Docker for DS

W W H

What Why How

Why What How

Why

Why

~~Why~~ Problems Docker Solves

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- Reproducibility.

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- Reproducibility.
- Scalable computational backend.

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- Persistent computational environment.

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- Shared dependency management.

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- Reproducibility.
- Scalable computational backend.
- Persistent computational environment.
- Shared dependency management.
- Lack of appropriate permissions on a server.

Reproducibility

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- The container used to run the code for the model can be restarted in the exact state it was left, and code re-run.

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- The container used to run the code for the model can be restarted in the exact state it was left, and code re-run.
- This complements the Makefile, by ensuring that the build process does not fail due to dependencies.

Scalable computational backend

Scalable computational backend

- Running code our macbooks works well, and is very flexible, but is limited by the hardware on our machines. Docker has to potential to scale to the size of the machine it is run on.

Persistent computational environment

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- Often models will train overnight, or code otherwise needs to keep running (displaying results in a dashboard, for example).

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- Relying on the Caffeine app doesn't always work (laptops sometimes just reset, we want to take them home, etc).

Shared dependency management

Shared dependency management

- We each set up our laptops ourselves, often requiring substantial work (see https://gist.github.com/andyreagan/32c737fd315e70ccb3b4a4387a466c85) and doing so inconsistently.

Shared dependency management

- We each set up our laptops ourselves, often requiring substantial work (see https://gist.github.com/andyreagan/32c737fd315e70ccb3b4a4387a466c85) and doing so inconsistently.
- If we can share installations of common tools, that would reduce the workload for individual data scientists or maintaining personal setups.

Lack of permissions

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- Happens both on some servers, and on managed macs!

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- This can be fixed, but is nonetheless a real life hurdle.

Problems Docker Creates

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- Performance overhead?

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- Performance overhead?
- Maintenance of docker environment itself.

Performance overhead

- This is a bit unknown (and yes, on both sides). Docker running inside a VM locally, or on a server, has access to share memory and compute (I've seen all N cores get used locally training a model).

Maintenance of docker environment itself

- Will this be less work than managing an individual setup? It is surely at least a bit harder to set up Docker (using the RUN commands, etc) than a local environment.

Alternatives (when *not* to use Docker)

- Python virtualenv.
- Julia user home package installation.
- Packrat?

What

What is Docker?

magic

What is Docker?

~~magic~~

What is Docker?

What is Docker?

plumbing!

What is Docker?

What is Docker?

- RedHat <-> linux as Docker <-> runC

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- RedHat <-> linux as   Docker <-> runC
- Underlying tech ~~LXC~~ runC/libcontainer.

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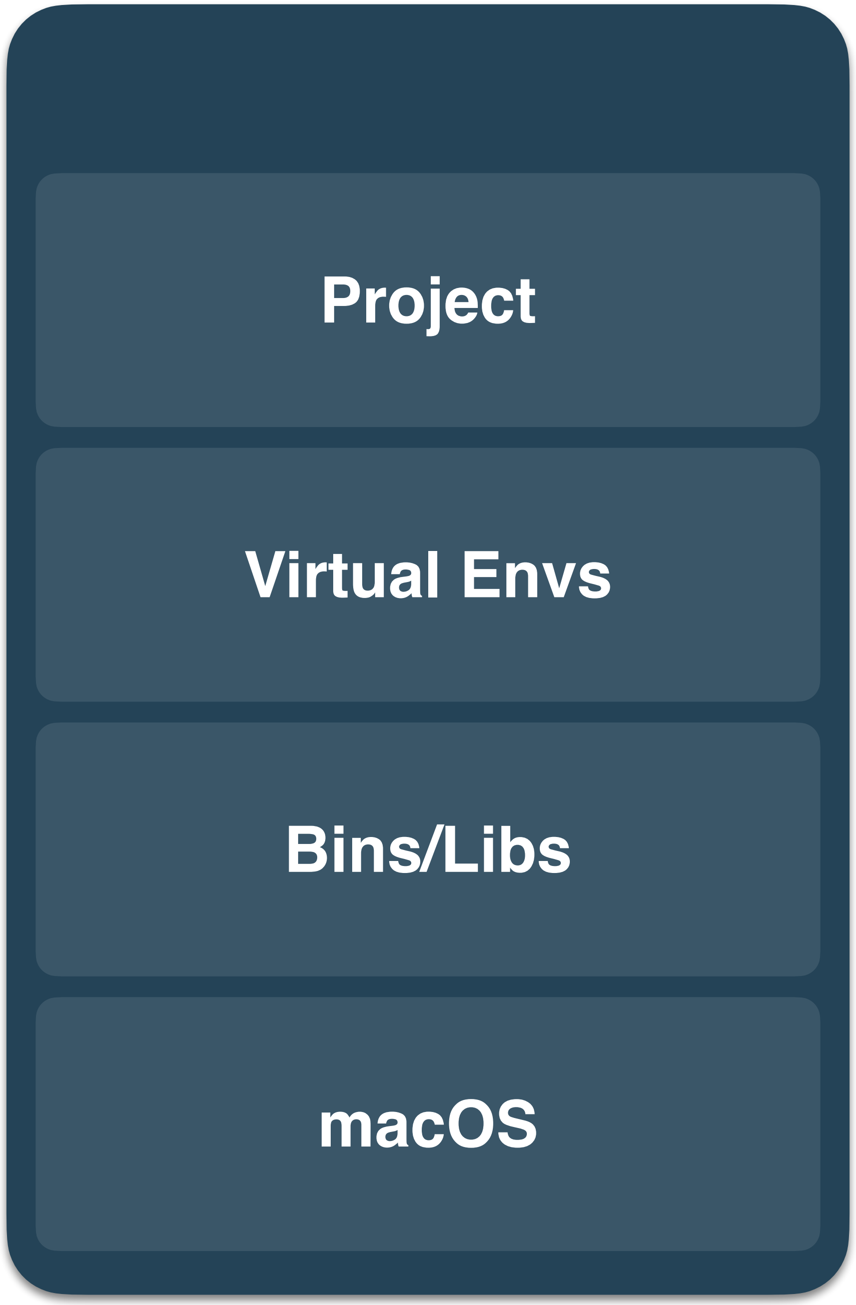
- RedHat <-> linux as Docker <-> runC
- Underlying tech ~~LXC~~ runC/libcontainer.
- ~~AuFS~~ OverlayFS file system driver

Your laptop



Project

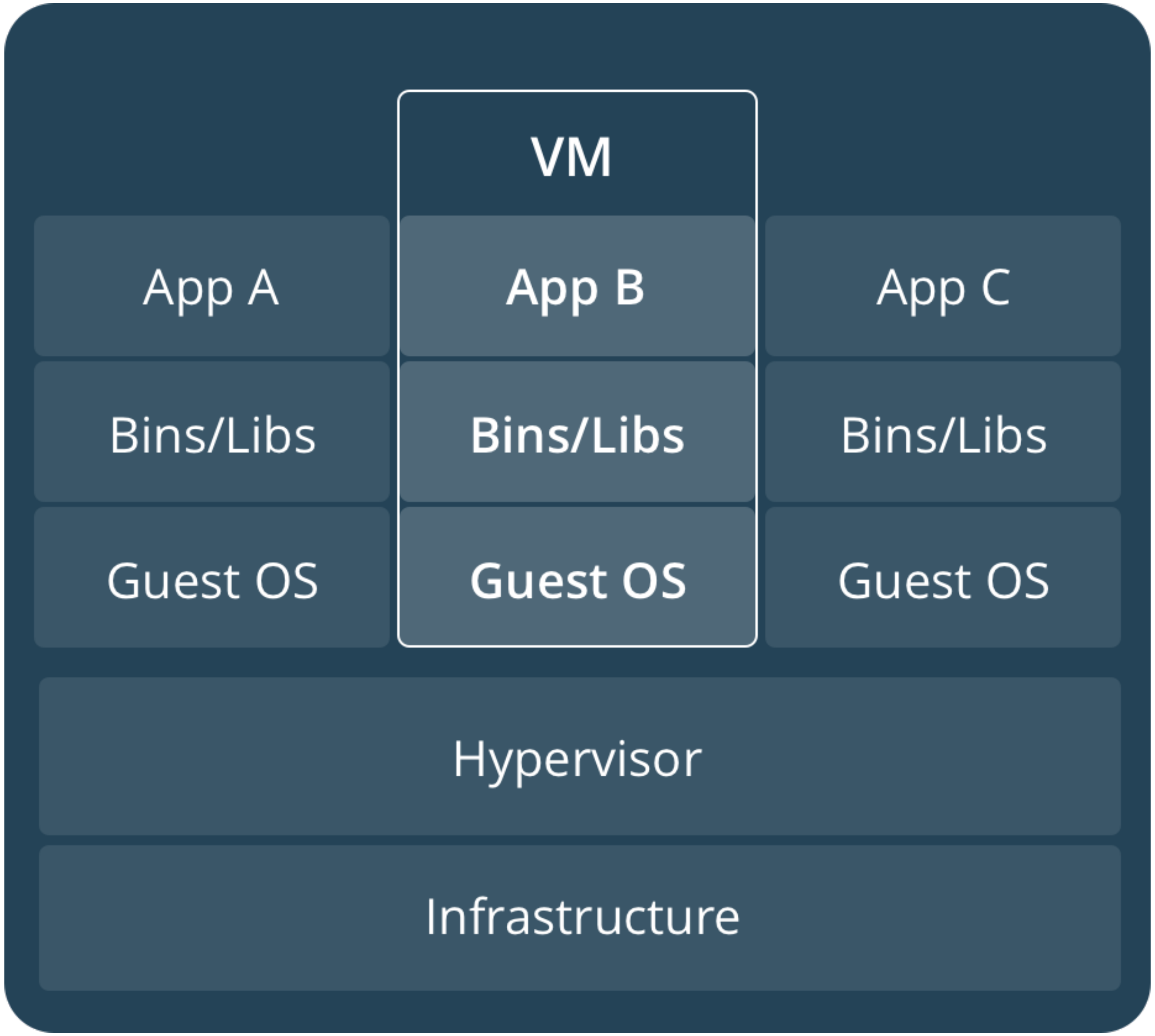
Virtual Envs

Bins/Libs

macOS

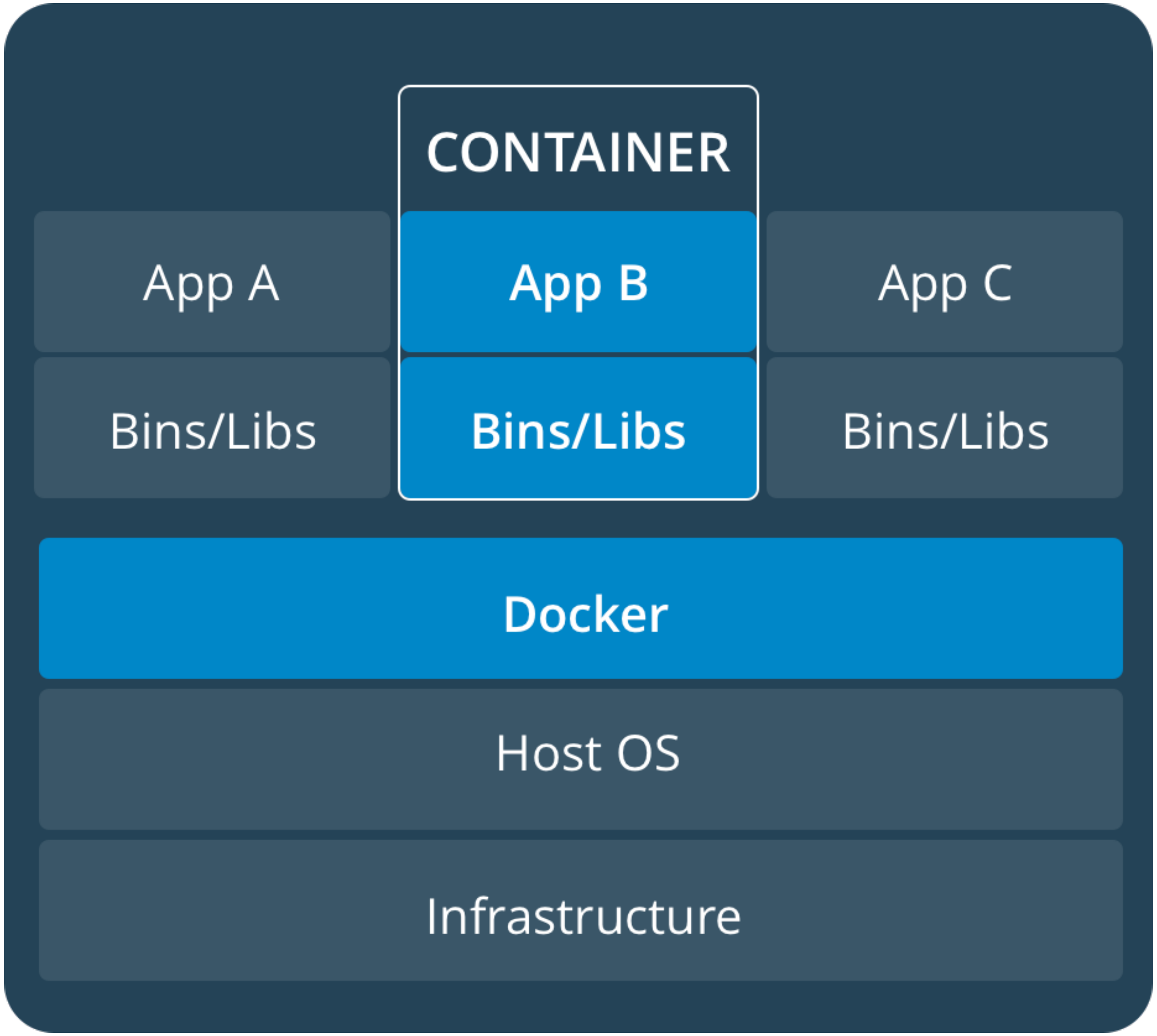
Your laptop

Your laptop

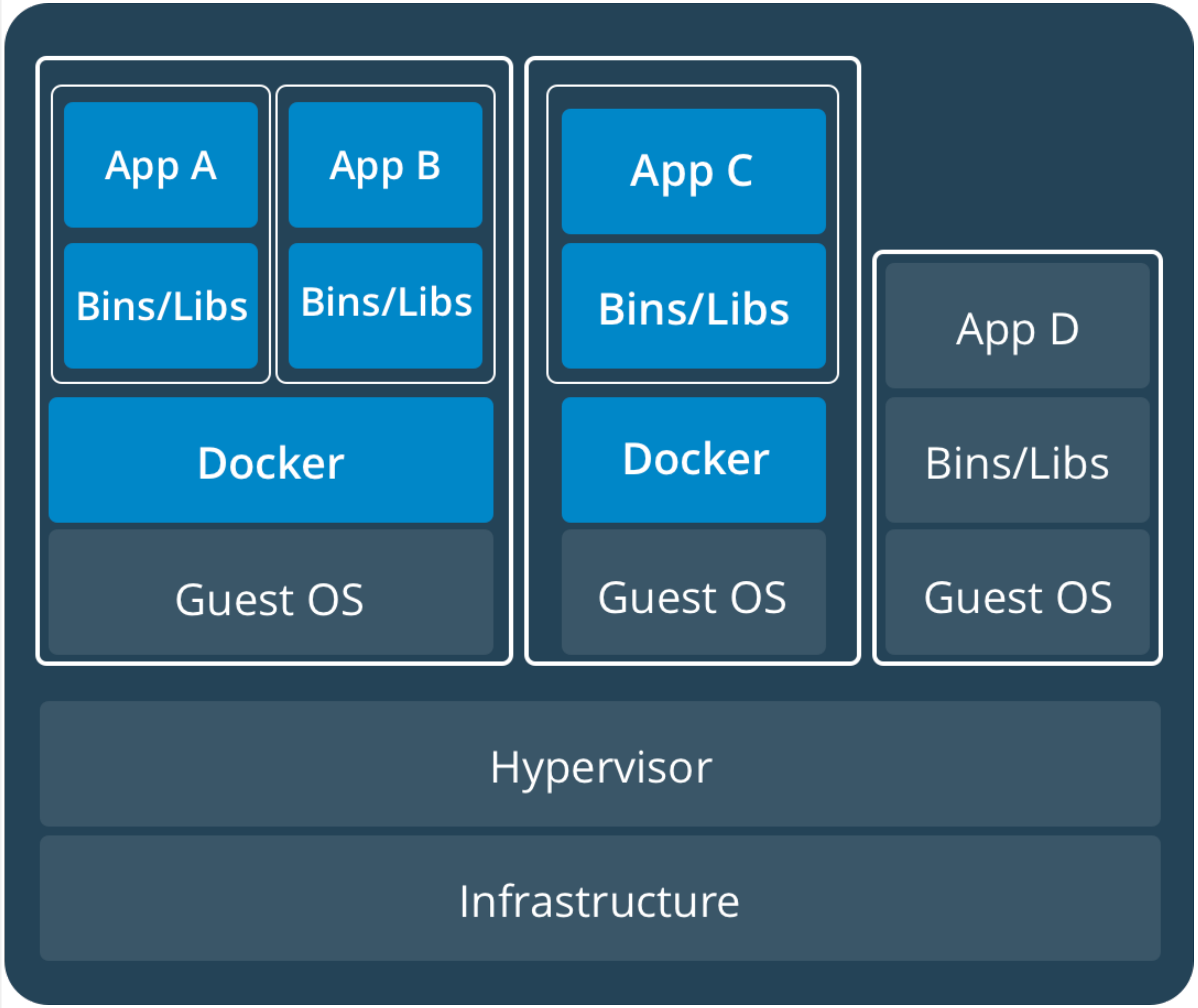


VM
App A
App B
App C
Bins/Libs
Bins/Libs
Bins/Libs
Guest OS
Guest OS
Guest OS
Hypervisor
Infrastructure

with containers

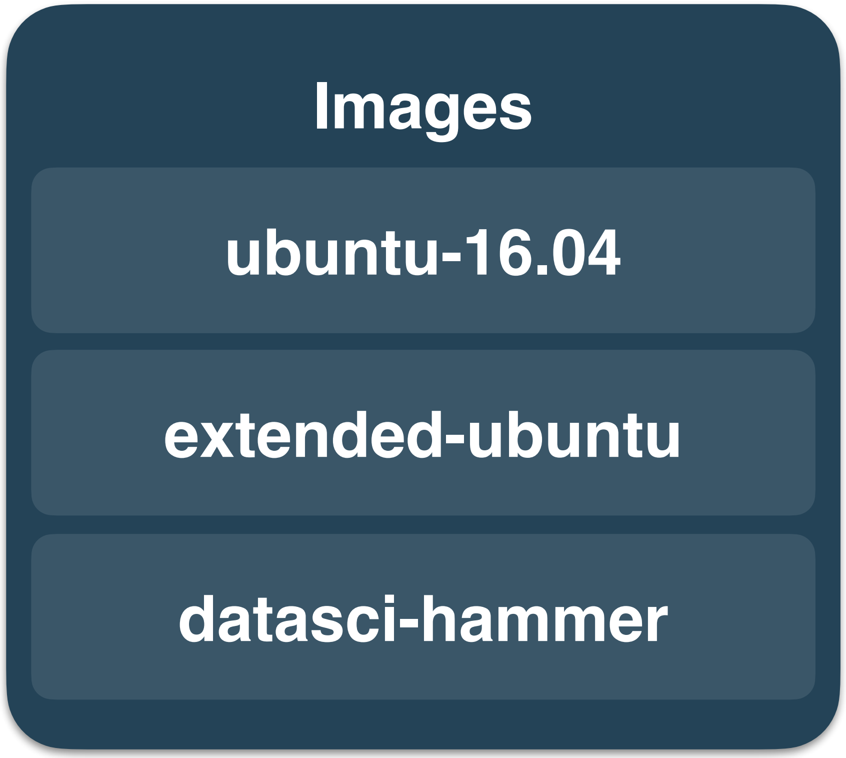


on your laptop



Two key concepts

Two key concepts



Images

ubuntu-16.04

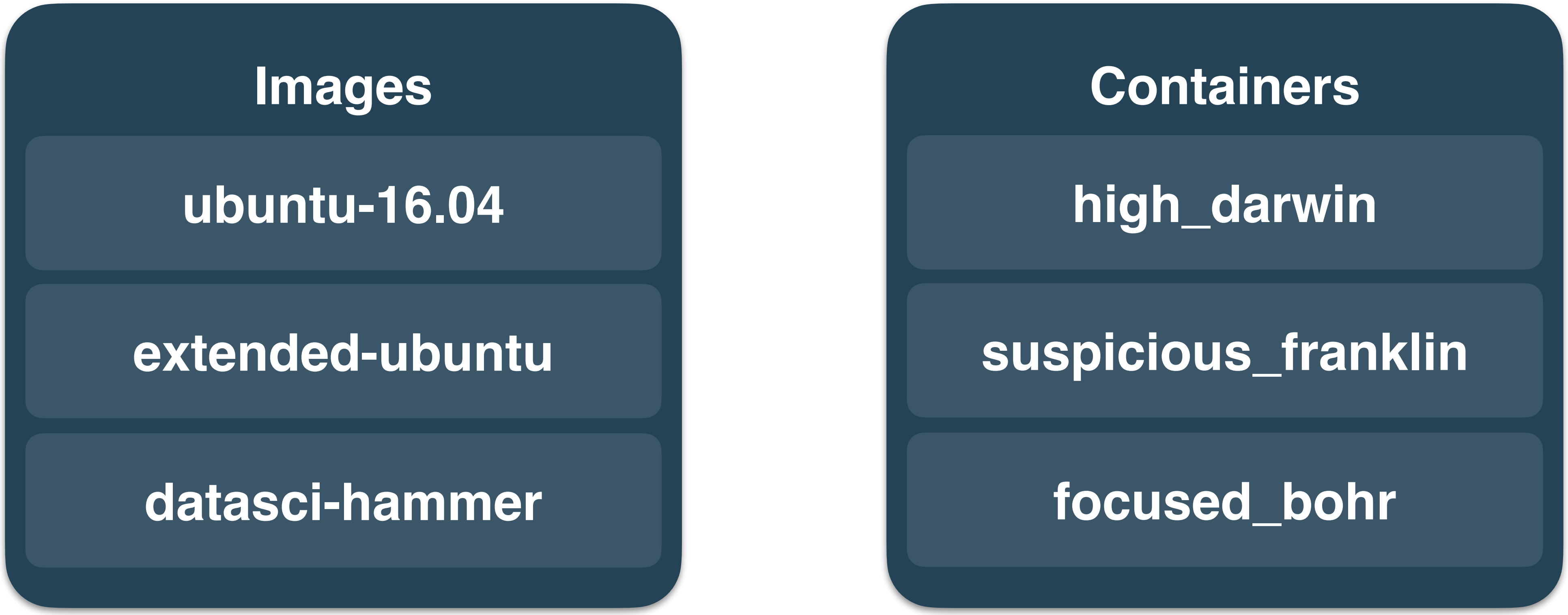
extended-ubuntu

datasci-hammer

Two key concepts

Images	Containers
ubuntu-16.04	sick_einstein
extended-ubuntu	reverent_fermat
datasci-hammer	naughty_heisenberg

Two key concepts



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- ubuntu-16.04
- extended-ubuntu
- datasci-hammer

Containers

- high_darwin
- suspicious_franklin
- focused_bohr

docker images

Two key concepts

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docker ps [-a]

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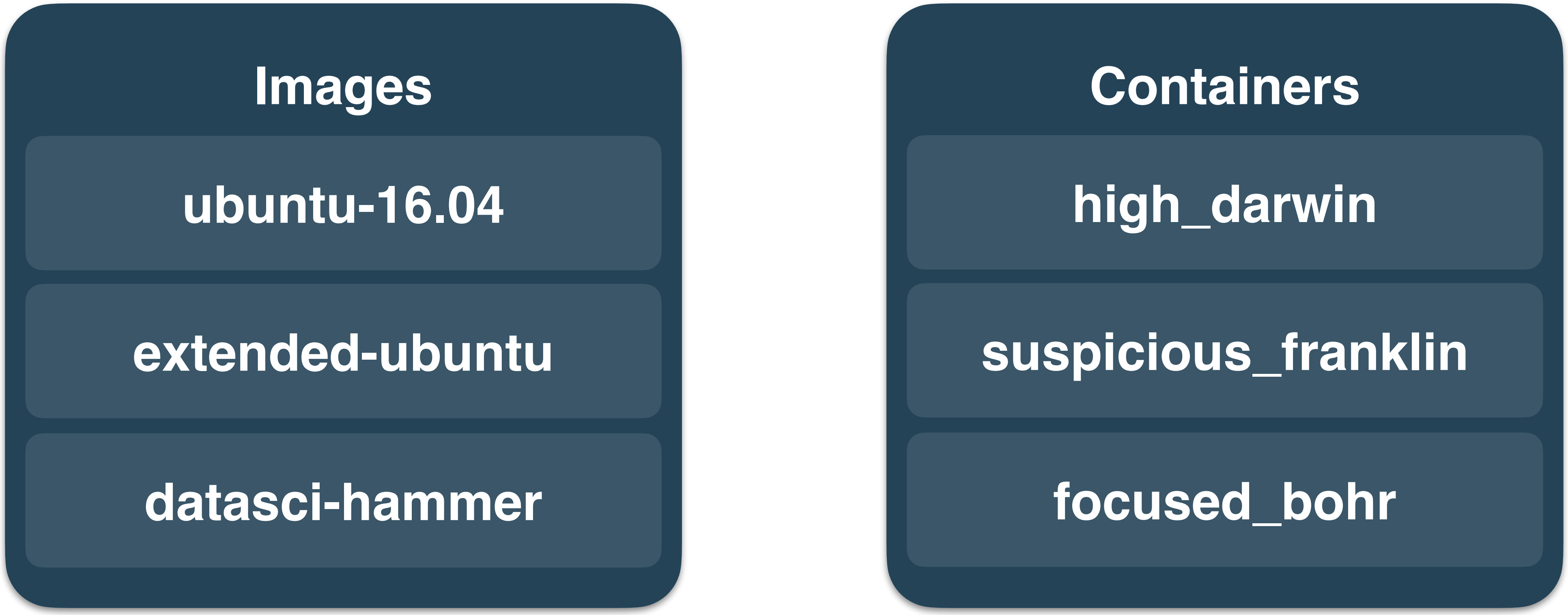

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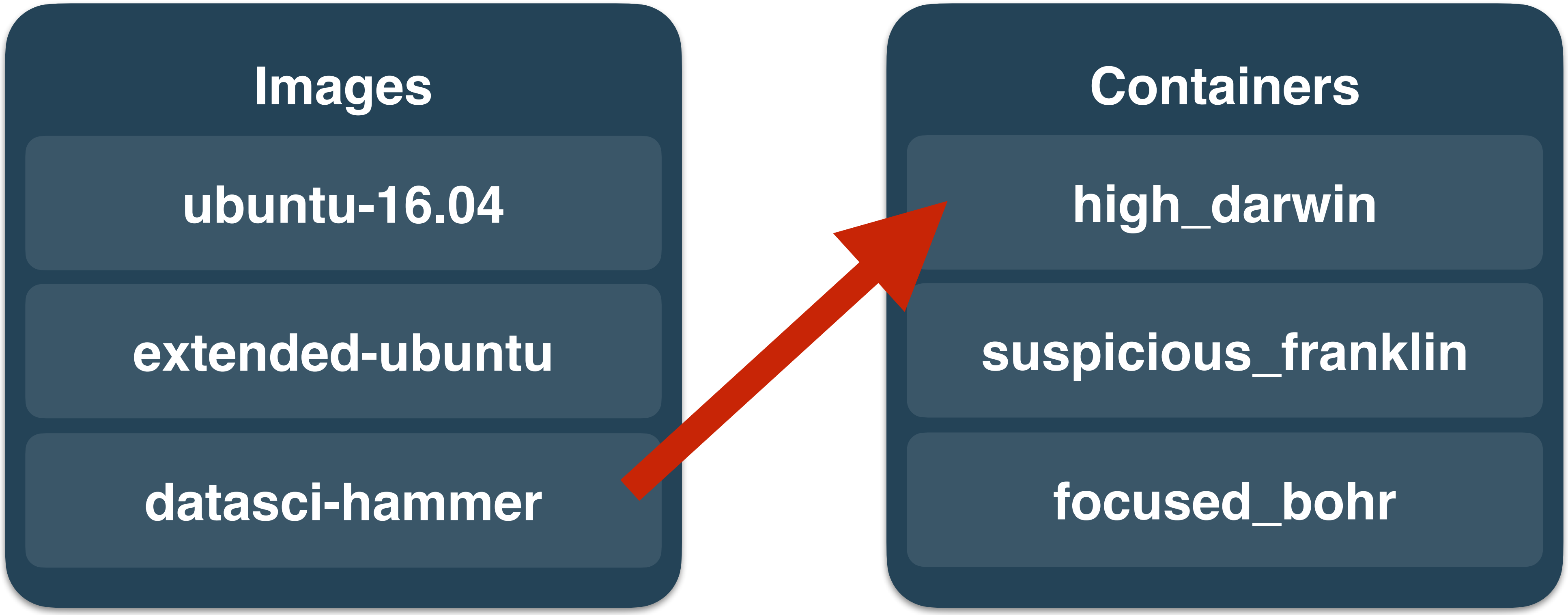

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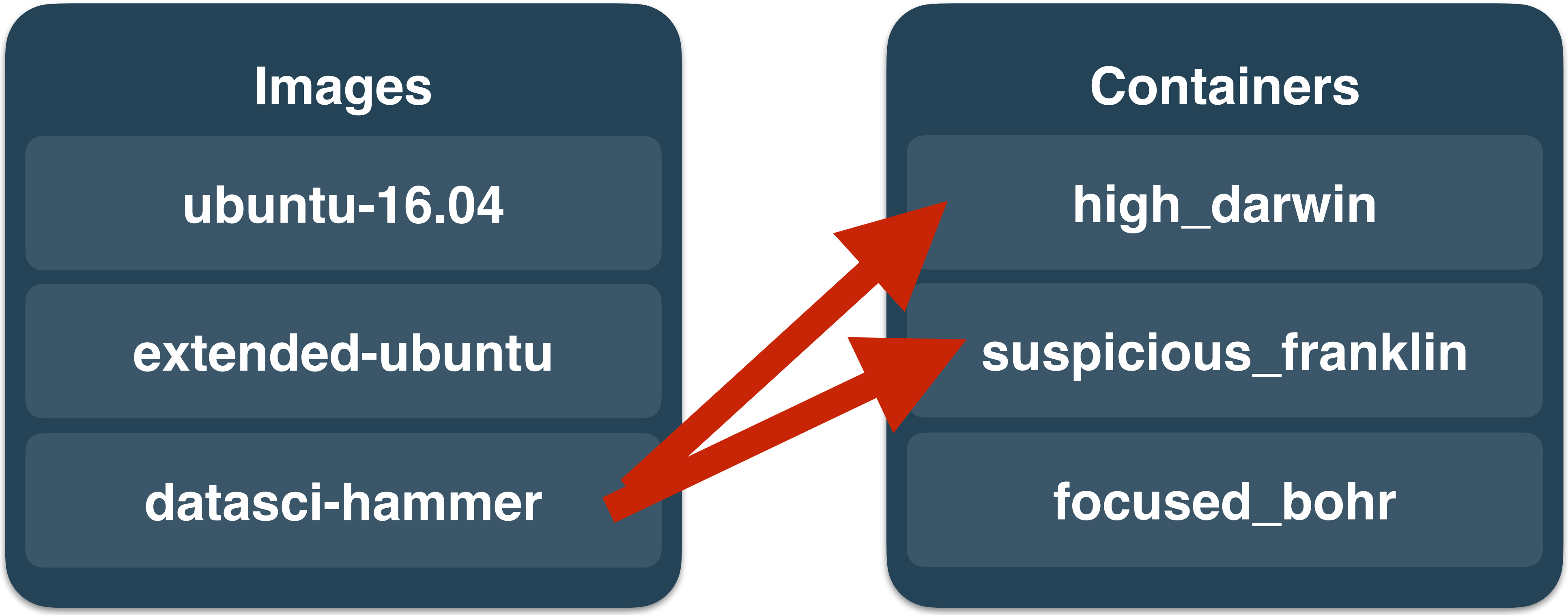

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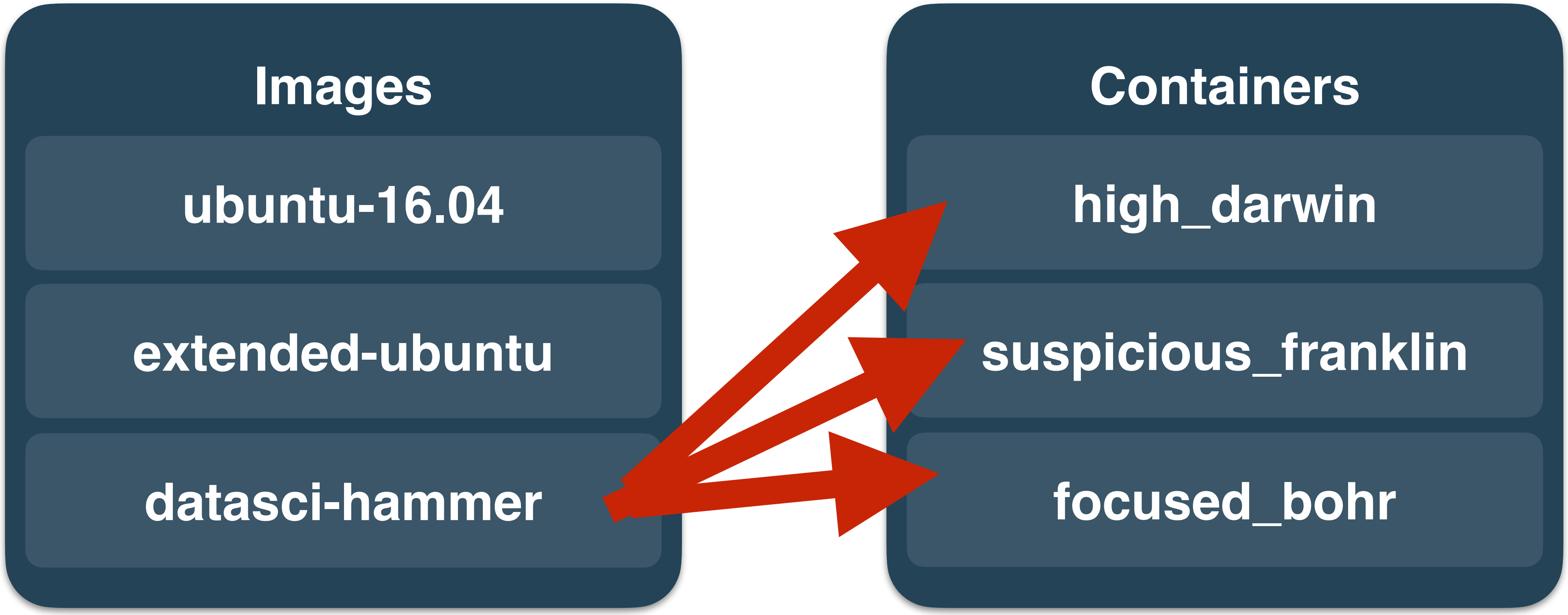

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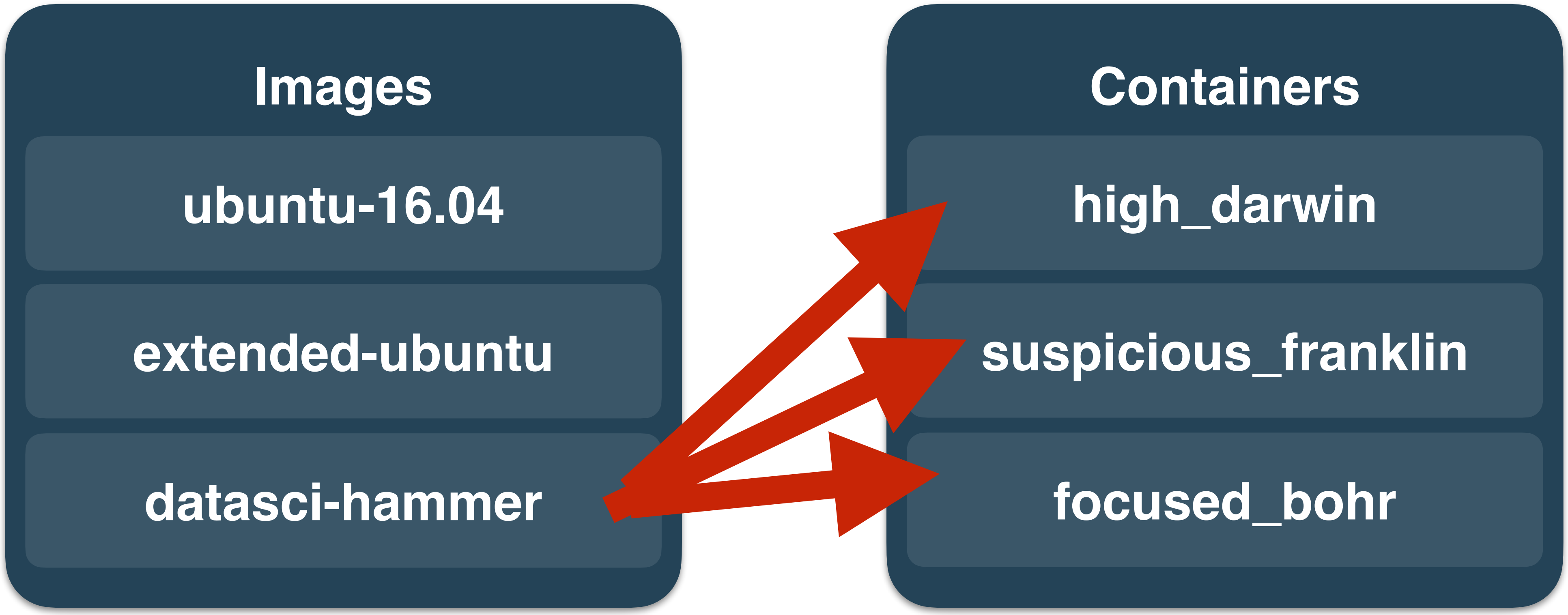

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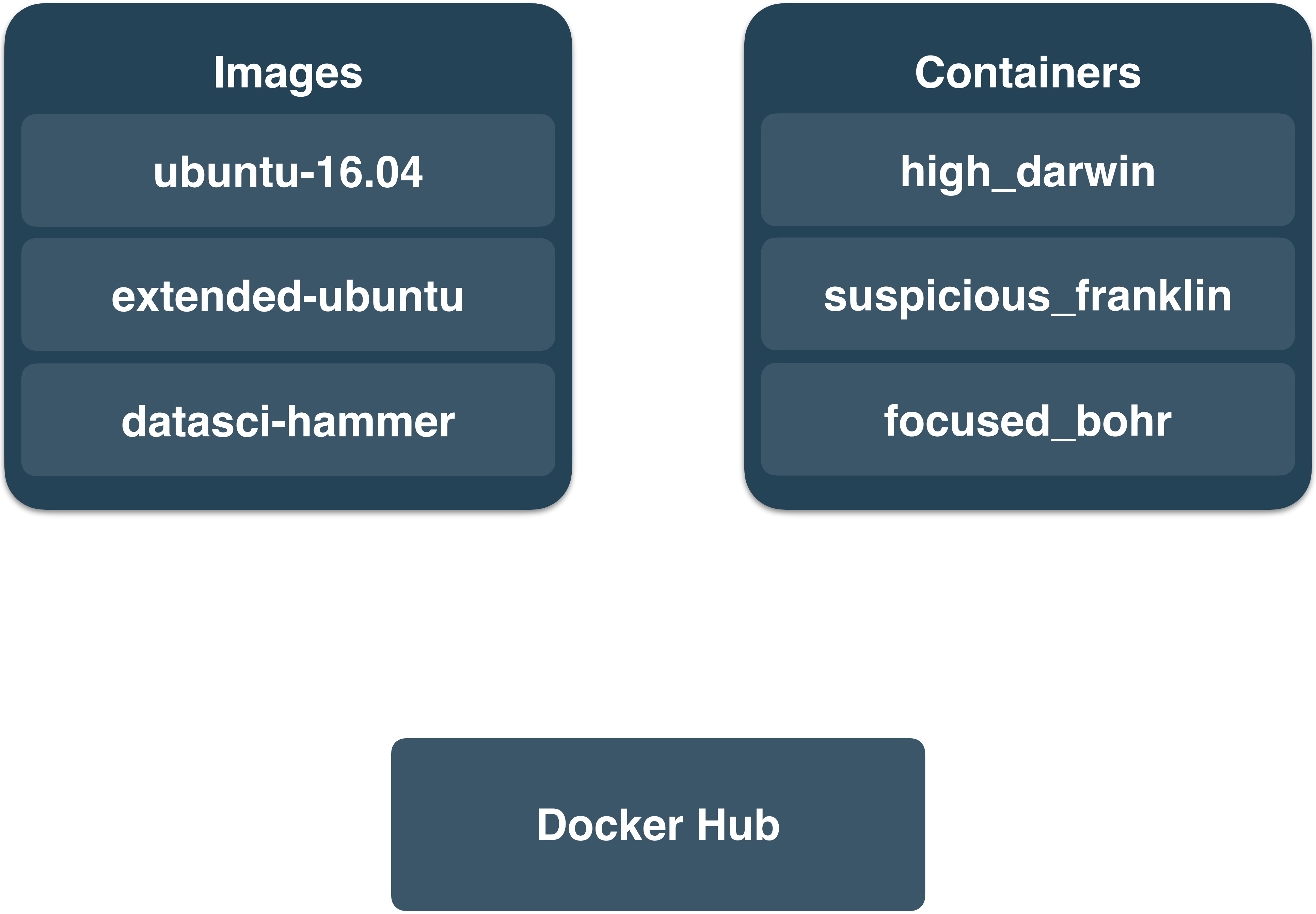
```
docker run datasci-hammer
```

Two key concepts



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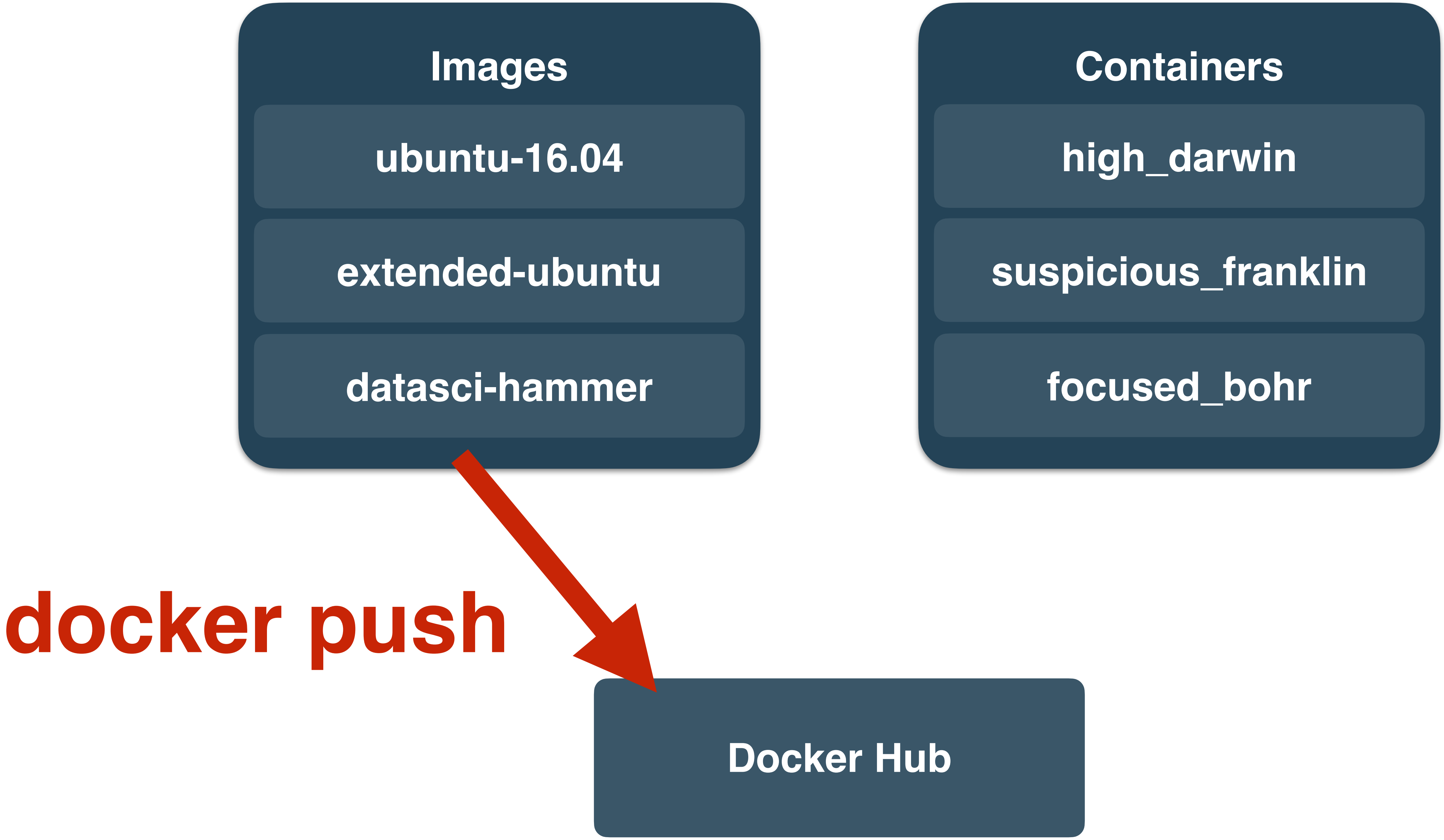
Docker Hub

Two key concepts



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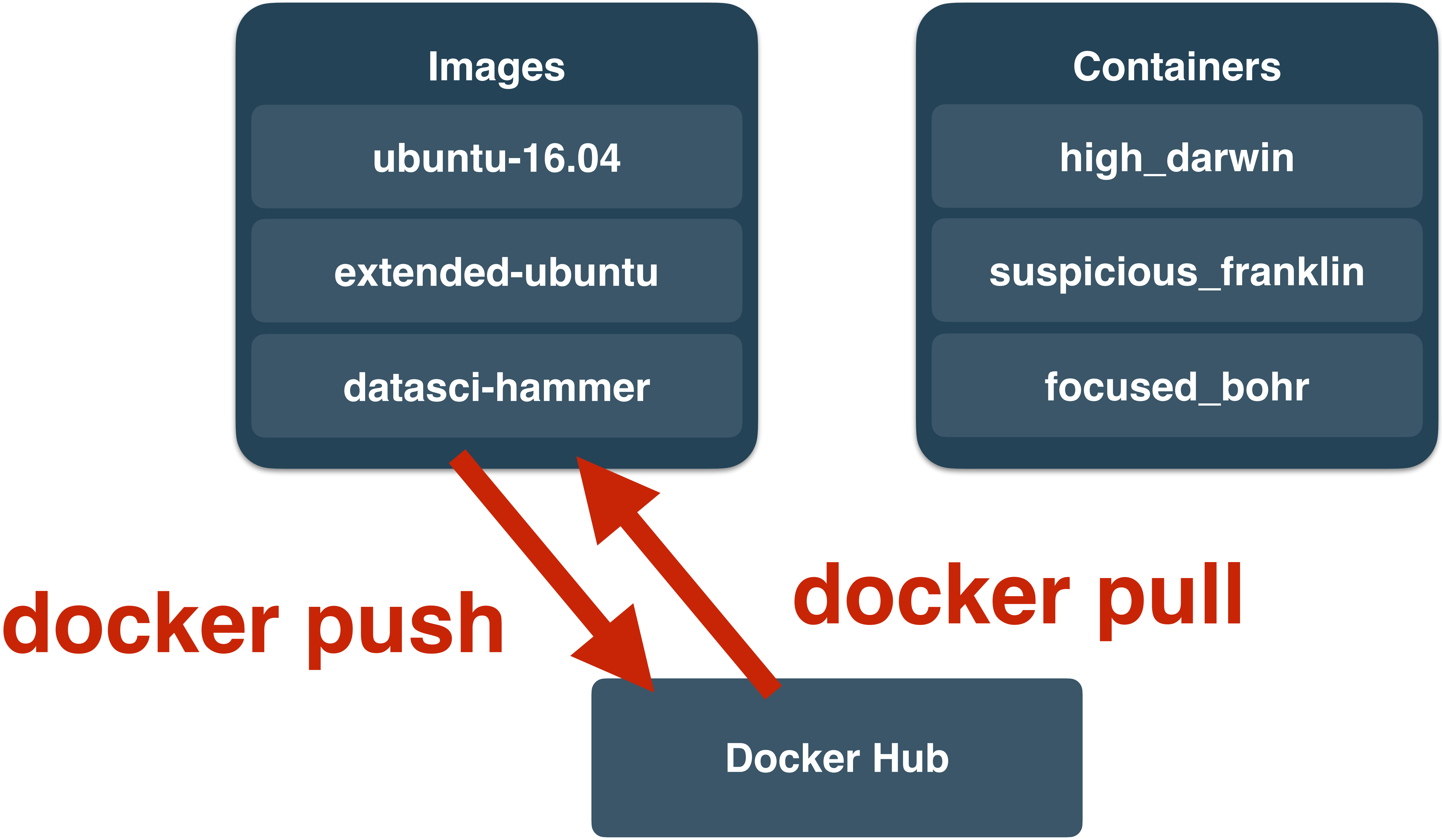

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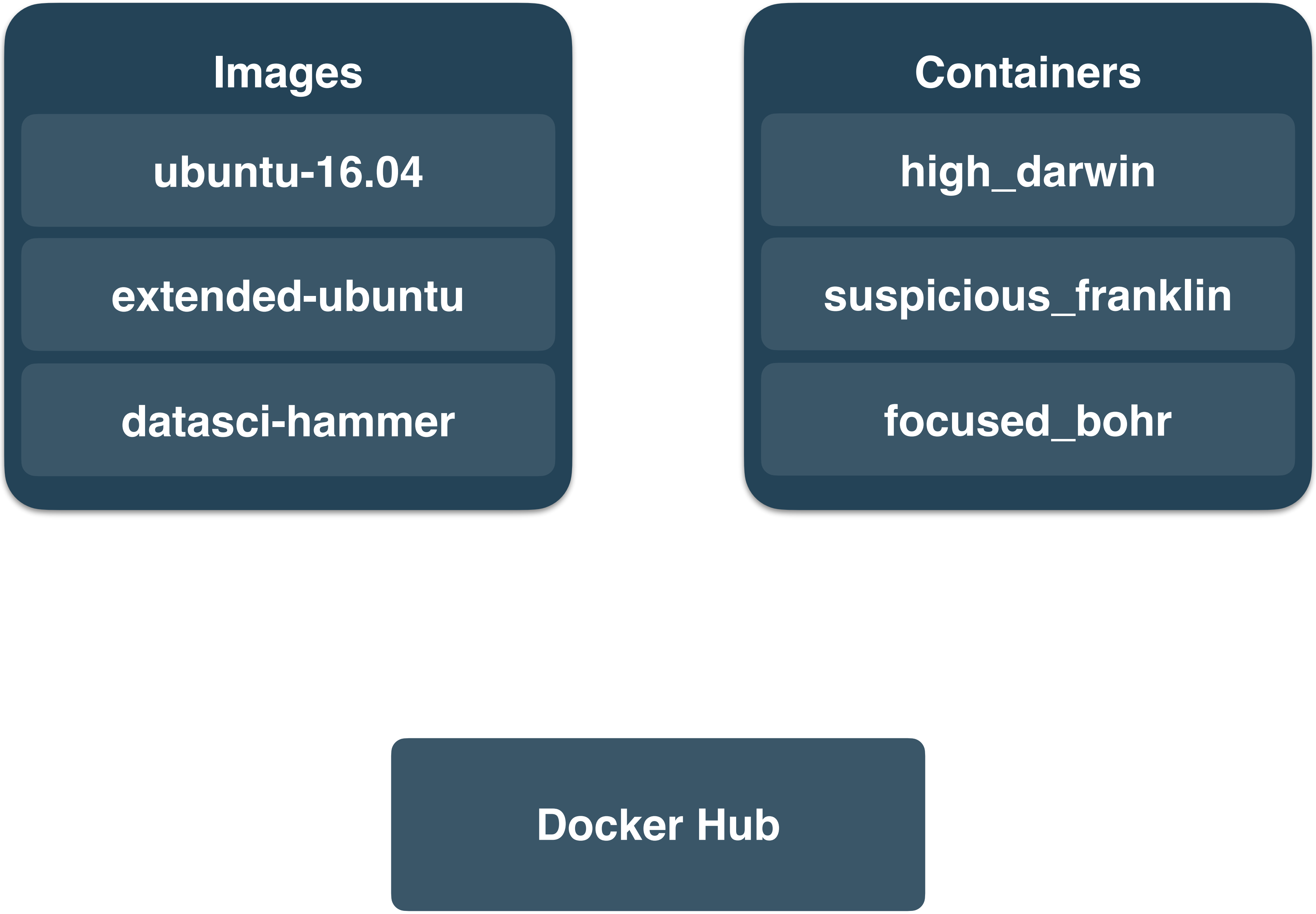
docker push

docker pull

Docker Hub



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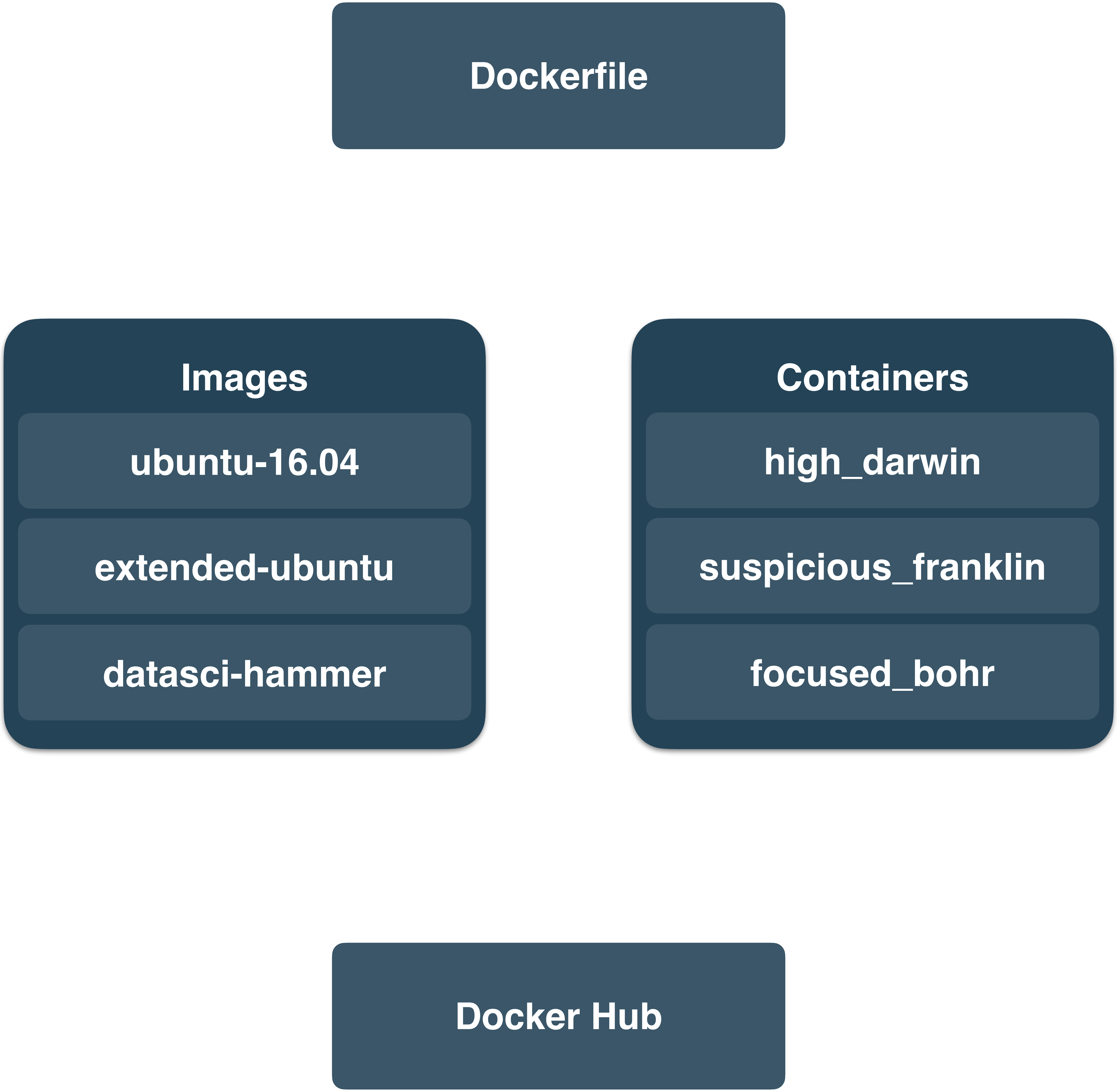

Dockerfile

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extended-ubuntu

datasci-hammer

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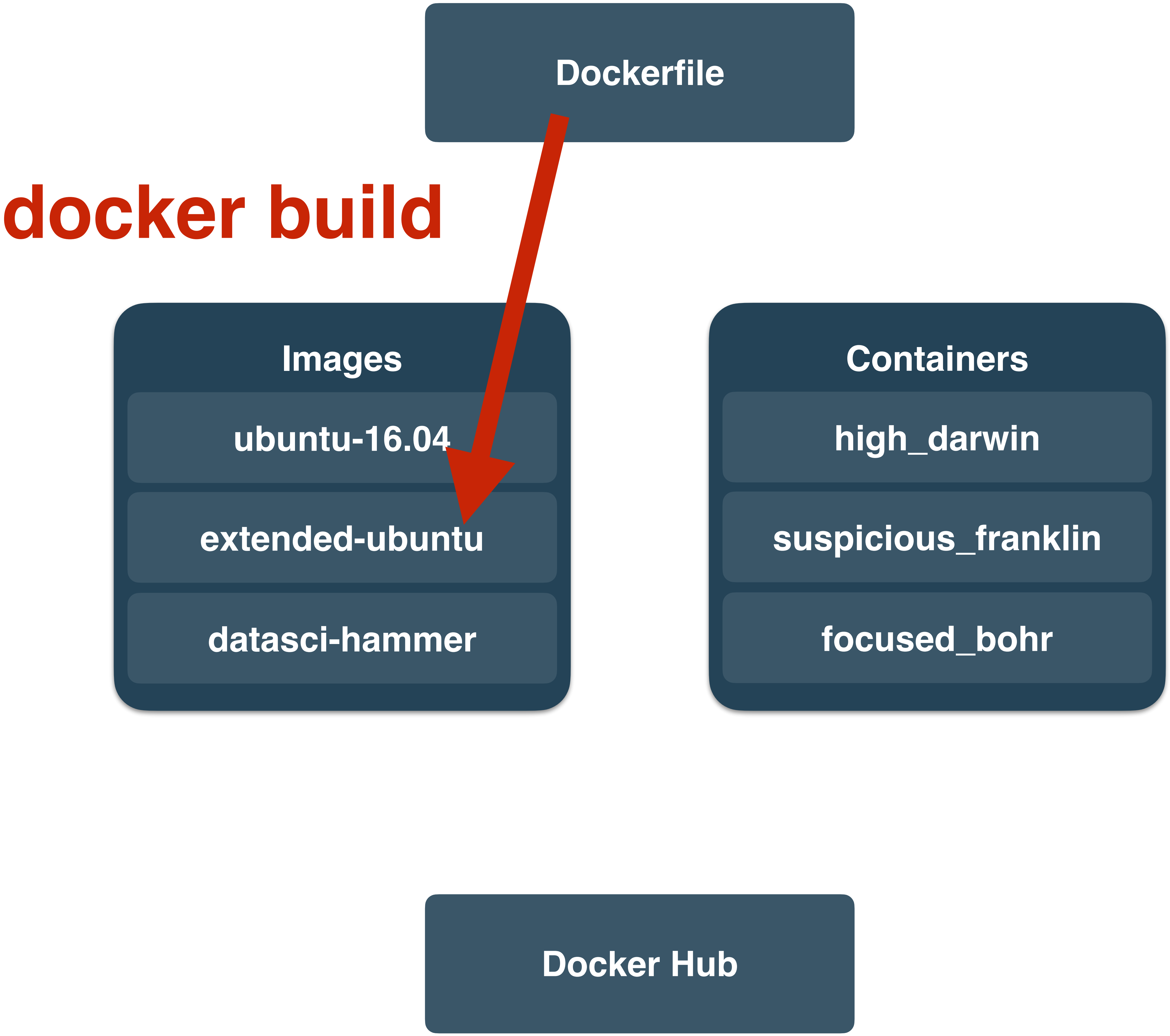
Docker Hub


Dockerfile
docker build
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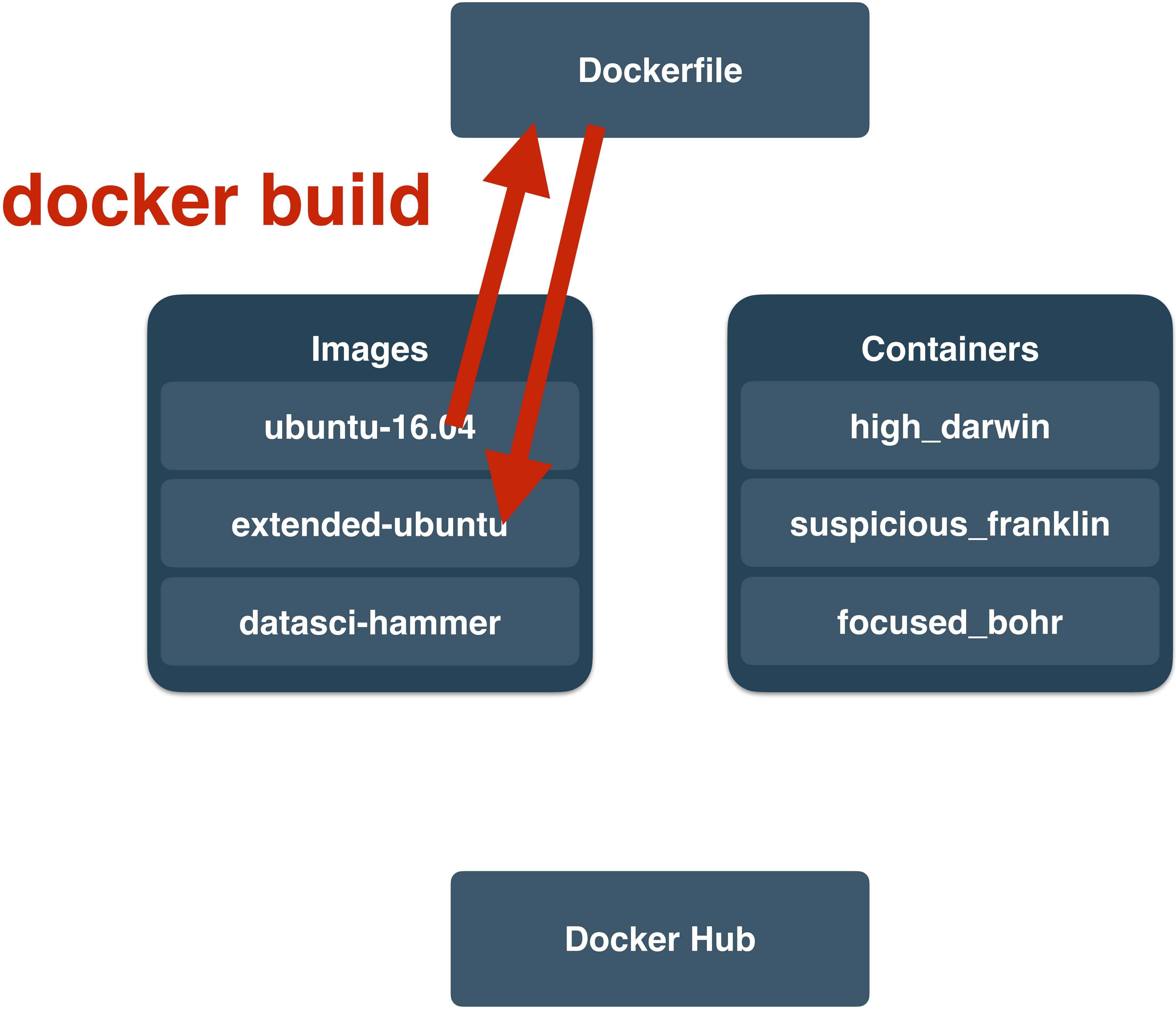

docker build

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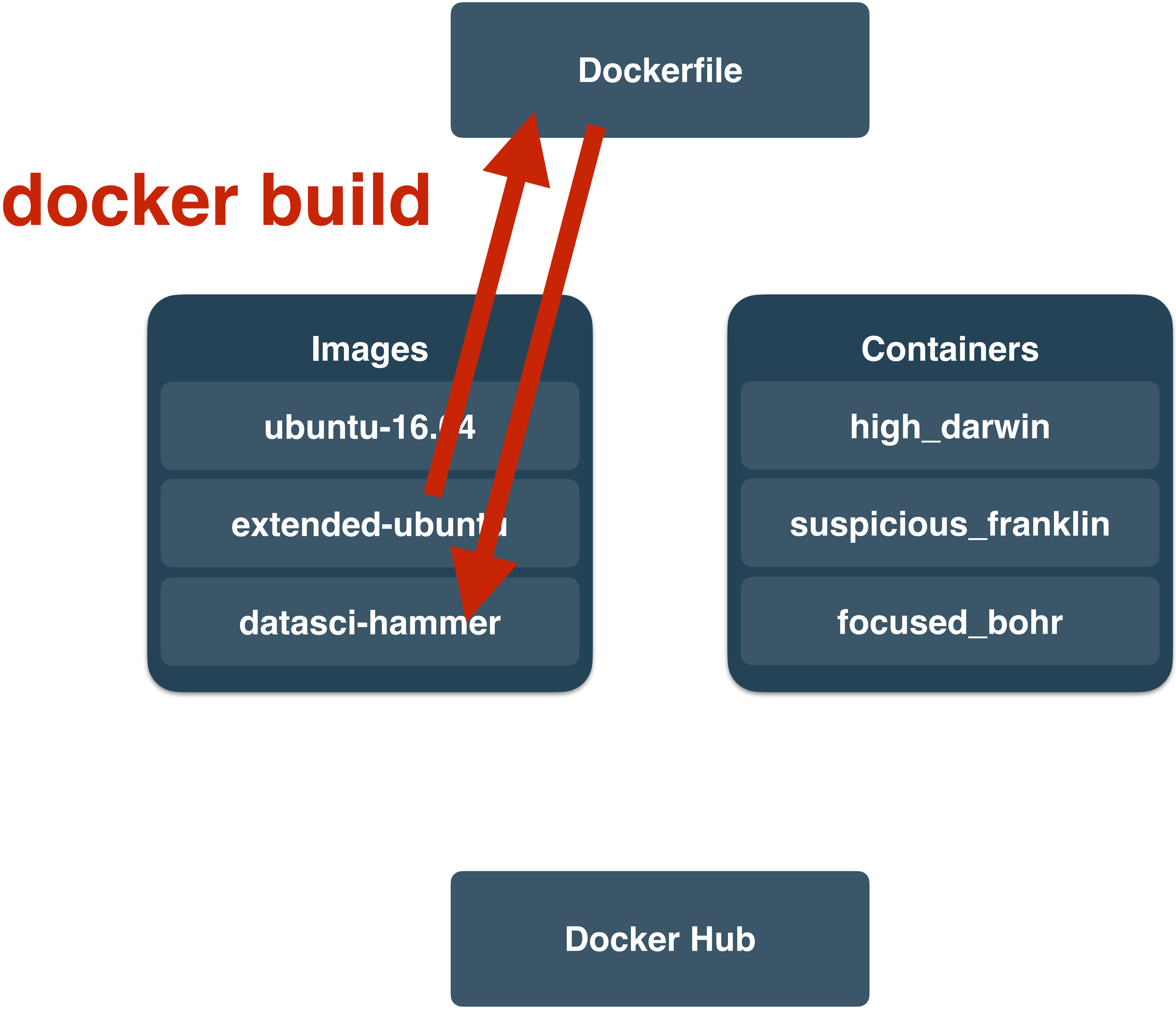

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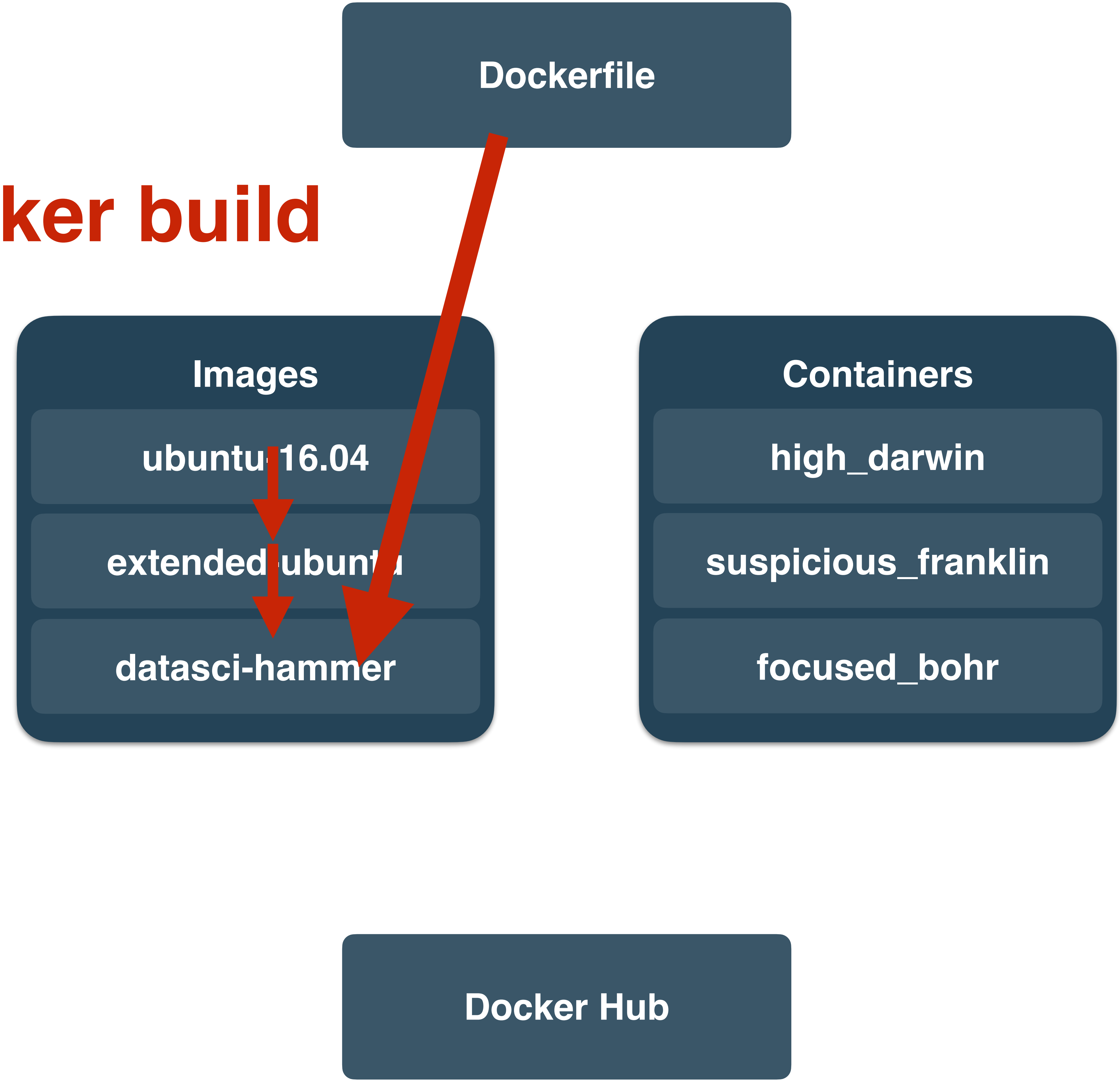

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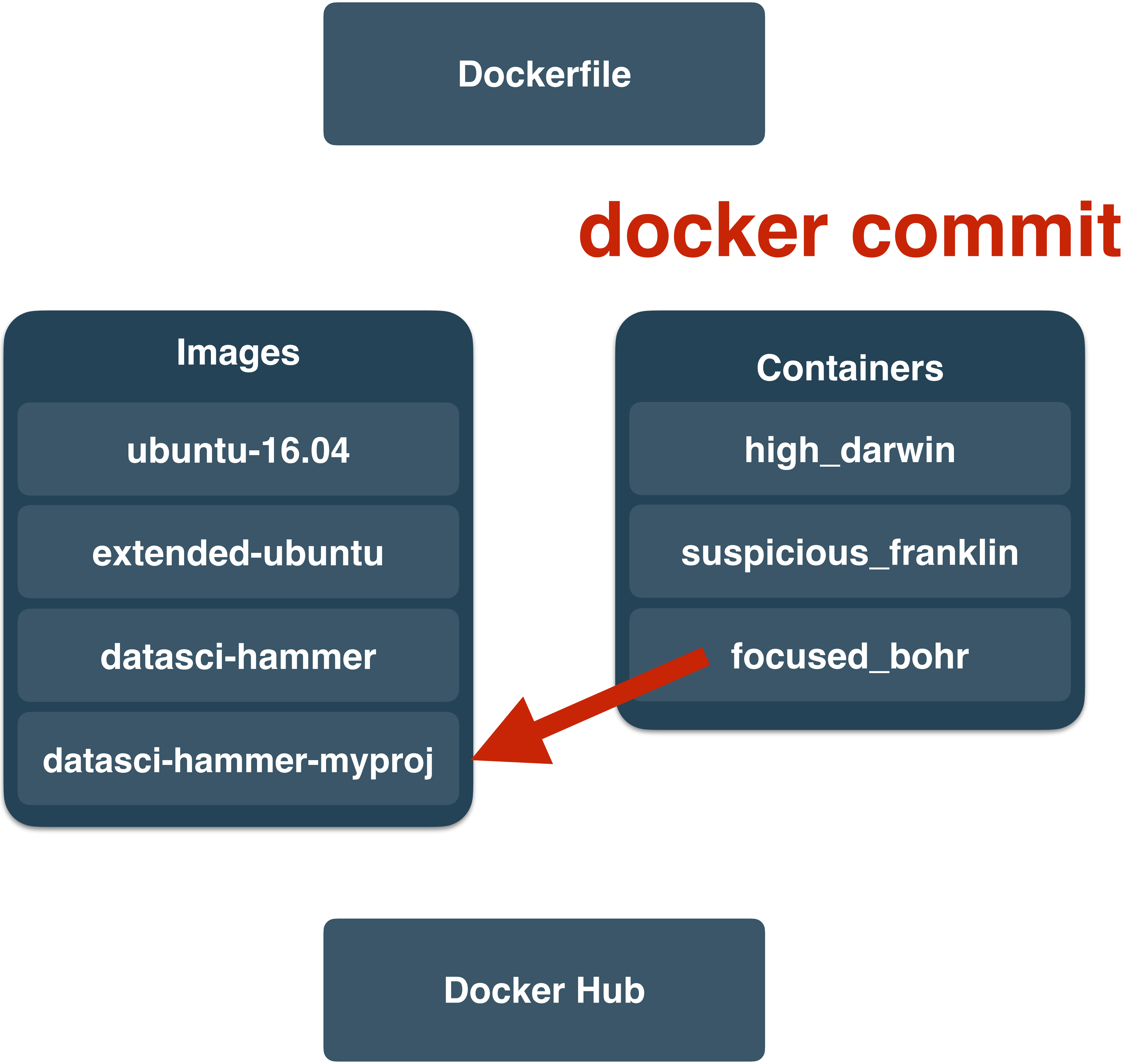

Dockerfile

docker commit

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ubuntu-16.04

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datasci-hammer

datasci-hammer-myproj

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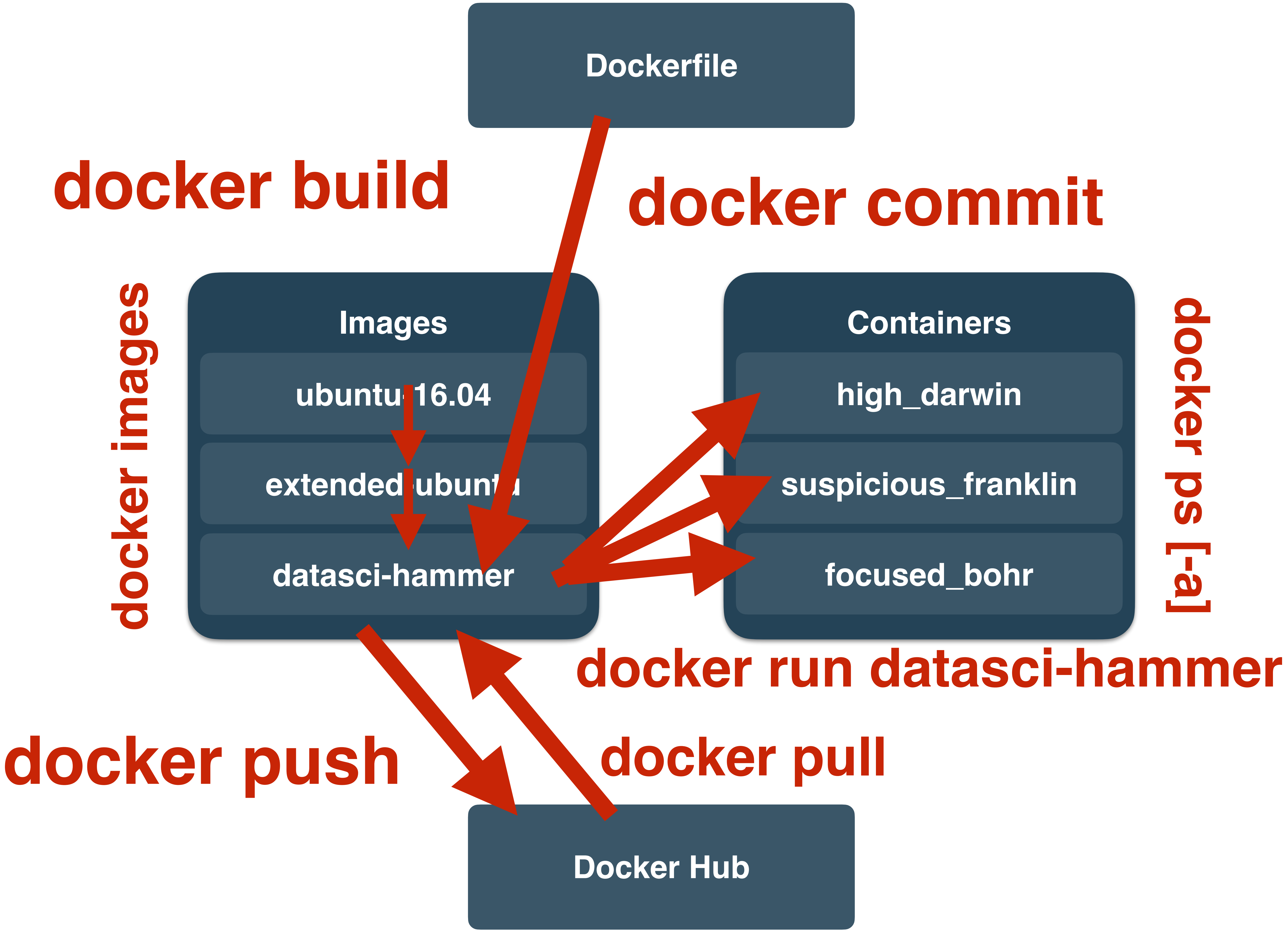
Docker Hub



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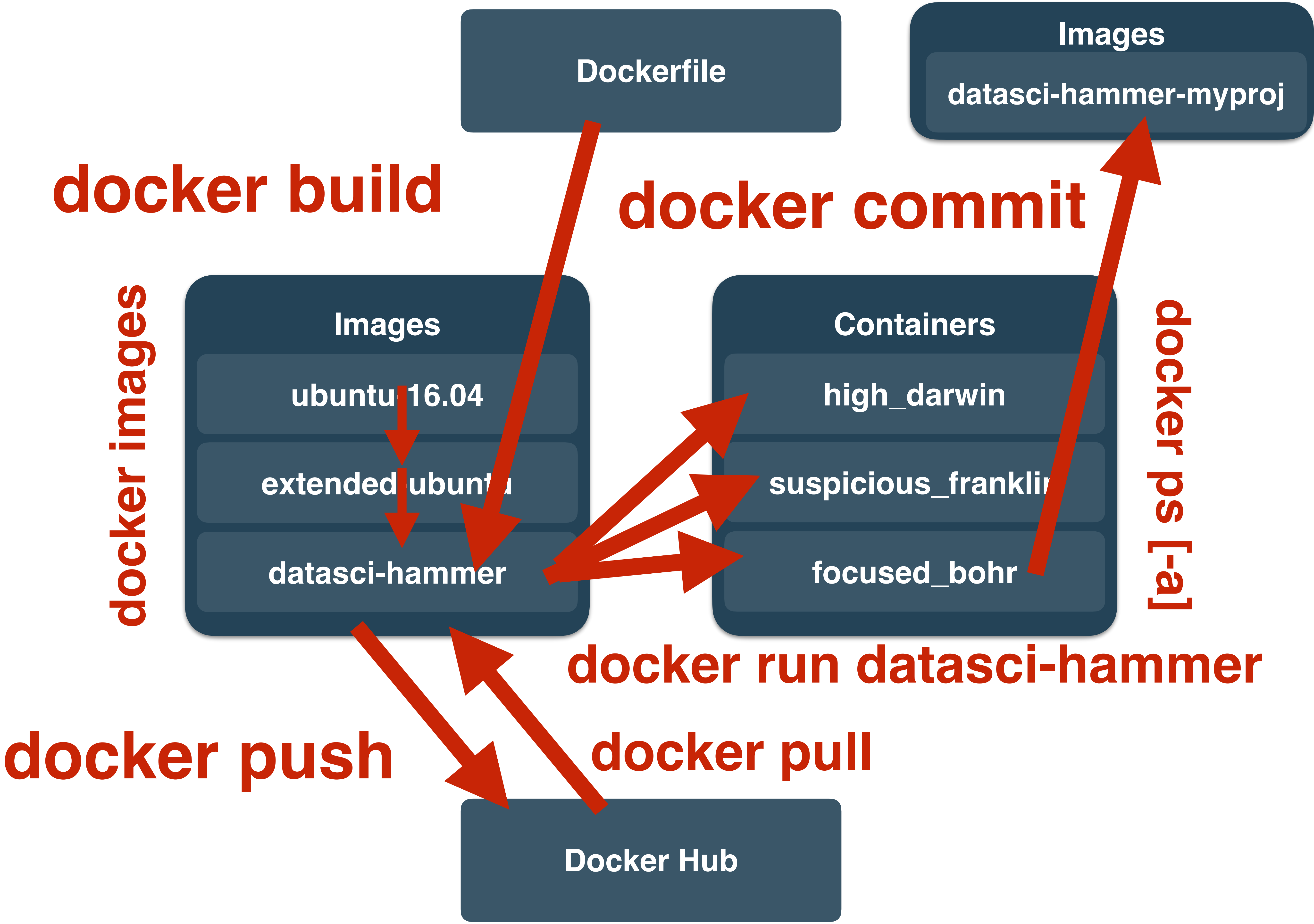
docker ps [-a]

docker run datasci-hammer

docker push

docker pull

Docker Hub



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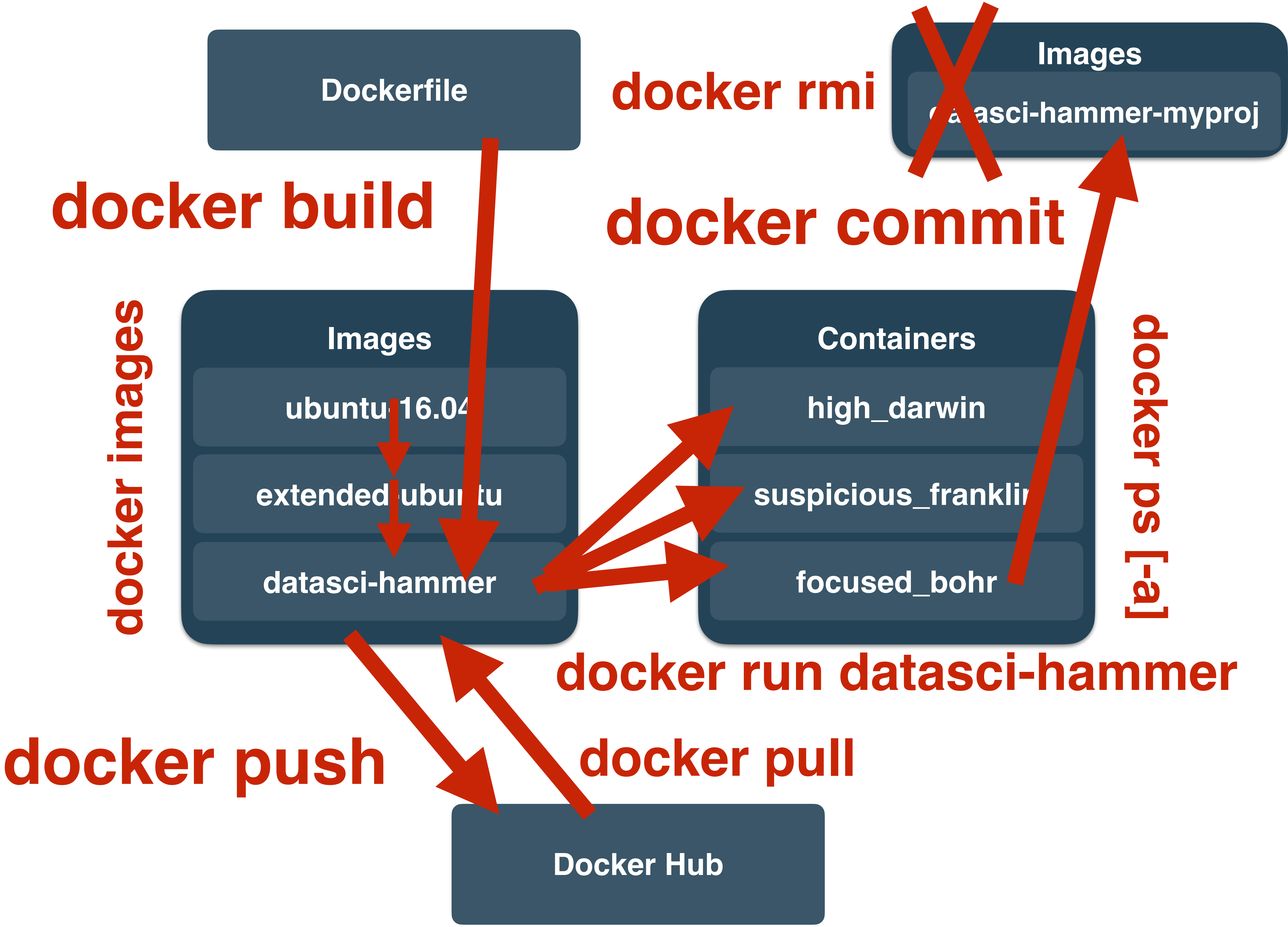

Dockerfile

docker rmi

Images

datasci-hammer-myproj

docker build

docker commit

docker images

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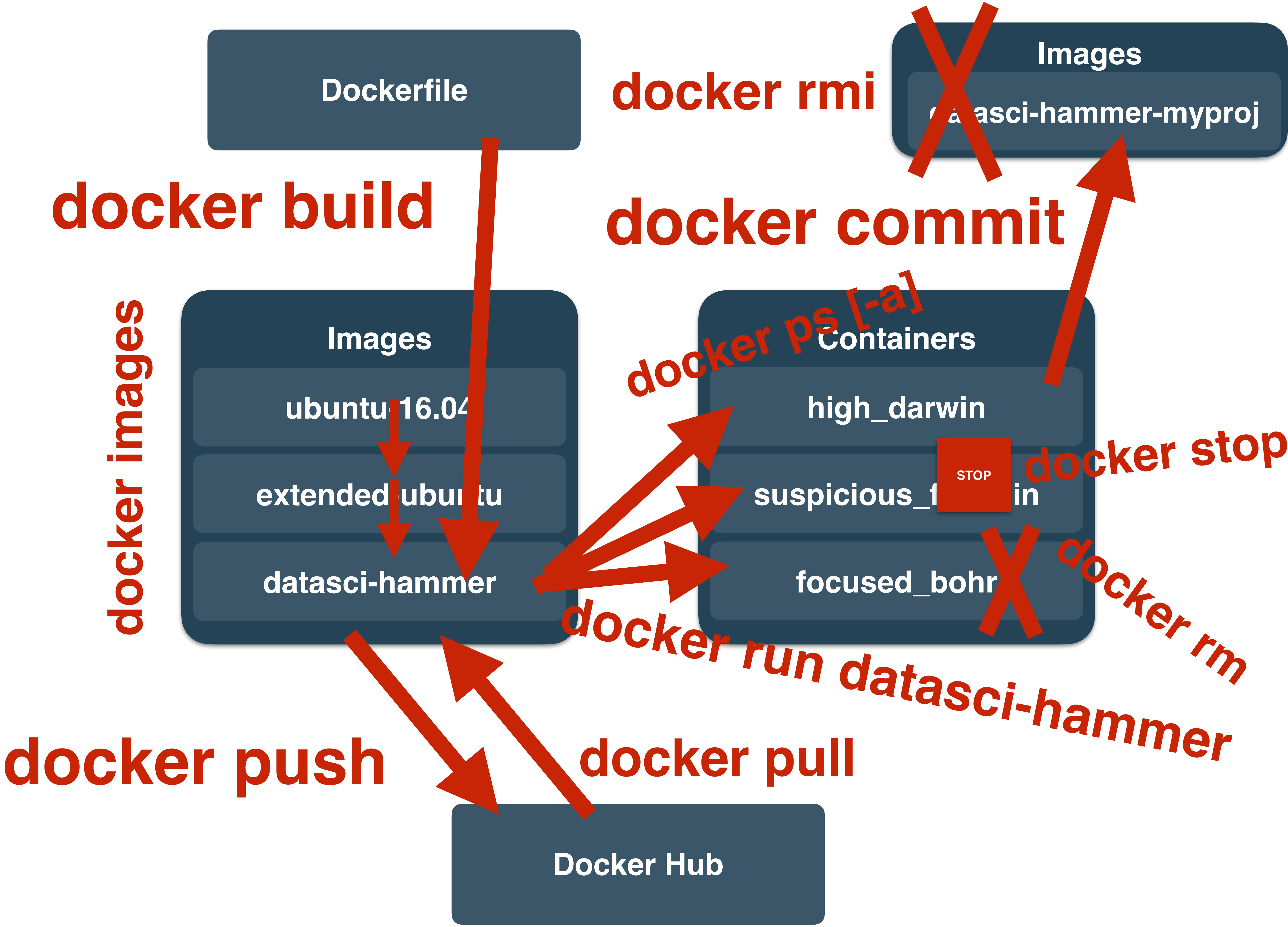

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datasci-hammer

docker ps [-a]

Containers

high_darwin

suspicious_f in

STOP

docker stop

focused_bohr

docker rm

docker run datasci-hammer

docker push

docker pull

Docker Hub

How

How to use Docker

In three steps:

1. Build or pull an image.
2. Run a container.
3. Execute code against container.

Build or pull an image

- Pull: easy!
  - This happens automatically with `docker run` or `docker build`
  - `docker pull andyreagan:datasci-hammer-ubuntu`
  - `docker pull centos:latest`

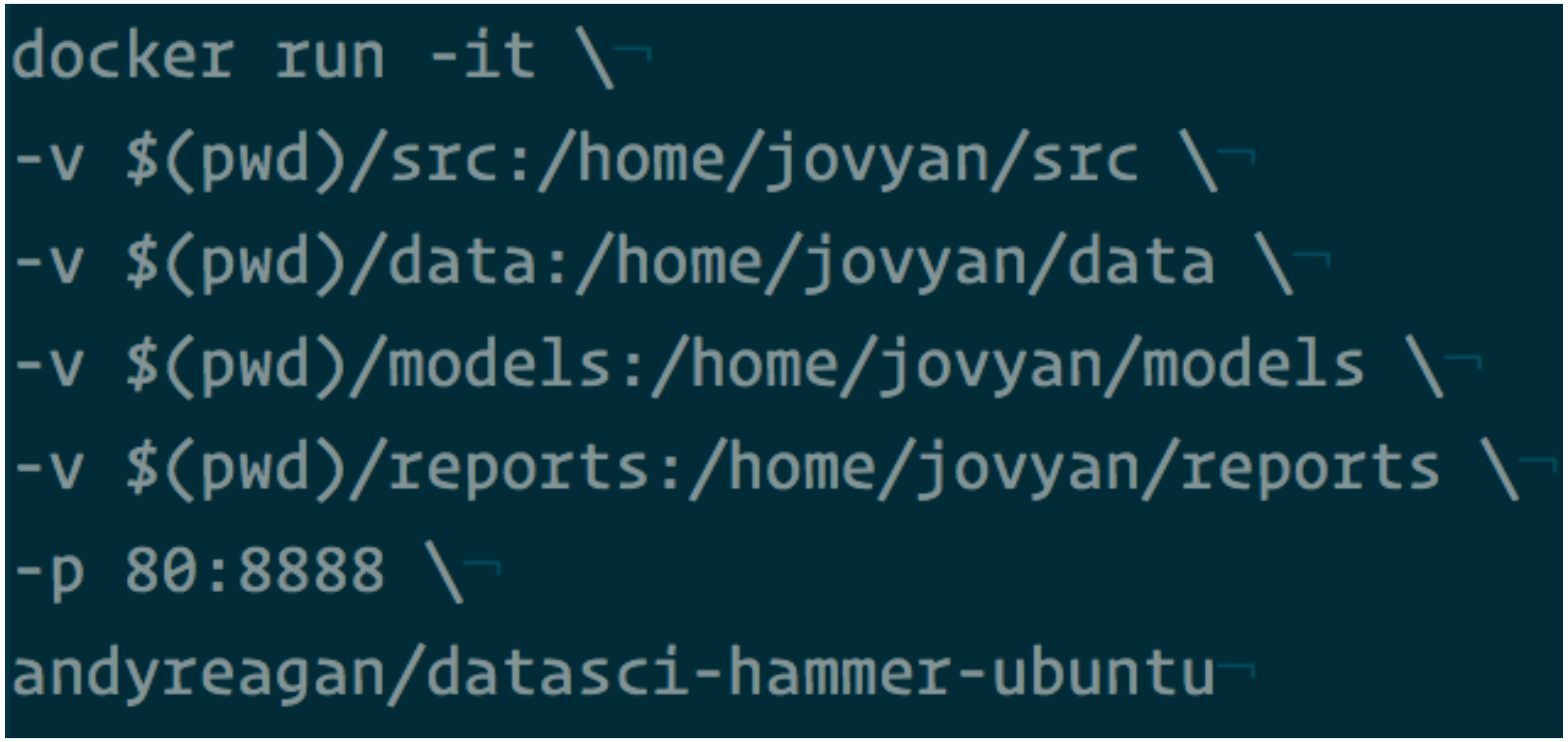
Build or pull an image

- Build: much more work
  - Dockerfile
    - Dockerfile language: RUN, COPY, USER, ADD, ENV...

Run a container

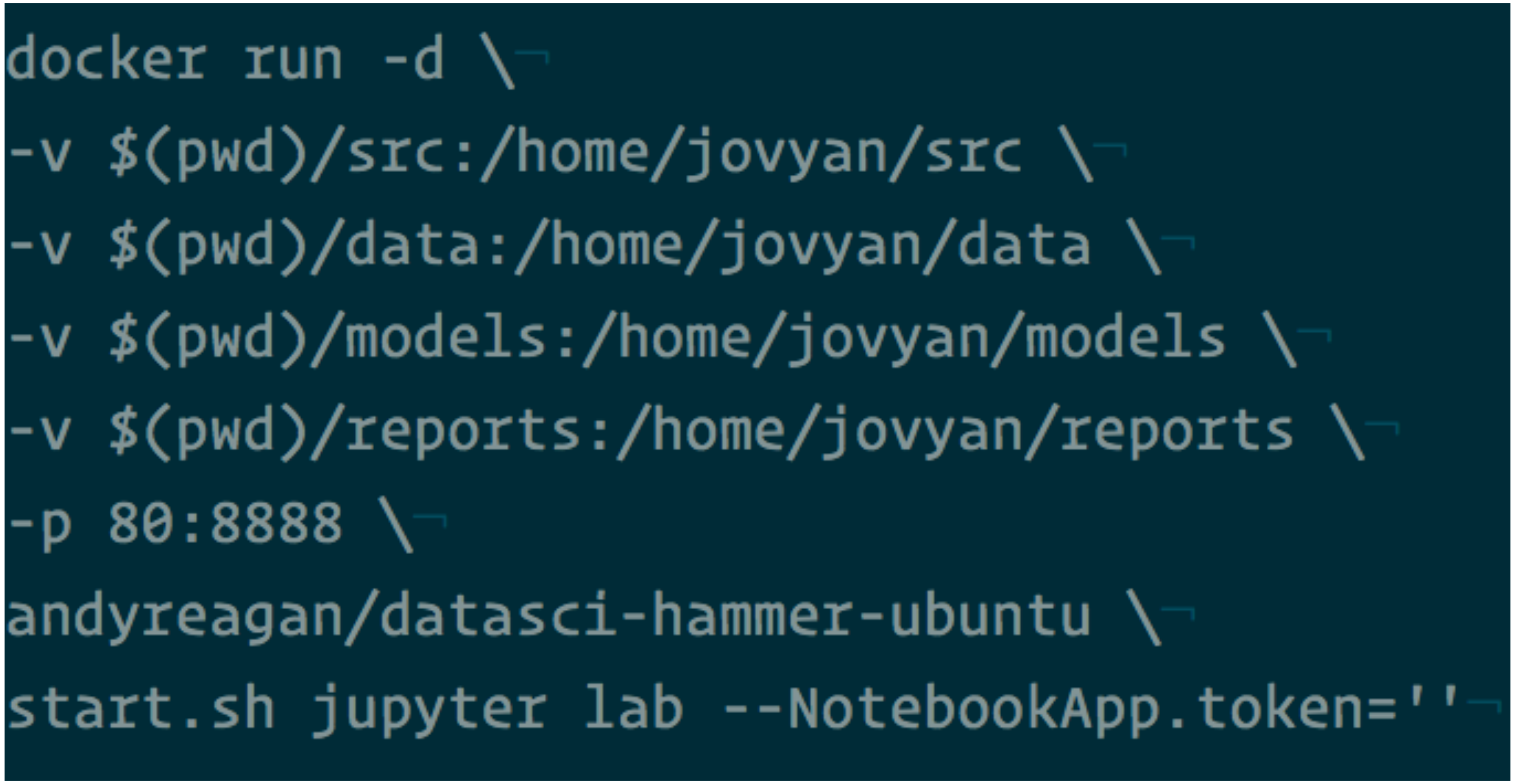
- Single command: `docker run`
- Many options
    - -d: daemon mode
    - -it: interactive mode
    - -v: mount volume
    - -p: map port
    - -e: pass env vars (I don't use this, but others might)

Run a container



```
docker run -it \
-v $(pwd)/src:/home/jovyan/src \
-v $(pwd)/data:/home/jovyan/data \
-v $(pwd)/models:/home/jovyan/models \
-v $(pwd)/reports:/home/jovyan/reports \
-p 80:8888 \
andyreagan/datasci-hammer-ubuntu
```

Run a container



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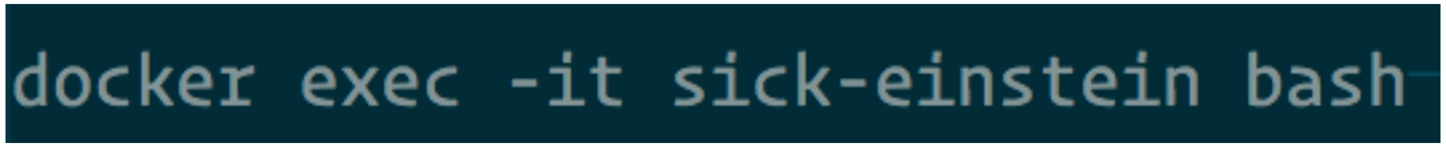
-v $(pwd)/data:/home/jovyan/data \
-v $(pwd)/models:/home/jovyan/models \
-v $(pwd)/reports:/home/jovyan/reports \
-p 80:8888 \
andyreagan/datasci-hammer-ubuntu \
start.sh jupyter lab --NotebookApp.token=''
```

Reconnect



```
docker exec -it sick-einstein bash
```

Execute code!

As you wish!

Performance of Docker

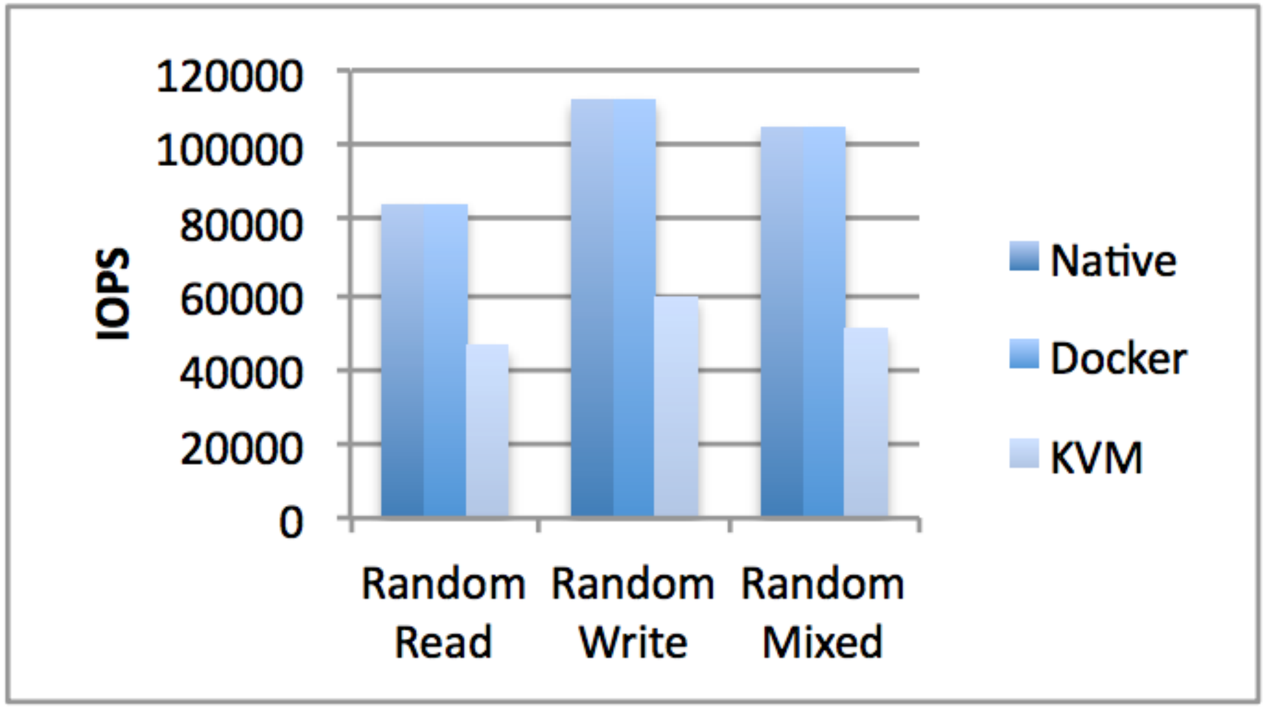


Fig. 6. Random I/O throughput (IOPS).

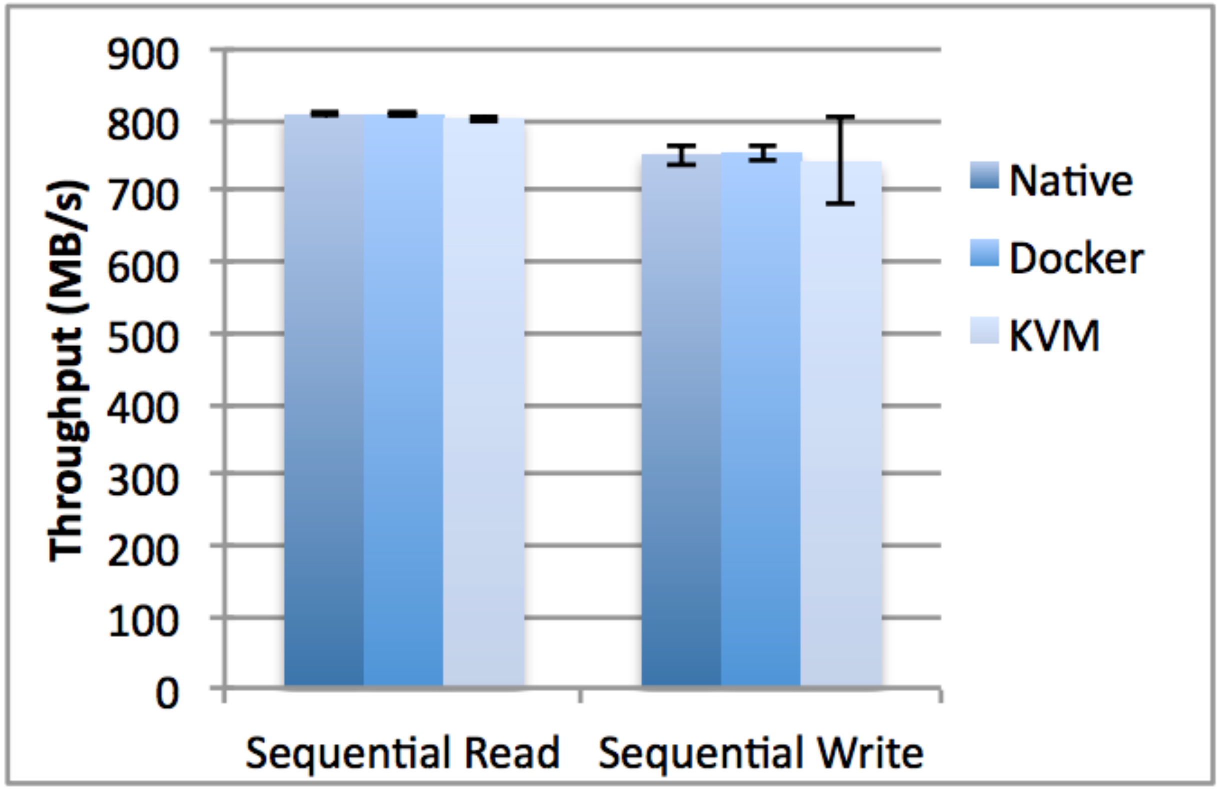


Fig. 5. Sequential I/O throughput (MB/s).

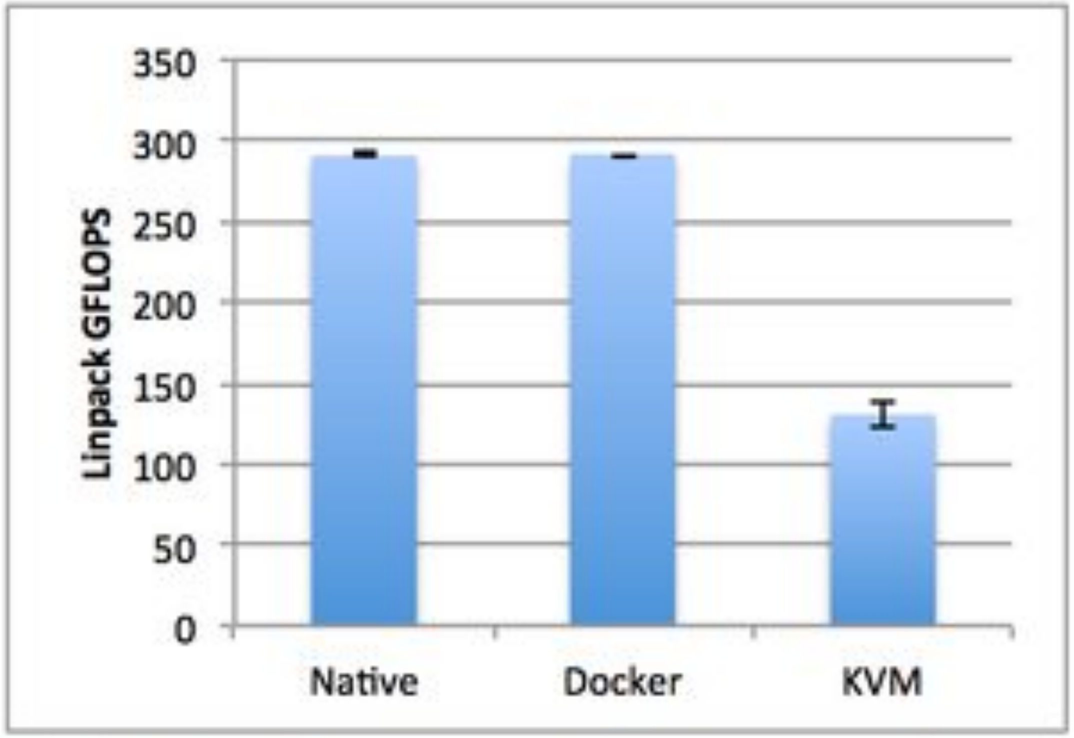


Figure 1. Linpack performance on two sockets (16 cores). Each data point is the arithmetic mean obtained from ten runs. Error bars indicate the standard deviation obtained over all runs.

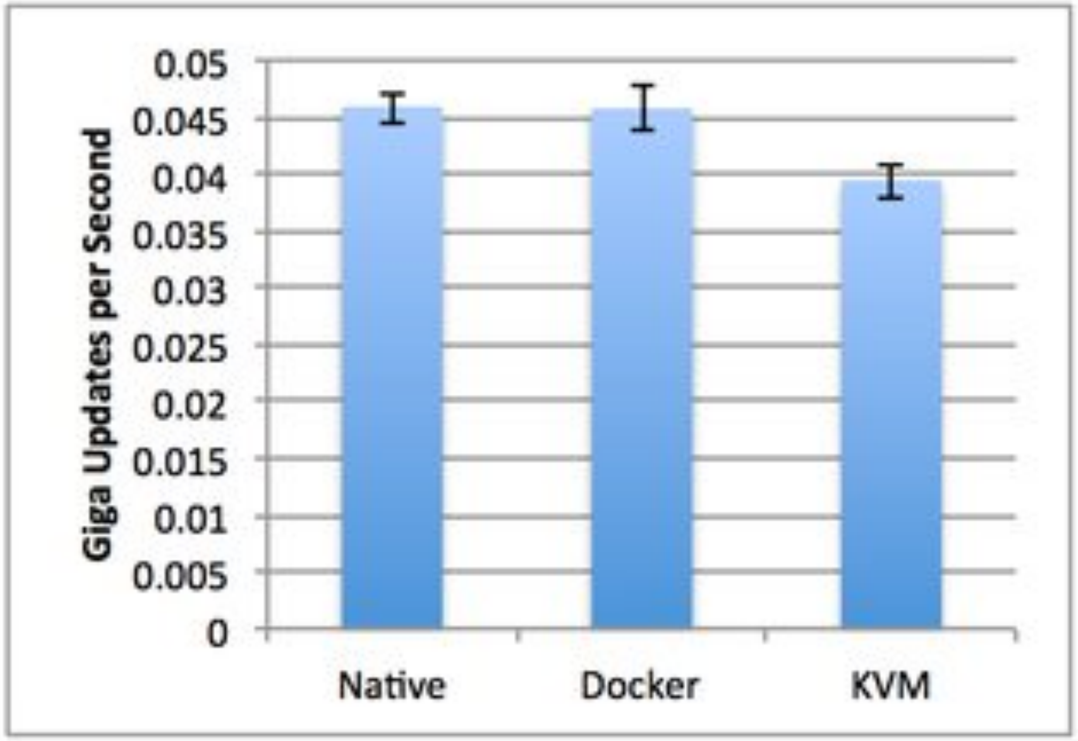


Figure 4. RandomAccess performance on a single socket (8 cores). Each data point is the arithmetic mean obtained from ten runs. Error bars indicate the standard deviation obtained over all runs.

Did we solve these problems?
You tell me!

- Reproducibility.
- Scalable computational backend.
- Persistent computational environment.
- Shared dependency management.
- Lack of appropriate permissions on a server.