fffbd8a22d75728bb1f06af30fc79f533f27c096eda8993 424B / 424B
=> => sha256:c3d1a34325805c22bf44a5157224bcff58dc6a8868558c7746d6a2ea64eb191c 2.31kB / 2.31kB
=> => sha256:5b17151e9710ed47471b3928b05325fa4832121a395b9647b7e50d3993e17ce0 28.89MB / 28.89MB
=> extracting sha256:5b17151e9710ed47471b3928b05325fa4832121a395b9647b7e50d3993e17ce0
=> [2/4] RUN apt update
=> [3/4] RUN apt install -y r-base
=> [4/4] RUN Rscript -e "install.packages('tibble')"
=> exporting to image
=> => exporting layers
=> => writing image sha256:10932419c2d9dfbf583a04aa8c57fac1a8634261ef53b7f9d5368bbaecf5e978
=> => naming to docker.io/library/example
```

### **Images**

10

10 i

```
> docker images
REPOSITORY
             TAG
                       IMAGE ID
                                       CREATED
                                                        SIZE
example
            latest
                      10932419c2d9
                                      56 seconds ago
                                                       1.06GB
 > docker run --rm -it example:latest
R version 4.3.3 (2024-02-29) -- "Angel Food Cake"
Copyright (C) 2024 The R Foundation for Statistical Computing
Platform: aarch64-unknown-linux-gnu (64-bit)
. . .
> library(tibble)
> tibble(a=1:10,b=letters[1:10])
# A tibble: 10 x 2
       a b
   <int> <chr>
       1 a
       2 b
 3
       3 c
       4 d
       5 e
 6
       6 f
       7 g
 8
       8 h
 9
       9 i
```

### Some helpful hints

- Using ENV DEBIAN\_FRONTEND=noninteractive prevents apt from stopping things to prompt for input
  - This is not needed with rpm / dnf since rpms are not supposed to prompt for input
- Using the –y flag with apt, rpm, or dnf skips prompting about installing additional dependencies
- If not specified docker build will use the latest tag

## A slightly different example

ex2/Dockerfile

```
1 FROM ubuntu:24.04
2
3 ENV DEBIAN_FRONTEND=noninteractive
4
5 RUN apt update && \
6    apt install -y r-base && \
7    Rscript -e "install.packages('tibble')" && \
8    rm -rf /var/cache/apt/archives /var/lib/apt/lists/*
9
10 CMD ["R", "--vanilla"]
```

### **Building**

```
build -t example .

[+] Building 102.6s (7/7) FINISHED

=> [internal] load build definition from Dockerfile

=> => transferring dockerfile: 311B

=> [internal] load metadata for docker.io/library/ubuntu:24.04

=> [auth] library/ubuntu:pull token for registry-1.docker.io

=> [internal] load .dockerignore

=> => transferring context: 2B

=> CACHED [1/2] FROM docker.io/library/ubuntu:24.04@sha256:72297848456d5d37d1262630108ab308d3e9ec

=> [2/2] RUN apt update && apt install -y r-base && Rscript -e "install.packages('tibble' exporting to image

=> => exporting layers

=> exporting image sha256:3ed77d00186595e102de575e37cbb846b4008f9e1c249477d3e0cdf26fcb9dd0
```

#### > docker Images

REPOSITORY	TAG	IMAGE ID	CREATED	SIZE
example	latest	3ed77d001865	About a minute ago	1.01GB
<none></none>	<none></none>	b73484b7a407	8 minutes ago	1.06GB

=> => naming to docker.io/library/example

## **Docker History**

#### > docker history 3ed77d001865

IMAGE	CREATED	CREATED BY	SIZE	COMMENT
3ed77d001865	2 minutes ago	CMD ["R" "vanilla"]	0B	buildkit.
<missing></missing>	2 minutes ago	RUN /bin/sh -c apt update && apt install…	912MB	buildkit.
<missing></missing>	2 minutes ago	<pre>ENV DEBIAN_FRONTEND=noninteractive</pre>	0B	buildkit.
<missing></missing>	2 months ago	/bin/sh -c #(nop) CMD ["/bin/bash"]	0B	
<missing></missing>	2 months ago	/bin/sh -c #(nop) ADD file:68158f1ff76fd4de9	101MB	
<missing></missing>	2 months ago	/bin/sh -c #(nop) LABEL org.opencontainers	0B	
<missing></missing>	2 months ago	/bin/sh -c #(nop) LABEL org.opencontainers	0B	
<missing></missing>	2 months ago	/bin/sh -c #(nop) ARG LAUNCHPAD_BUILD_ARCH	0B	
<missing></missing>	2 months ago	/bin/sh -c #(nop) ARG RELEASE	0B	

#### > docker history b73484b7a407

IMAGE	CREATED	CREATED BY	SIZE	COMMENT
b73484b7a407	9 minutes ago	CMD ["R" "vanilla"]	0B	buildkit
<missing></missing>	9 minutes ago	RUN /bin/sh -c rm -rf /var/cache/apt/archive	0B	buildkit
<missing></missing>	27 minutes ago	RUN /bin/sh -c Rscript -e "install.packages(	15.3MB	buildkit
<missing></missing>	27 minutes ago	RUN /bin/sh -c apt install -y r-base # build	897MB	buildkit
<missing></missing>	28 minutes ago	RUN /bin/sh -c apt update # buildkit	46.5MB	buildkit
<missing></missing>	28 minutes ago	ENV DEBIAN_FRONTEND=noninteractive	0B	buildkit
<missing></missing>	2 months ago	/bin/sh -c #(nop) CMD ["/bin/bash"]	0B	
<missing></missing>	2 months ago	/bin/sh -c #(nop) ADD file:68158f1ff76fd4de9	101MB	
<missing></missing>	2 months ago	/bin/sh -c #(nop) LABEL org.opencontainers	0B	
<missing></missing>	2 months ago	/bin/sh -c #(nop) LABEL org.opencontainers	0B	
<missing></missing>	2 months ago	/bin/sh -c #(nop) ARG LAUNCHPAD_BUILD_ARCH	0B	
<missing></missing>	2 months ago	/bin/sh -c #(nop) ARG RELEASE Sta 663 - Spring 2023	0B	

## Dangling images

When an image (and tag) is replaced with a newer versiomn this can result in a dangling image (e.g. b73484b7a407)

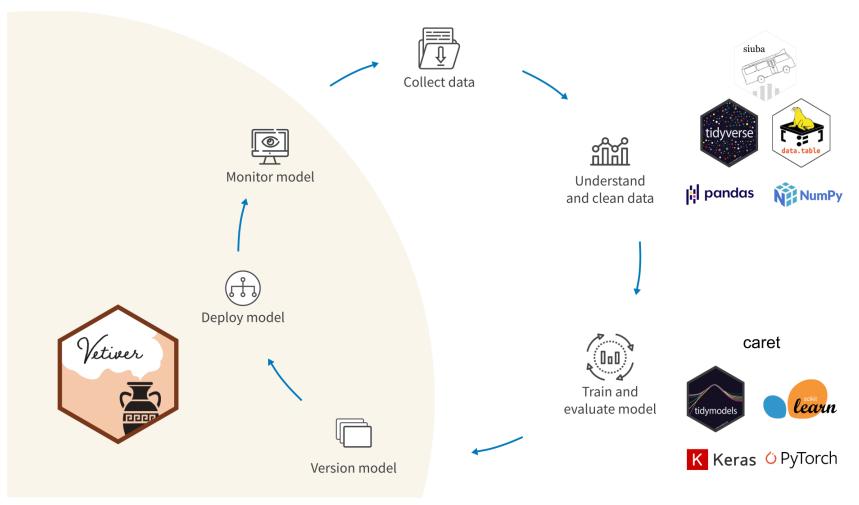
This image can be deleted directly via docker rmi b73484b7a407 or using docker image prune to remove all dangling images.

```
WARNING! This will remove all dangling images.
Are you sure you want to continue? [y/N] y
Deleted Images:
deleted: sha256:b73484b7a407bbd2d1e49983bf987147db9531b940d3169ad9b33a0a6101a4a8
Total reclaimed space: 0B
```

# Vetiver

### **MLOps with Vetiver**

The goal of vetiver is to provide fluent tooling to version, deploy, and monitor a trained model. Functions handle both recording and checking the model's input data prototype, and predicting from a remote API endpoint.



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### **Vetiver for R and Python**

There are vetiver packages for both R and Python that provide similar functionality. Vetiver supports the following modeling frameworks from each language:

#### R

- tidymodels workflows
- caret
- mlr3
- XGBoost
- ranger
- lm() and glm()
- GAMS from mgcv

#### **Python**

- scikit-learn
- PyTorch
- XGBoost
- statsmodels
- spacy

### Train a model

Back to our tried and true MNIST model, using sklearn's logistic regression model:

```
1 from sklearn.datasets import load_digits
   from sklearn.model_selection import train test split
   digits = load_digits()
 5 X, y = digits.data, digits.target
 6
   X_train, X_test, y_train, y_test = train_test_split(
       X, y, test_size=0.20, shuffle=True, random_state=1234
 9
10
   from sklearn.linear_model import LogisticRegression
   from sklearn.metrics import accuracy score
13
   m = LogisticRegression(
     penalty=None
16 ).fit(
     X train, y train
17
18 )
```

### Create a vetiver model

A vetiver model is a light wrapper around a supported model that comes with extra meta data (e.g. data prototype, metrics, etc.)

```
import vetiver
vetiver.VetiverModel(
m, model_name = "mnist_log_reg",
prototype_data = X_train
)
v.description
```

<sup>&#</sup>x27;A scikit-learn LogisticRegression model'

### Pinning models

Model objects can be saved (and versioned) using a pins board

```
import pins
    board = pins.board_temp(versioned = True, allow_pickle_read = True)
    board.board
'/var/folders/v7/wrxd7cdj6l5gzr0191 m9lr0000gr/T/tmpj7lajl6a'
  1 vetiver_vetiver_pin_write(board, v)
Model Cards provide a framework for transparent, responsible reporting.
 Use the vetiver `.qmd` Quarto template as a place to start,
 with vetiver.model card()
Writing pin:
Name: 'mnist log reg'
Version: 20250402T095413Z-02741
    board.pin versions("mnist log reg")
              created
                        hash
                                             version
0 2025-04-02 09:54:13 02741 20250402T095413Z-02741
```

### **Board contents**

### Models from boards

Once a model has been saved (pinned) to a board it can be loaded by vetiver using VetiverModels from\_pin() method.

### Pinning data

Just like models we can also pin (and version) data

```
1 board.pin_write(X_train, "mnist_X_train", type = "joblib")
Writing pin:
Name: 'mnist X train'
Version: 20250402T095413Z-3083a
Meta(title='mnist X train: a pinned ndarray object', description=None, created='20250402T095413Z',
    board.pin write(y train, "mnist y train", type = "joblib")
Writing pin:
Name: 'mnist y train'
Version: 20250402T095413Z-07062
Meta(title='mnist y train: a pinned ndarray object', description=None, created='20250402T095413Z',
    board.pin write(X test, "mnist X test", type = "joblib")
Writing pin:
Name: 'mnist X test'
Version: 20250402T095413Z-5fbe8
Meta(title='mnist X test: a pinned ndarray object', description=None, created='20250402T095413Z',
    board.pin write(y test, "mnist y test", type = "joblib")
Writing pin:
Name: 'mnist_y_test'
Version: 20250402T095413Z-1cd99
Meta(title='mnist y test: a pinned ndarray object', description=None, created='20250402T095413Z',
```

### **Updated contents**

Structure

data.txt

> tree mnist\_log\_reg 20250401T092253Z-02741 — data.txt mnist\_log\_reg.joblib mnist X test 20250401T094626Z-5fbe8 — data.txt mnist\_X\_test.joblib mnist X train \_\_\_\_ 20250401T094620Z-3083a — data.txt — mnist X train.joblib mnist y test 20250401T094626Z-1cd99 — data.txt — mnist y test.joblib mnist y train 20250401T094624Z-07062 — data.txt — mnist y train.joblib

### **Deploying models**

For supported model types, vetiver can generate a basic model api for you using plumber (R) or FastAPI (Python),

```
1 app = vetiver.VetiverAPI(v, check_prototype=True)
2 app.run(port = 8080)
```

If everything is working as expected you should see something like the following:

```
INFO: Started server process [81869]
INFO: Waiting for application startup.
INFO: VetiverAPI starting...
INFO: Application startup complete.
INFO: Uvicorn running on http://127.0.0.1:8080 (Press CTRL+C to quit)
```

The predict endpoint can be accessed using the server submodule,

```
1 endpoint = vetiver.server.vetiver_endpoint("http://127.0.0.1:8080/predict")
2 res = vetiver.server.predict(endpoint, pd.DataFrame(X_test[:10]))
3 res.predict.values
[6 8 5 3 5 6 6 4 5 0]
```

```
1 y_test[:10]
```

[6 8 5 3 5 6 6 4 5 0]

### Prepare a Dockerfile

```
1 os.makedirs("docker/", exist_ok=True)
2 prepare_docker(board, "mnist_log_reg", path="docker/")
```

```
☐ app.py ☐ vetiver_requirements.txt ☐ Dockerfile
```

```
from vetiver import VetiverModel
from dotenv import load_dotenv, find_dotenv
import vetiver
import pins

load_dotenv(find_dotenv())

b = pins.board_folder('board', allow_pickle_read=True)
v = VetiverModel.from_pin(b, 'mnist_log_reg', version = '20250331T101211Z-02741')

vetiver_api = vetiver.VetiverAPI(v)
api = vetiver_api.app
```

### Build

```
> cd docker/
 > docker build -t mnist .
[+] Building 31.9s (10/10) FINISHED
=> [internal] load build definition from Dockerfile
=> => transferring dockerfile: 573B
=> [internal] load metadata for docker.io/library/python:3.12
=> [internal] load .dockerignore
=> => transferring context: 2B
=> [1/5] FROM docker.io/library/python:3.12@sha256:4e7024df2f2099e87d0a41893c299230d2a974c3474e6{
=> => resolve docker.io/library/python:3.12@sha256:4e7024df2f2099e87d0a41893c299230d2a974c3474e6{
=> => sha256:4e7024df2f2099e87d0a41893c299230d2a974c3474e681b0996f141951f9817 10.04kB / 10.04kB
=> => sha256:4378a6c11dea5043896b9425853a850807e5845b0018fe01ddee56c16245fc3c 23.54MB / 23.54MB
=> => sha256:3340b5550573c063816b90ec36245946fb68ad9780d223ff526cb93279631b21 2.33kB / 2.33kB
=> => sha256:0cac921bfee1587757ce9e51a5480012877e020ba9ad1b0269747b0b78534b81 6.41kB / 6.41kB
=> => sha256:545aa82ec479fb0ff3a196141d43d14e5ab1bd1098048223bfd21e505b70581f 48.30MB / 48.30MB
=> => sha256:140d15be2fea6dcd21c20cadae2601a118c08a938168718b2612ad6aca91f74a 64.36MB / 64.36MB
=> => extracting sha256:545aa82ec479fb0ff3a196141d43d14e5ab1bd1098048223bfd21e505b70581f
=> => sha256:1d9d474cce081e468bc6f85727459852112ba732fbbfe3236fae66c5fa8a5ed5 202.75MB / 202.75ME
=> extracting sha256:4378a6c11dea5043896b9425853a850807e5845b0018fe01ddee56c16245fc3c
=> => sha256:3ac7d2d82d1801308a369fcd2a58cadcff5e2c88bf92089c61a74309774d76c8 6.24MB / 6.24MB
=> => sha256:7ca5d982b4a5e69d0cfbae58dab889e32fc7601f34888a1047dfddb815d8e3cc 24.91MB / 24.91MB
=> => sha256:5c1ef3e2d60a1e9bb7a0718e08d9e24bf523c6dcc1f8224baf1b42593b587b9e 249B / 249B
=> => extracting sha256:140d15be2fea6dcd21c20cadae2601a118c08a938168718b2612ad6aca91f74a
=> => extracting sha256:1d9d474cce081e468bc6f85727459852112ba732fbbfe3236fae66c5fa8a5ed5
=> => extracting sha256:3ac7d2d82d1801308a369fcd2a58cadcff5e2c88hf92089c61a74309774d76c8
```

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### Docker run

```
> docker images
REPOSITORY
            TAG
                     IMAGE ID
                                   CREATED
                                                   SIZE
mnist
            latest
                     ae6791f6ab84
                                   36 seconds ago
                                                   1.51GB
 > docker run --rm mnist:latest
Traceback (most recent call last):
  File "/usr/local/bin/uvicorn", line 8, in <module>
   sys.exit(main())
            ^^^^
  File "/usr/local/lib/python3.12/site-packages/click/core.py", line 1161, in __call__
   return self.main(*args, **kwargs)
          ^^^^^
  File "/usr/local/lib/python3.12/site-packages/click/core.py", line 1082, in main
   rv = self.invoke(ctx)
        ^^^^^
 File "/usr/local/lib/python3.12/site-packages/click/core.py", line 1443, in invoke
    return ctx.invoke(self.callback, **ctx.params)
          ^^^^^
  File "/usr/local/lib/python3.12/site-packages/click/core.py", line 788, in invoke
   return callback(*args, **kwargs)
          ^^^^^
  File "/usr/local/lib/python3.12/site-packages/uvicorn/main.py", line 412, in main
   run(
  File "/usr/local/lib/python3.12/site-packages/uvicorn/main.py", line 579, in run
   server_run()
 File "/usr/local/lib/python3.12/site-packages/uvicorn/server.py", line 66, in run
   return asyncio.run(self.serve(sockets=sockets))
```

### Failure?

The error messages are a bit convoluted but, the issue amounts to pins errors PinsError: Pin mnist\_log\_reg either does not exist, which implies that app py in the Docker image wasn't able to find our mnist\_log\_reg pin.

This should not be terribly surpising since the pin lives in the board/ folder locally and we have not copied that folder or its contents into the Dockerfile.

We have two options to resolve this,

- 1. Modify our Dockerfile to include a COPY to move board/ into /vetiver in the container.
- 2. Make use of a Docker volume to give our container access to the local board folder when we run it.

### **Docker volumes**

are passed to docker run via the -v or --volume flag and uses the syntax:

```
> docker run -v [<volume-name>:]<mount-path>[:opts]
```

where <volume-name> is the path on the local system, <mount-path> is the path inside the container, and opts are options like ro for readonly access.

#### A helpful note:

Local and container paths must be absolute paths - you can use the `pwd` expansion to simplify things

### **Corrected run**

```
> docker run --rm -v `pwd`/../broad:/vetiver/broad mnist:latest
```

INFO: Started server process [1]

INFO: Waiting for application startup.

INFO: VetiverAPI starting...

INFO: Application startup complete.

INFO: Uvicorn running on http://0.0.0.0:8080 (Press CTRL+C to quit)

Everything now appears to be running, but can you connect to http://0.0.0.0:8080 or http://localhost:8080?

### **Docker ports**

Similar to volumes, Docker makes a distinction between ports being used within a container and the ports used by the host machine.

Our Dockerfile included EXPOSE 8080 to expose port 8080 but currently there is no mapping between that container port and our machine's network.

Syntax is similar to volumes and uses the -p or --publish flags to specify a mapping between the host and container ports

> docker run -p HOST\_PORT:CONTAINER\_PORT

### Corrected run w/ ports

```
1 endpoint = vetiver.server.vetiver_endpoint("http://0.0.0.0:8080/predict")
2 res = vetiver.server.predict(endpoint, pd.DataFrame(X_test[:10]))
3 res.predict.values
```

```
[6 8 5 3 5 6 6 4 5 0]
```

```
1 y_test[:10]
```

[6 8 5 3 5 6 6 4 5 0]

## Finalizing deployment

You may notice that when we use docker run here we see the Uvicorn output but we are not taken back to our prompt. We can use Ctrl+C to exit but this kills the container. If run remotely (via ssh) the container will also be killed when we disconnect.

A couple of additional flags are useful with docker run here

- −d, −−detach run container in background
- --restart specifies a container's restart policy, possible policies are:
  - no (Default) container does not restart
  - on-failure[:max-retries] restarts on errors (based on exit code) up to max-retries
  - always restarts unless manually stopped (docker stop)
  - unless-stopped similar to always but does not restart when daemon restarts

### **Detached container**

```
> docker run -d --restart=on-failure -v `pwd`/../board:/vetiver/board -p 8080:8080 mnist:latest
998718e4a28a95afd46903df2e5b40642b4fb2245425804f2dd1f4d5f1525f9c
```

We can see our running container with docker ps, use the —a flag to see all containers (running and stopped),

If we need to debug or mess with the running container we can run new command inside with docker exec,

## Stopping and cleaning up

When we're done with the container (or want to replace it) we can stop the container by name or id with docker stop, a stopped container can be restarted via docker start, and a container can be deleted via docker rm.

```
> docker stop eager knuth
eager knuth
 > docker ps -a
CONTAINER ID
               IMAGE
                              COMMAND
                                                       CREATED
                                                                        STATUS
998718e4a28a
               mnist:latest
                              "uvicorn app.app:api..."
                                                       6 minutes ago
                                                                       Exited (0) 14 seconds ago
   docker rm 998718e4a28a
998718e4a28a
 > docker ps -a
CONTAINER ID
               IMAGE
                         COMMAND
                                   CREATED
                                             STATUS
                                                       PORTS
                                                                 NAMES
```

### Some comments about HW5

- We will be pushing the deadline for HW5 back to Friday, April 11th at 5 pm
- Parts of Vetiver can be made to work with pytorch but it is clunky at best
  - e.g. Transforming X\_train to be a flat numpy array lets you create a
     VetiverModel that can be pinned
- Parts of Vetiver cannot be made to work with pytorch at moment
  - VetiverAPI's predict endpoint is not able to correctly serialize and unserialize the prediction data for torch

The current plan is on Friday is a complete demo involving:

- Briefly introducing FastAPI
- Bootstraping a basic prediction API using a saved torch model
- Combine these pieces into a custom Dockerfile

### Container on the vm

Based on the content of the last lecture, you should be able to get Docker up and running on the VM and also be able to install any additional necessary packages to be able to build your image on the VM.

A couple of points,

- Files can be copied to the VM using scp via the command line or any number of GUI tools using this protocol
- Feel free to commit your Dockerfile and pins board to your GitHub repository, the repo can then be cloned on the VM
  - Do be mindful of the size of your board files GitHub has a individual file size limit of ~100MB