Scaling

Machine Learning

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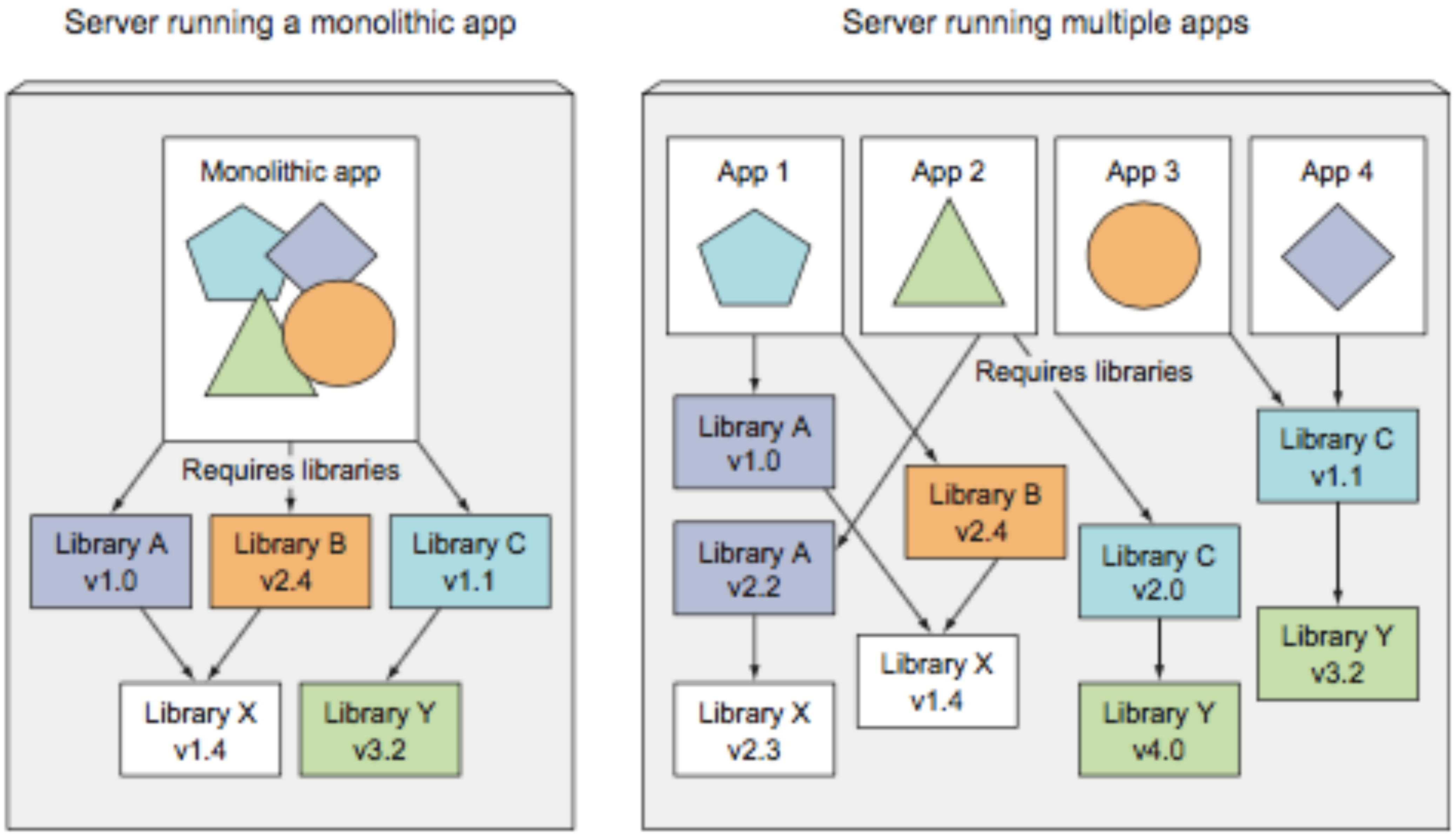
What is scaling?

- Running experiments reproducibly, and keeping track
- Running in parallel, for speed and resilience
- Dealing with large data sets
- Grid or other Hyper-parameter optimization
- optimizing Gradient Descent

Running Experiments

The multiple libraries problem



Conda

- create a conda environment for each new project
- put an `environment.yml` in each project folder
- at least have one for each new class, or class of projects
- envoronment for class of projects may grow organically, but capture its requirements from time-to-time.

see here

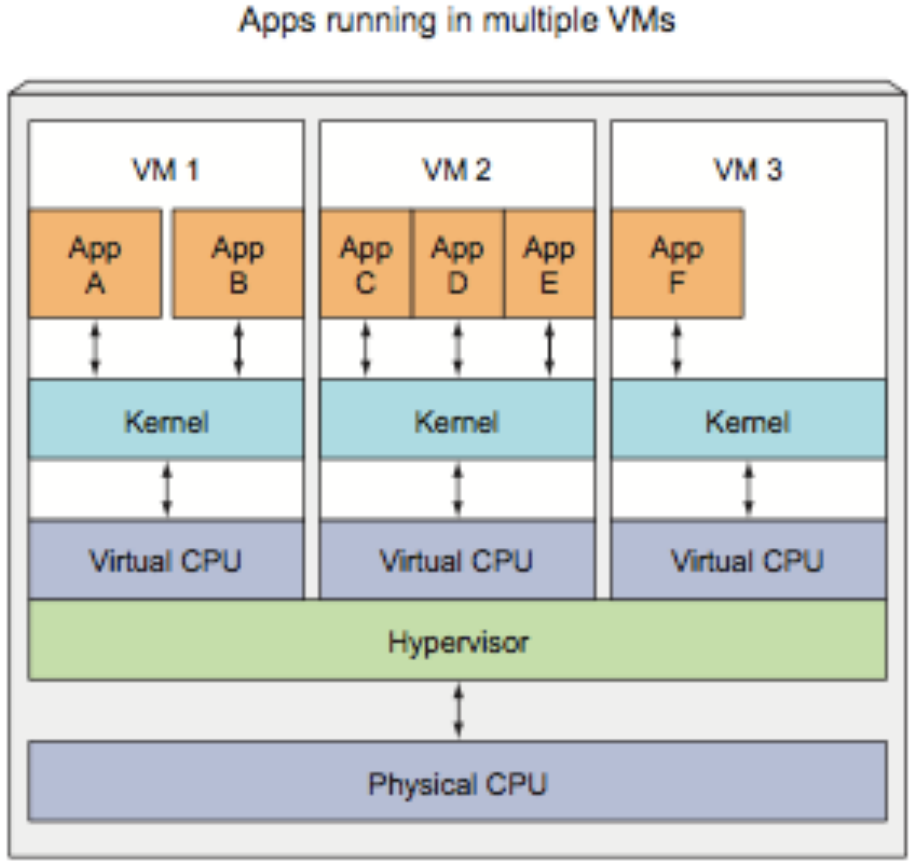
```yaml
# file name: environment.yml

# Give your project an informative name
name: project-name

# Specify the conda channels that you wish to grab packages from, in order of priority.
channels:
- defaults
- conda-forge

# Specify the packages that you would like to install inside your environment.
#Version numbers are allowed, and conda will automatically use its dependency
#solver to ensure that all packages work with one another.
dependencies:
- python=3.7
- conda
- scipy
- numpy
- pandas
- scikit-learn

# There are some packages which are not conda-installable. You can put the pip dependencies here instead.
- pip:
    - tqdm  # for example only, tqdm is actually available by conda.
```

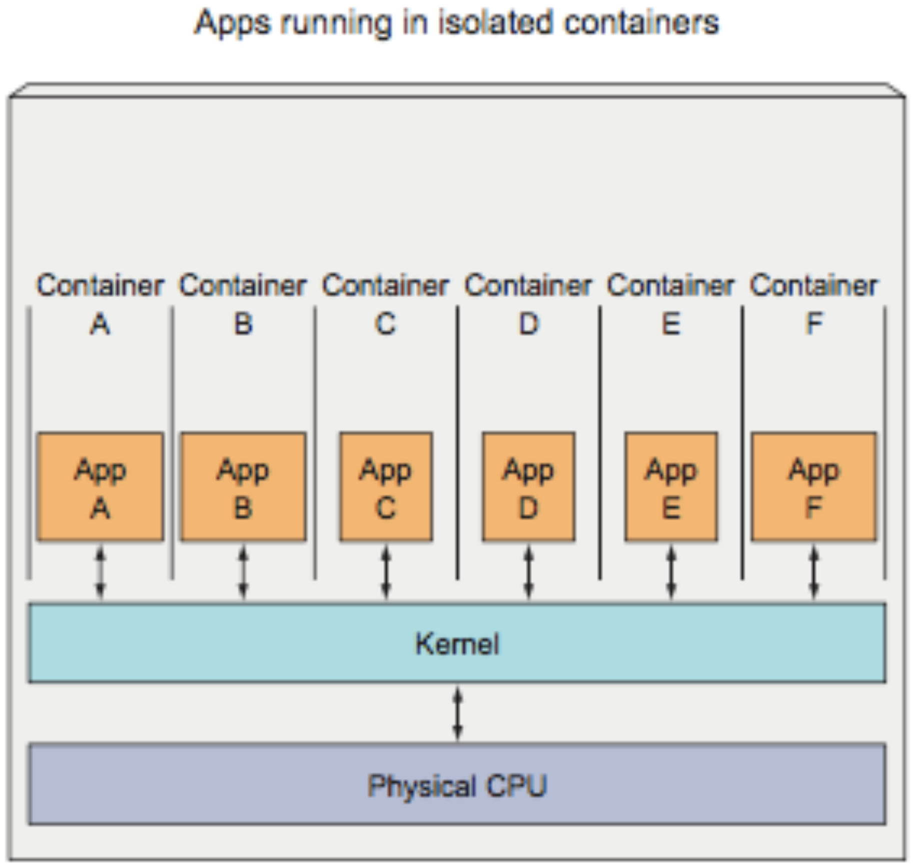
(from http://ericmjl.com/blog/2018/12/25/conda-hacks-for-data-science-efficiency/)

- `conda create --name environment-name [python=3.6]`
- `source[conda] activate environment-name` or project-name in the 1 environment per project paradigm
- `conda env create` in project folder
- `conda install <packagename>`
- or add the package to spec file, type `conda env update environment.yml` in appropriate folder
- `conda env export > environment.yml`

Docker

More than python libs

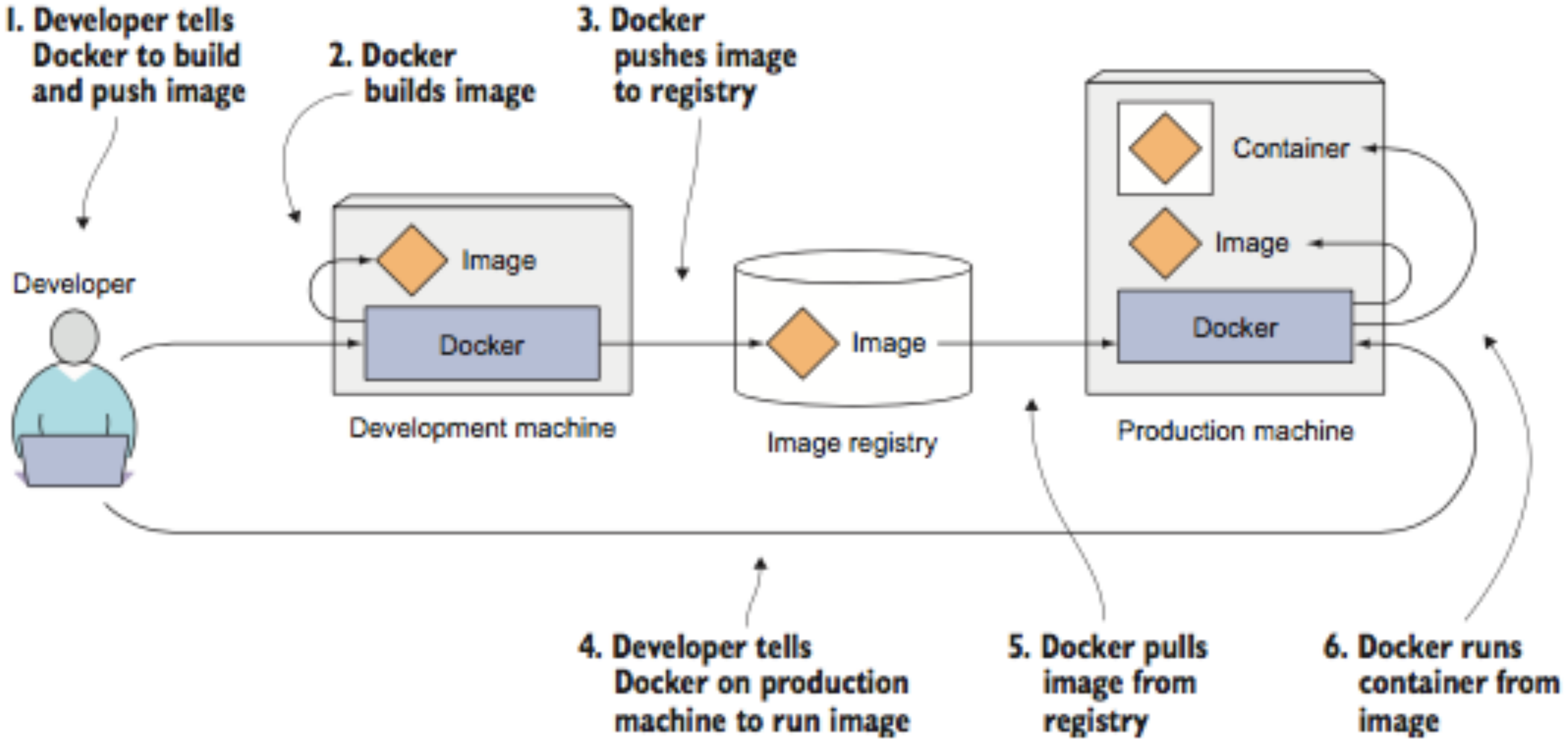




Containers vs Virtual Machines

- VMs meed an OS level "hypervisor"
- are more general, but more resource hungry
- containers provide process isolation, process throttling
- but work at library and kernel level, and can access hardware more easily
- hardware access important for gpu access
- containers can run on VMS, this is how docker runs on mac

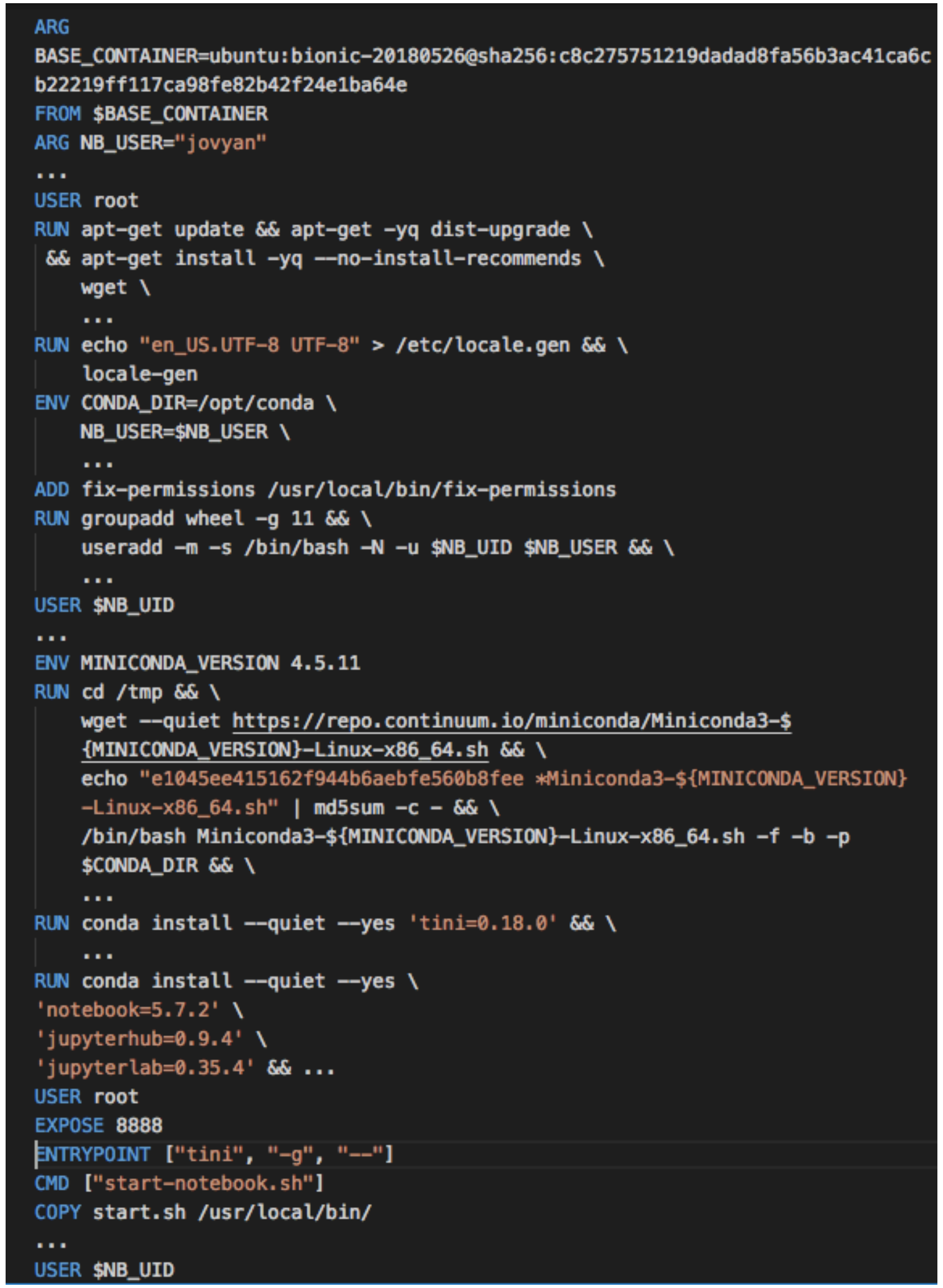
Docker Architecture


1. Developer tells Docker to build and push image
2. Docker builds image
3. Docker pushes image to registry
Developer
Image
Docker
Development machine
Image
Image registry
Container
Image
Docker
Production machine
4. Developer tells Docker on production machine to run image
5. Docker pulls image from registry
6. Docker runs container from image

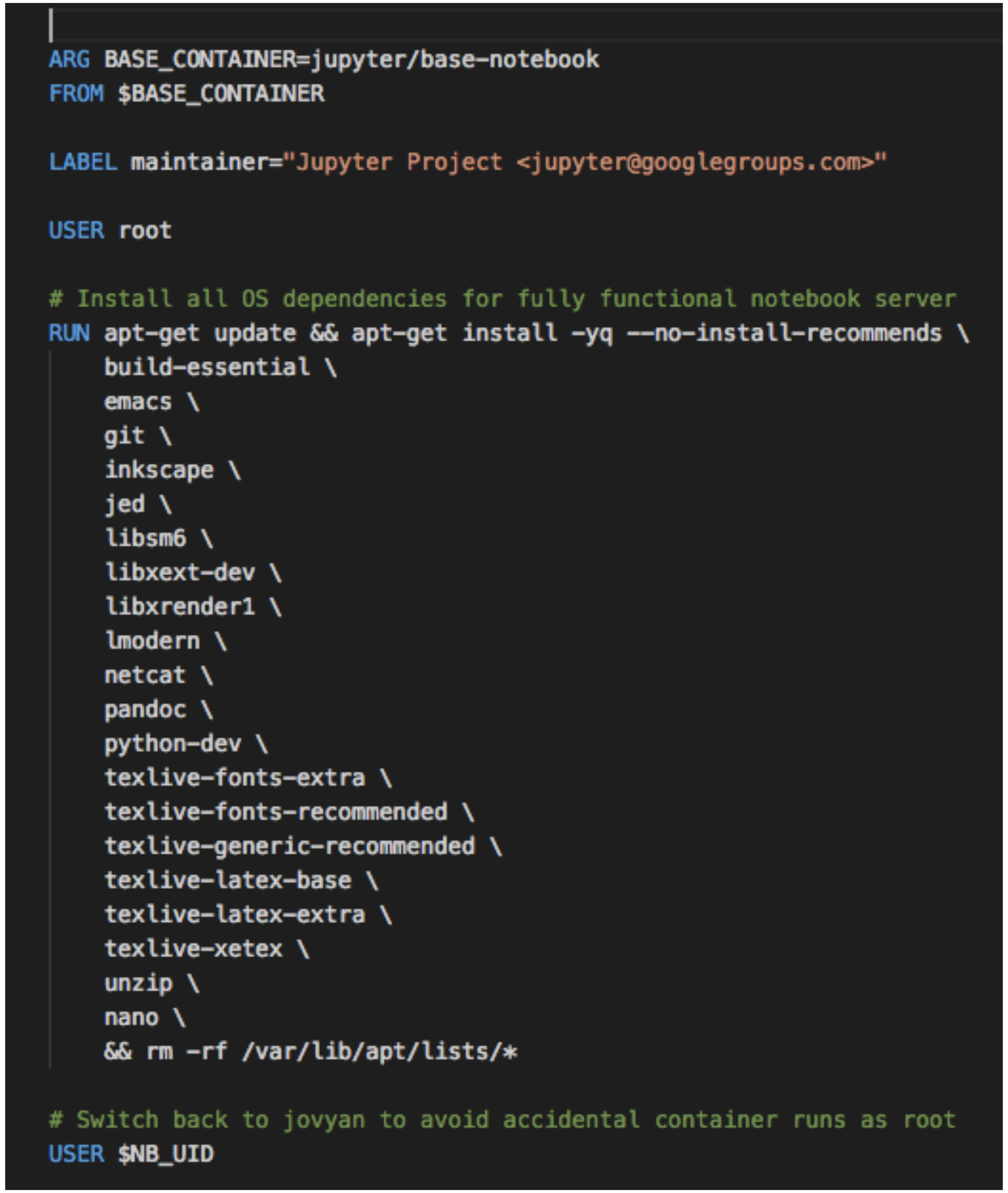
Docker images

- docker is linux only, but other OS's now have support
- allow for environment setting across languages and runtimes
- can be chained together to create outcomes
- base image is a linux (full) image, others are just layers on top

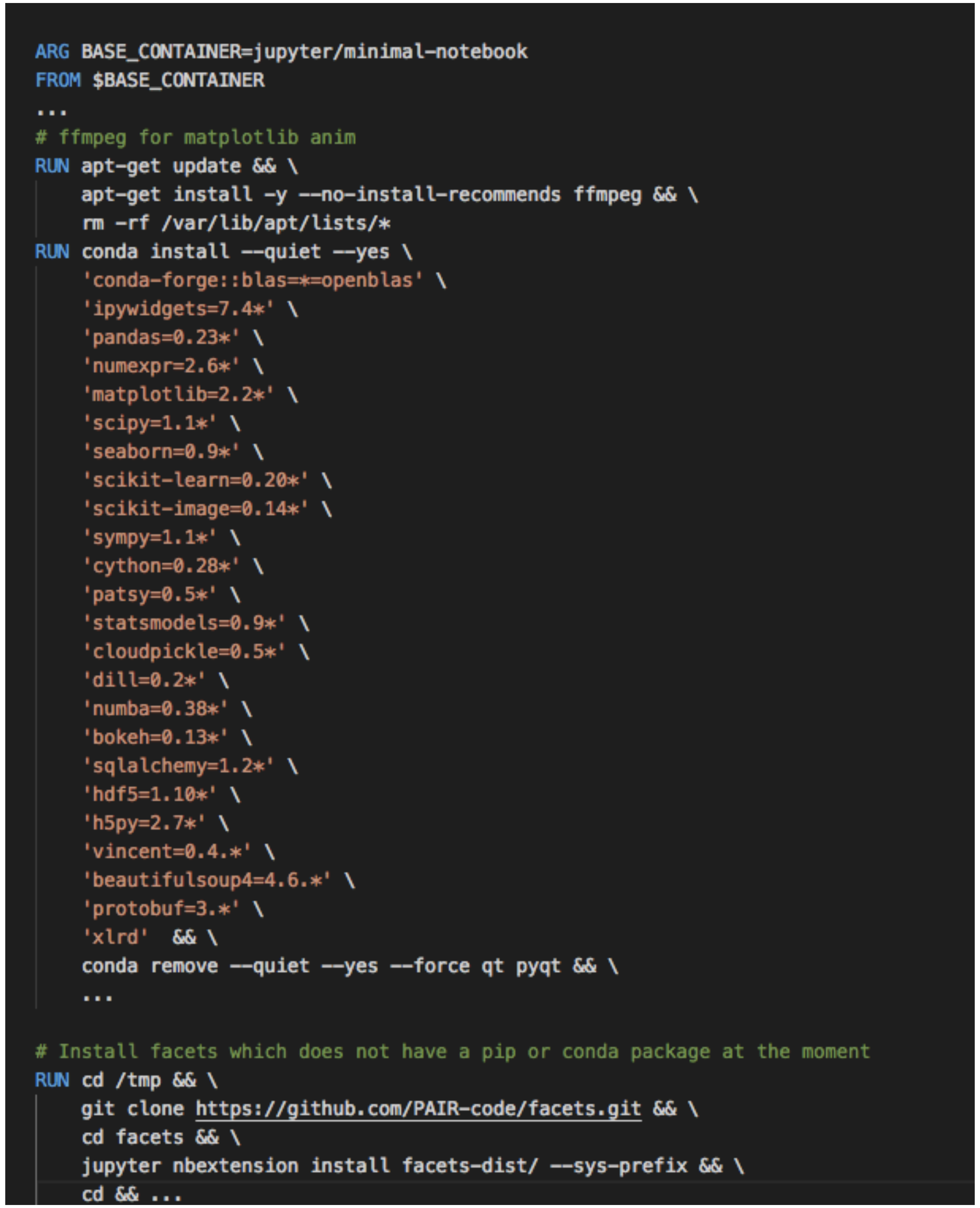
Example: base notebook -> minimal notebook -> scipy notebook -> tensorflow notebook



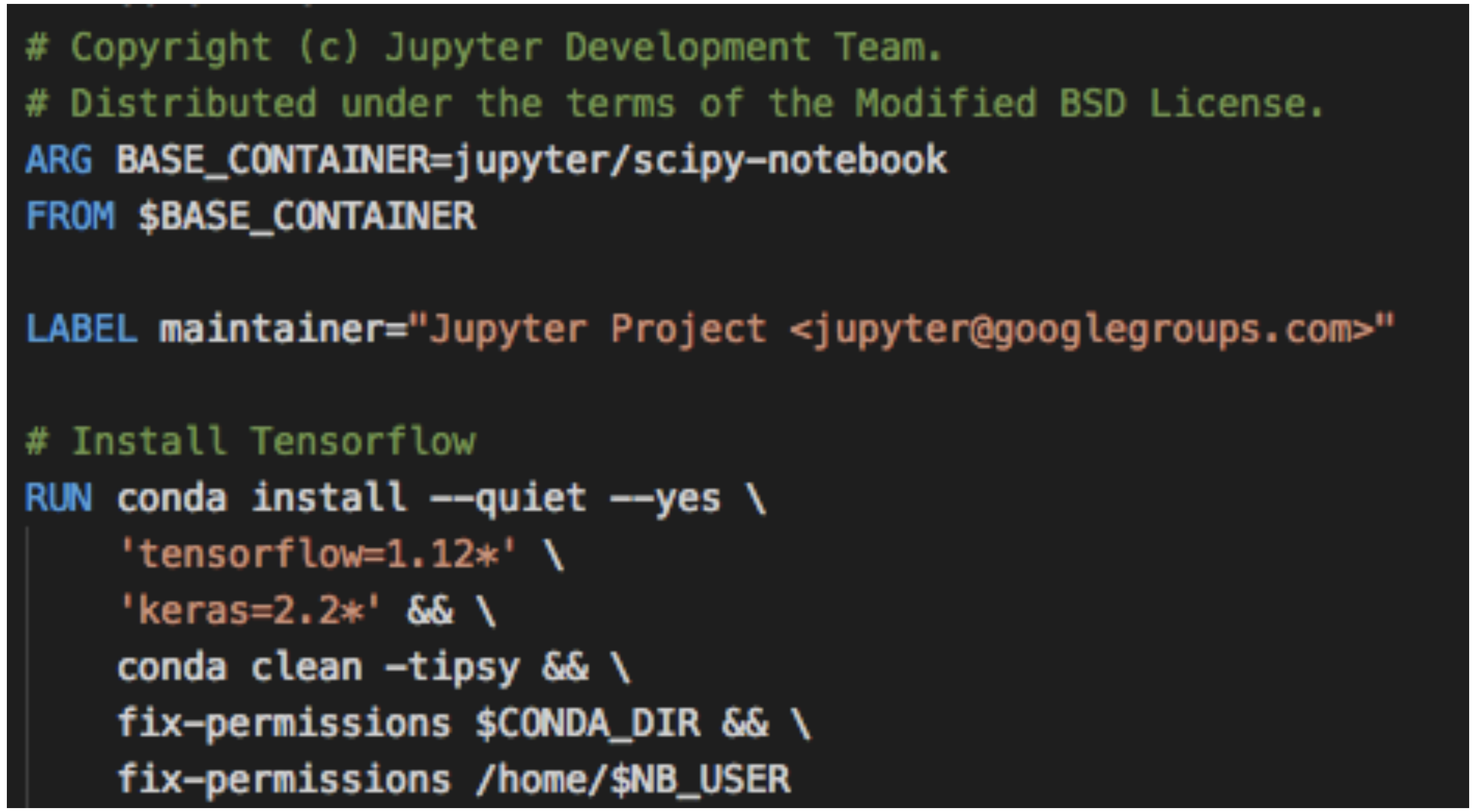
```
ARG
BASE_CONTAINER=ubuntu:bionic-20180526@sha256:c8c275751219dadad8fa56b3ac41ca6c
b22219ff117ca98fe82b42f24e1ba64e
FROM $BASE_CONTAINER
ARG NB_USER="jovyan"
...
USER root
RUN apt-get update && apt-get -yq dist-upgrade \
 && apt-get install -yq --no-install-recommends \
    wget \
    ...
RUN echo "en_US.UTF-8 UTF-8" > /etc/locale.gen && \
    locale-gen
ENV CONDA_DIR=/opt/conda \
    NB_USER=$NB_USER \
    ...
ADD fix-permissions /usr/local/bin/fix-permissions
RUN groupadd wheel -g 11 && \
    useradd -m -s /bin/bash -N -u $NB_UID $NB_USER && \
    ...
USER $NB_UID
...
ENV MINICONDA_VERSION 4.5.11
RUN cd /tmp && \
    wget --quiet https://repo.continuum.io/miniconda/Miniconda3-$
    {MINICONDA_VERSION}-Linux-x86_64.sh && \
    echo "e1045ee415162f944b6aebfe560b8fee *Miniconda3-${MINICONDA_VERSION}
    -Linux-x86_64.sh" | md5sum -c - && \
    /bin/bash Miniconda3-${MINICONDA_VERSION}-Linux-x86_64.sh -f -b -p
    $CONDA_DIR && \
    ...
RUN conda install --quiet --yes 'tini=0.18.0' && \
    ...
RUN conda install --quiet --yes \
'notebook=5.7.2' \
'jupyterhub=0.9.4' \
'jupyterlab=0.35.4' && ...
USER root
EXPOSE 8888
ENTRYPOINT ["tini", "-g", "--"]
CMD ["start-notebook.sh"]
COPY start.sh /usr/local/bin/
...
USER $NB_UID
```



```
ARG BASE_CONTAINER=jupyter/base-notebook
FROM $BASE_CONTAINER

LABEL maintainer="Jupyter Project <jupyter@googlegroups.com>"

USER root

# Install all OS dependencies for fully functional notebook server
RUN apt-get update && apt-get install -yq --no-install-recommends \
    build-essential \
    emacs \
    git \
    inkscape \
    jed \
    libsm6 \
    libxext-dev \
    libxrender1 \
    lmodern \
    netcat \
    pandoc \
    python-dev \
    texlive-fonts-extra \
    texlive-fonts-recommended \
    texlive-generic-recommended \
    texlive-latex-base \
    texlive-latex-extra \
    texlive-xetex \
    unzip \
    nano \
    && rm -rf /var/lib/apt/lists/*

# Switch back to jovyan to avoid accidental container runs as root
USER $NB_UID
```



```
ARG BASE_CONTAINER=jupyter/minimal-notebook
FROM $BASE_CONTAINER
...
# ffmpeg for matplotlib anim
RUN apt-get update && \
    apt-get install -y --no-install-recommends ffmpeg && \
    rm -rf /var/lib/apt/lists/*
RUN conda install --quiet --yes \
    'conda-forge::blas=*=openblas' \
    'ipywidgets=7.4*' \
    'pandas=0.23*' \
    'numexpr=2.6*' \
    'matplotlib=2.2*' \
    'scipy=1.1*' \
    'seaborn=0.9*' \
    'scikit-learn=0.20*' \
    'scikit-image=0.14*' \
    'sympy=1.1*' \
    'cython=0.28*' \
    'patsy=0.5*' \
    'statsmodels=0.9*' \
    'cloudpickle=0.5*' \
    'dill=0.2*' \
    'numba=0.38*' \
    'bokeh=0.13*' \
    'sqlalchemy=1.2*' \
    'hdf5=1.10*' \
    'h5py=2.7*' \
    'vincent=0.4.*' \
    'beautifulsoup4=4.6.*' \
    'protobuf=3.*' \
    'xlrd'  && \
    conda remove --quiet --yes --force qt pyqt && \
    ...

# Install facets which does not have a pip or conda package at the moment
RUN cd /tmp && \
    git clone https://github.com/PAIR-code/facets.git && \
    cd facets && \
    jupyter nbextension install facets-dist/ --sys-prefix && \
    cd && ...
```



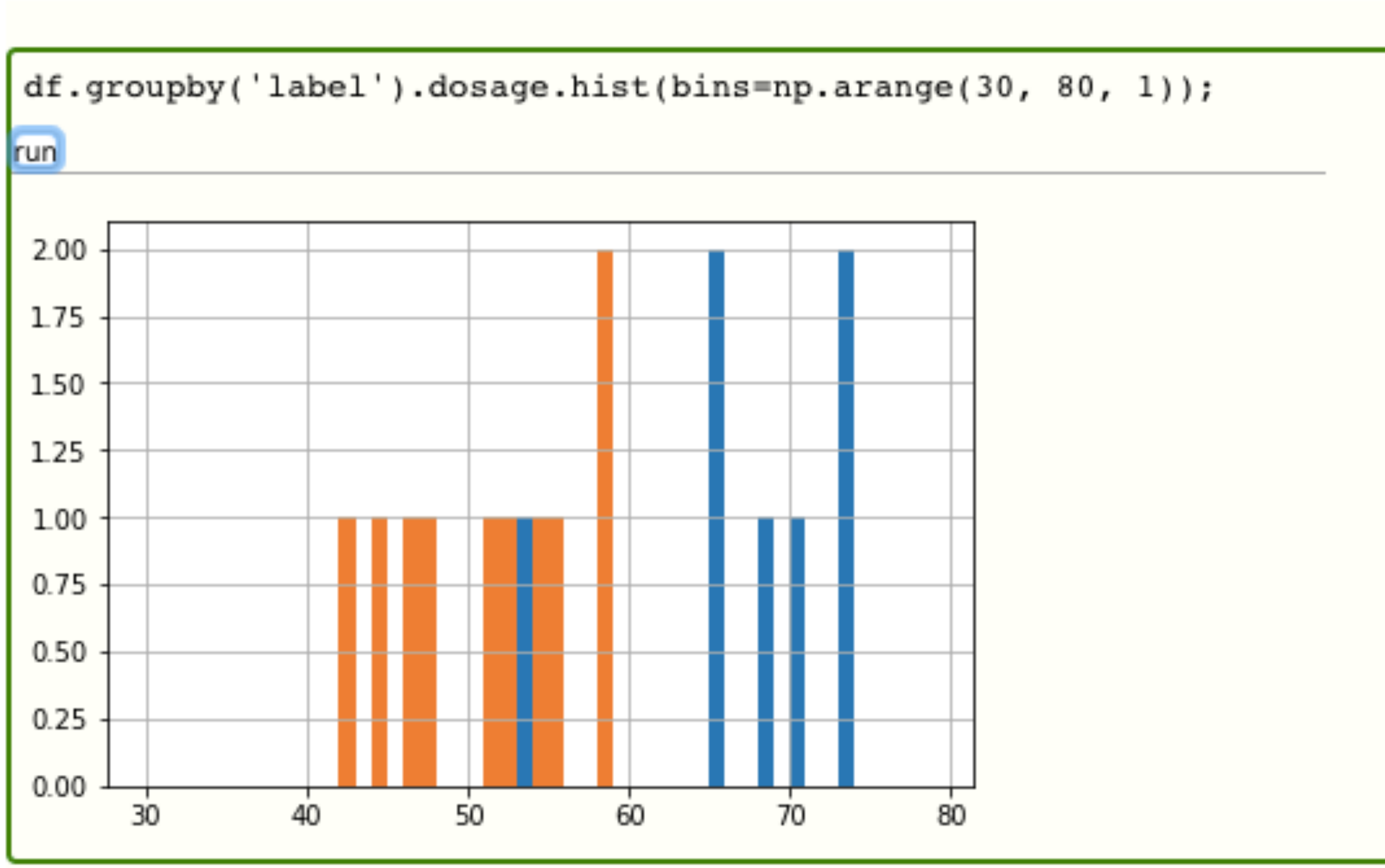
```
# Copyright (c) Jupyter Development Team.
# Distributed under the terms of the Modified BSD License.
ARG BASE_CONTAINER=jupyter/scipy-notebook
FROM $BASE_CONTAINER

LABEL maintainer="Jupyter Project <jupyter@googlegroups.com>"

# Install Tensorflow
RUN conda install --quiet --yes \
    'tensorflow=1.12*' \
    'keras=2.2*' && \
    conda clean -tipsy && \
    fix-permissions $CONDA_DIR && \
    fix-permissions /home/$NB_USER
```

repo2docker and binder

- building docker images is not dead simple
- the Jupyter folks created repo2docker for this.
- provide a github repo, and repo2docker makes a docker image and uploads it to the docker image repository for you
- binder builds on this to provide a service where you provide a github repo, and it gives you a working jupyterhub where you can "publish" your project/demo/etc

usage example: AM207 and thebe-lab

- see https://github.com/am207/shadowbinder , a repository with an environment file only
- this repo is used to build a jupyterlab with some requirements where you can work.
- see here for example
- uses thebelab



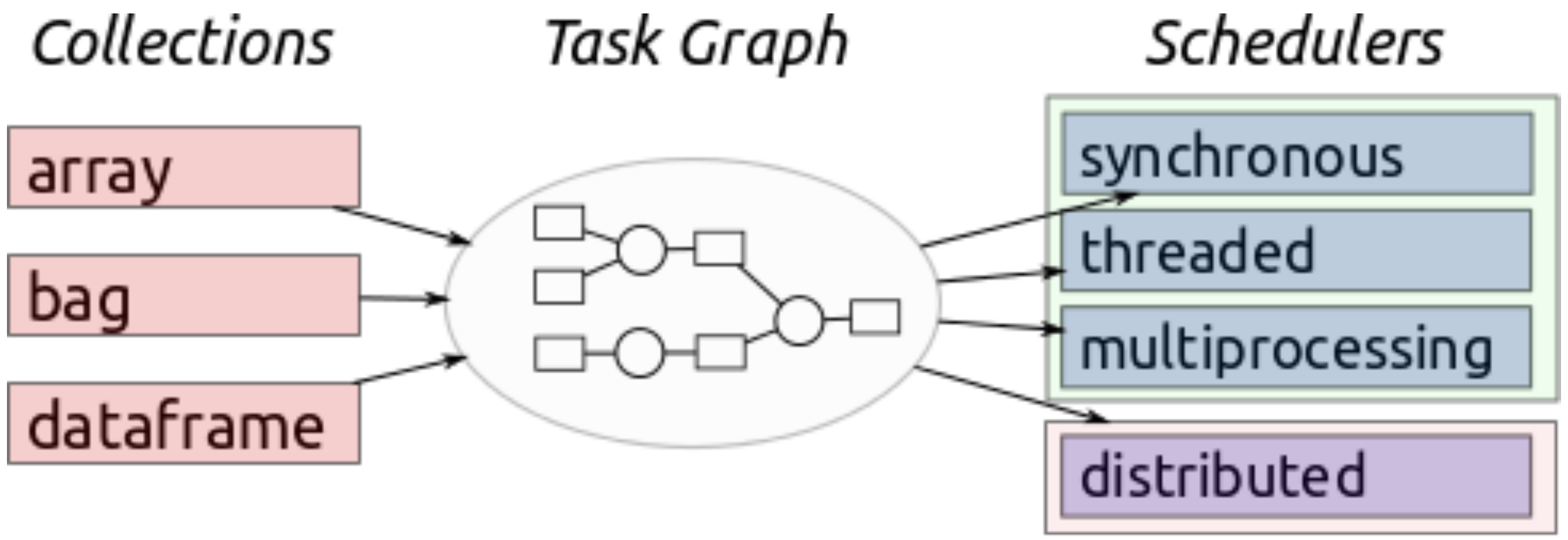
```
df.groupby('label').dosage.hist(bins=np.arange(30, 80, 1));
```

```
<script type="text/x-thebe-config">
      thebeConfig = {
        binderOptions: {
          repo: "AM207/shadowbinder",
        },
        kernelOptions: {
          name: "python3",
        },
        requestKernel: true
      }
    </script>
    <script src="/css/thebe_status_field.js" type="text/javascript"></script>
    <link rel="stylesheet" type="text/css" href="/css/thebe_status_field.css"/>
    <script>
      $(function() {
          var cellSelector = "pre.highlight code";

          if ($(cellSelector).length > 0) {
             $(' <span>|</span><span class="thebe_status_field"></span>')
                .appendTo('article p:first');
             thebe_place_activate_button();
          }
      });
    </script>
    <script>window.onload = function() { $("div.language-python pre.highlight code").attr("data-executable", "true")};</script>
```

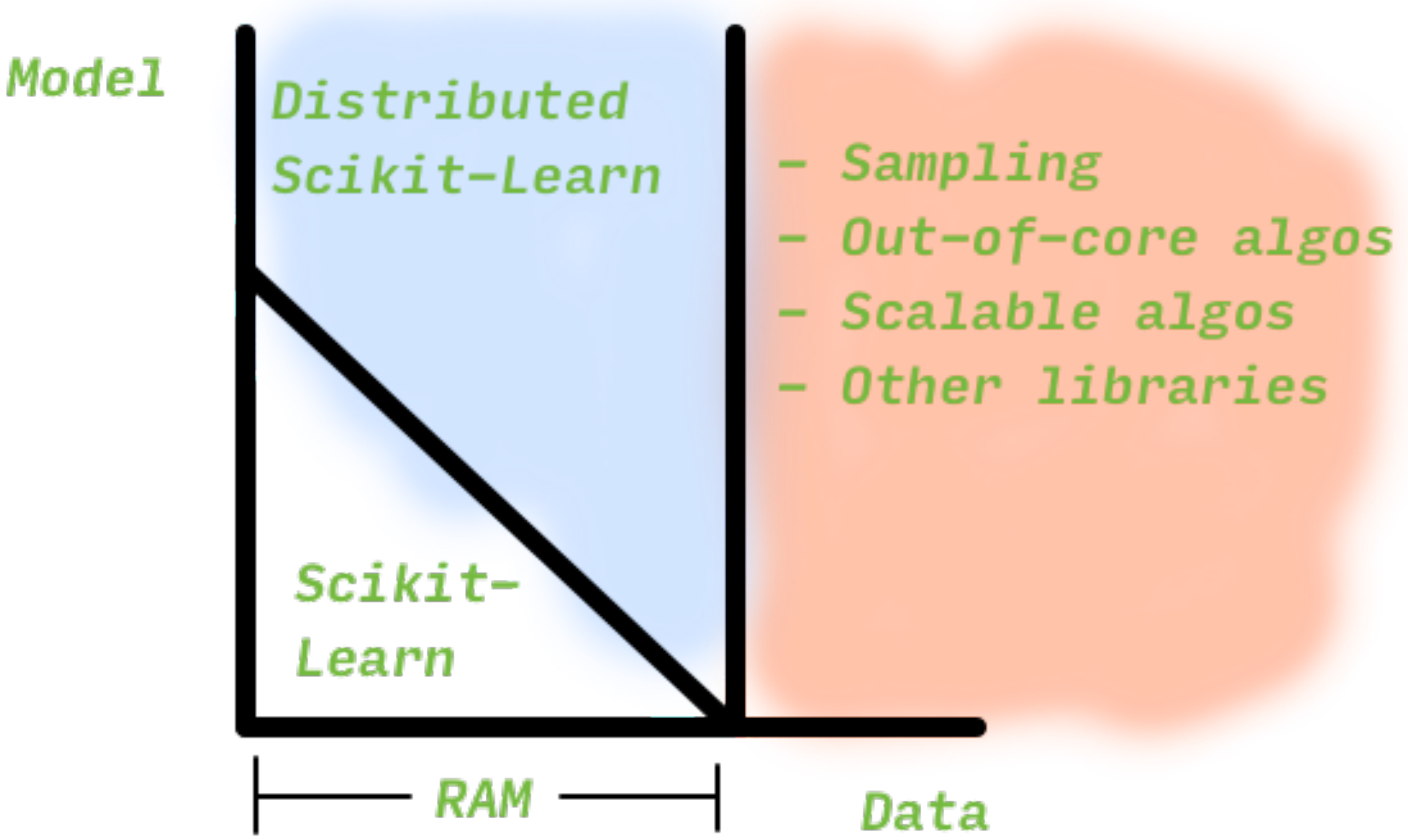
Dask

Running in parallel

Dask



- library for parallel computing in Python.
- 2 parts. Dynamic task scheduling optimized for computation like `Airflow`. “Big Data” collections like parallel (numpy) arrays, (pandas) dataframes, and lists
- scales up (1000 core cluster) and doqn (laptop)
- designed with interactive computing in mind, with web based diagnostics



(from https://github.com/TomAugspurger/dask-tutorial-pycon-2018)

Parallel Hyperparameter Optimization

Why is this bad?

```python
from sklearn.model_selection import GridSearchCV

vectorizer = TfidfVectorizer()
vectorizer.fit(text_train)

X_train = vectorizer.transform(text_train)
X_test = vectorizer.transform(text_test)

clf = LogisticRegression()
grid = GridSearchCV(clf, param_grid={'C': [.1, 1, 10, 100]}, cv=5)
grid.fit(X_train, y_train)
```

Grid search on pipelines

```python
from sklearn.feature_extraction.text import CountVectorizer, TfidfTransformer
from sklearn.linear_model import SGDClassifier
from sklearn.pipeline import Pipeline
from sklearn.model_selection import GridSearchCV
from sklearn.datasets import fetch_20newsgroups

categories = [
    'alt.atheism',
    'talk.religion.misc',
]
data = fetch_20newsgroups(subset='train', categories=categories)
pipeline = Pipeline([('vect', CountVectorizer()),
                     ('tfidf', TfidfTransformer()),
                     ('clf', SGDClassifier())])
grid = {'vect__ngram_range': [(1, 1)],
        'tfidf__norm': ['l1', 'l2'],
        'clf__alpha': [1e-3, 1e-4, 1e-5]}

if __name__=='__main__':
    grid_search = GridSearchCV(pipeline, grid, cv=5, n_jobs=-1)
    grid_search.fit(data.data, data.target)
    print("Best score: %0.3f" % grid_search.best_score_)
    print("Best parameters set:", grid_search.best_estimator_.get_params())
```

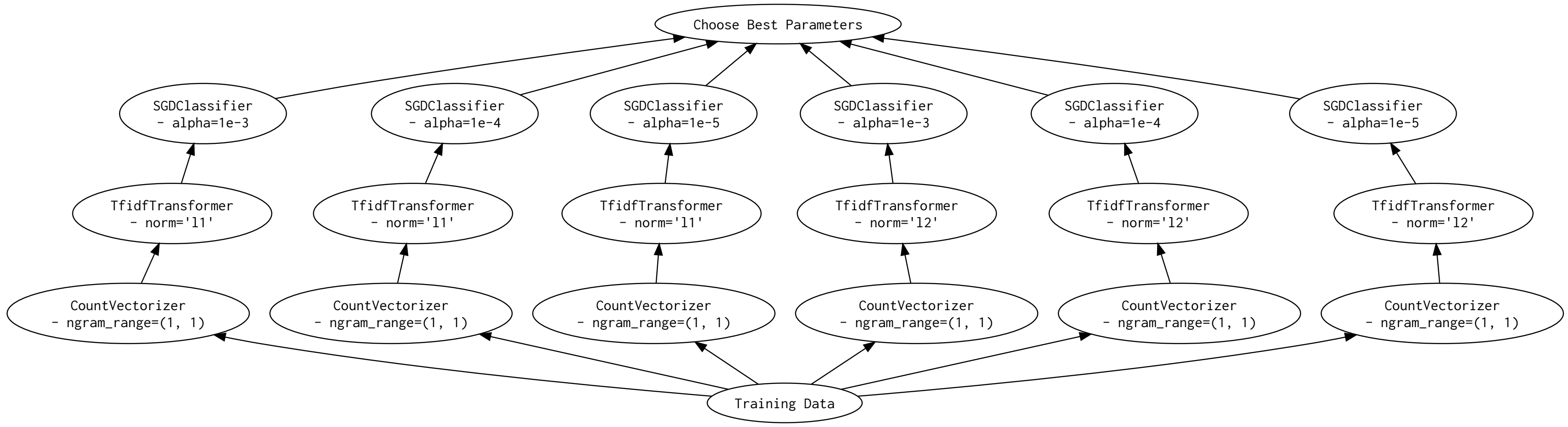
From sklearn.pipeline.Pipeline.html :

Sequentially apply a list of transforms and a final estimator. Intermediate steps of the pipeline must be 'transforms', that is, they must implement `fit` *and* `transform` *methods. The final estimator only needs to implement* `fit`*. The transformers in the pipeline can be cached using memory argument.*

The purpose of the pipeline is to assemble several steps that can be cross-validated together while setting different parameters.

sklearn pipelines: the bad

```
scores = []
for ngram_range in parameters['vect__ngram_range']:
    for norm in parameters['tfidf__norm']:
        for alpha in parameters['clf__alpha']:
            vect = CountVectorizer(ngram_range=ngram_range)
            X2 = vect.fit_transform(X, y)
            tfidf = TfidfTransformer(norm=norm)
            X3 = tfidf.fit_transform(X2, y)
            clf = SGDClassifier(alpha=alpha)
            clf.fit(X3, y)
            scores.append(clf.score(X3, y))
best = choose_best_parameters(scores, parameters)
```



Choose Best Parameters

SGDClassifier - alpha=1e-3

SGDClassifier - alpha=1e-4

SGDClassifier - alpha=1e-5

SGDClassifier - alpha=1e-3

SGDClassifier - alpha=1e-4

SGDClassifier - alpha=1e-5

TfidfTransformer - norm='l1'

TfidfTransformer - norm='l1'

TfidfTransformer - norm='l1'

TfidfTransformer - norm='l2'

TfidfTransformer - norm='l2'

TfidfTransformer - norm='l2'

CountVectorizer - ngram_range=(1, 1)

CountVectorizer - ngram_range=(1, 1)

CountVectorizer - ngram_range=(1, 1)

CountVectorizer - ngram_range=(1, 1)

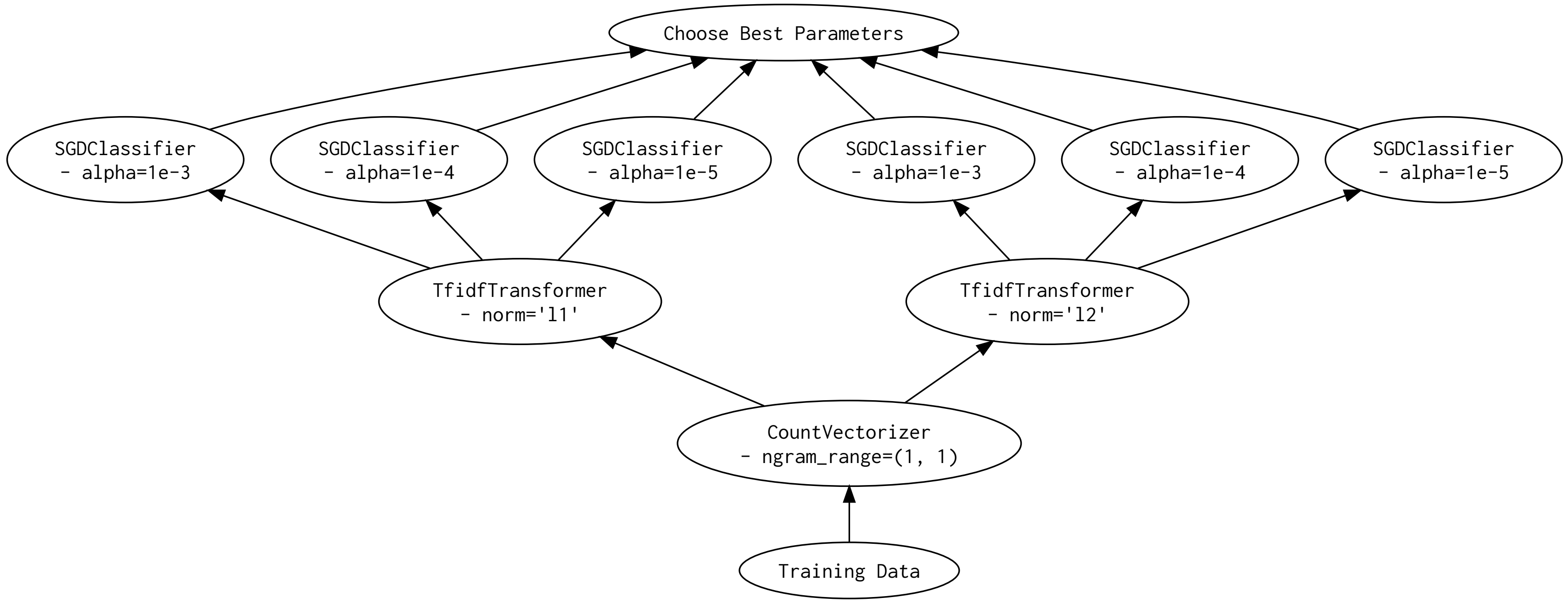
CountVectorizer - ngram_range=(1, 1)

CountVectorizer - ngram_range=(1, 1)

Training Data

dask pipelines: the good

```
scores = []
for ngram_range in parameters['vect__ngram_range']:
    vect = CountVectorizer(ngram_range=ngram_range)
    X2 = vect.fit_transform(X, y)
    for norm in parameters['tfidf__norm']:
        tfidf = TfidfTransformer(norm=norm)
        X3 = tfidf.fit_transform(X2, y)
        for alpha in parameters['clf__alpha']:
            clf = SGDClassifier(alpha=alpha)
            clf.fit(X3, y)
            scores.append(clf.score(X3, y))
best = choose_best_parameters(scores, parameters)
```


Choose Best Parameters
SGDClassifier - alpha=1e-3
SGDClassifier - alpha=1e-4
SGDClassifier - alpha=1e-5
SGDClassifier - alpha=1e-3
SGDClassifier - alpha=1e-4
SGDClassifier - alpha=1e-5
TfidfTransformer - norm='l1'
TfidfTransformer - norm='l2'
CountVectorizer - ngram_range=(1, 1)
Training Data

Now, lets parallelize

- for data that fits into memory, we simply copy the memory to each node and run the algorithm there

- if you have created a re-sizable cluster of parallel machines, `dask` can even dynamically send parameter combinations to more and more machines

- see PANGEO and Grisel for this

Hyperopt

```python
from keras.models import Sequential
from keras.layers import Dense
from keras.wrappers.scikit_learn import KerasClassifier
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
from dask_ml.model_selection import GridSearchCV
from dask.distributed import Client
from sklearn.externals import joblib

def simple_nn(hidden_neurons):
  model = Sequential()
  model.add(Dense(hidden_neurons, activation='relu', input_dim=30))
  model.add(Dense(1, activation='sigmoid'))
  model.compile(loss='binary_crossentropy', optimizer='rmsprop', metrics=['accuracy'])
  return model

param_grid = {'hidden_neurons': [100, 200, 300]}
if __name__=='__main__':
    client = Client()
    cv = GridSearchCV(KerasClassifier(build_fn=simple_nn, epochs=10), param_grid)
    X, y = load_breast_cancer(return_X_y=True)
    X_train, X_test, y_train, y_test = train_test_split(X, y)
    with joblib.parallel_backend("dask", scatter=[X_train, y_train]):
        cv.fit(X_train, y_train)
    print(f'Best Accuracy for {cv.best_score_:.4} using {cv.best_params_}')
    #score = cv.score(X_test, y_test)
    print('score = {} on train set with params={}.'.format(score, cv.best_params_))
```

Large

Data Sets

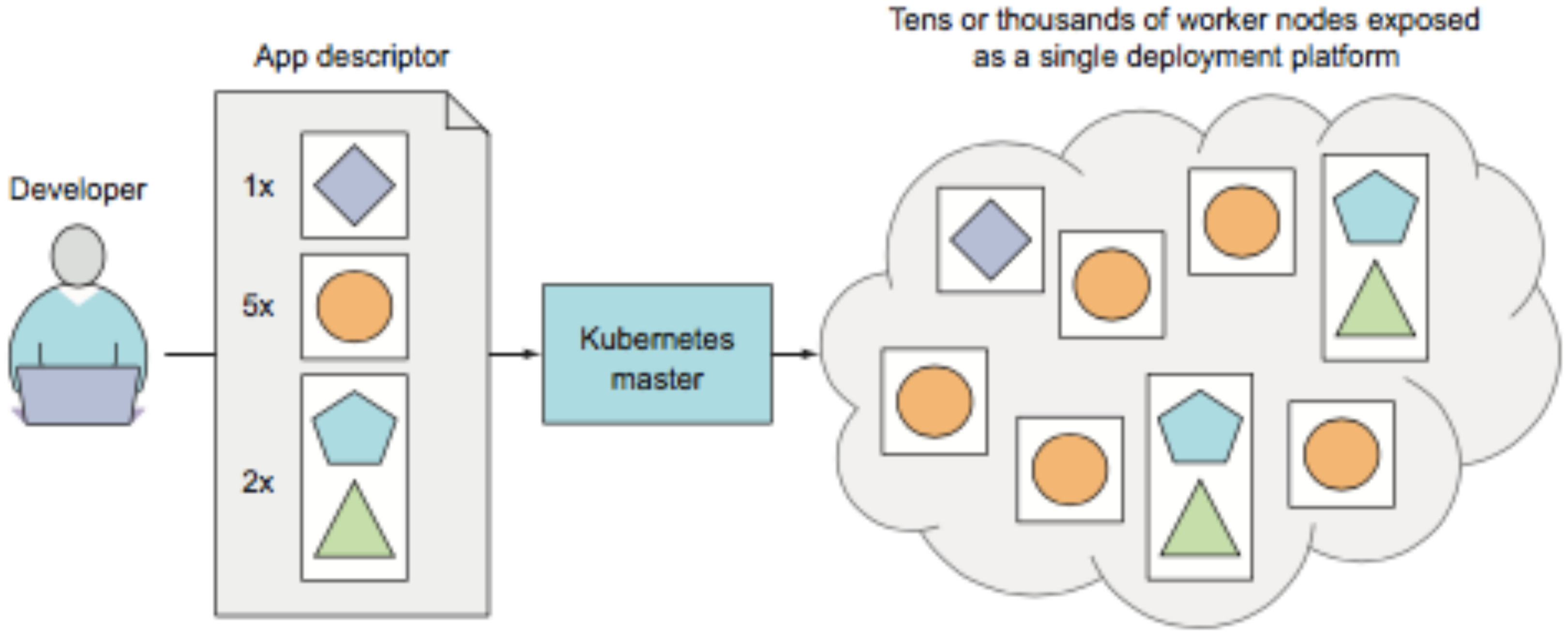
- important for pre-processing,
- also important for prediction on large data (test) sets
- dask provides scalable algoritms which can be run over clusters and are drop-in replacements for the `sklearn` equivalents
- Dask separates computation description (task graphs) from execution (schedulers).
- Write code once, and run it locally or scale it out across a cluster.

```python
# Setup a local cluster.
import dask.array as da
import dask.delayed
from sklearn.datasets import make_blobs
import numpy as np
from dask_ml.cluster import KMeans


n_centers = 12
n_features = 20
X_small, y_small = make_blobs(n_samples=1000, centers=n_centers, n_features=n_features, random_state=0)
centers = np.zeros((n_centers, n_features))
for i in range(n_centers):
    centers[i] = X_small[y_small == i].mean(0)
print(centers)

n_samples_per_block = 20000 # 0
n_blocks = 500
delayeds = [dask.delayed(make_blobs)(n_samples=n_samples_per_block,
                                     centers=centers,
                                     n_features=n_features,
                                     random_state=i)[0] for i in range(n_blocks)]
arrays = [da.from_delayed(obj, shape=(n_samples_per_block, n_features), dtype=X_small.dtype) for obj in delayeds]
X = da.concatenate(arrays)
print(X.nbytes / 1e9)
X = X.persist() #actually run the stuff

clf = KMeans(init_max_iter=3, oversampling_factor=10)
clf.fit(X)
print(clf.labels_[:10].compute()) #actually run the stuff
```

```python
# run using local distributed scheduler
import dask.array as da
import dask.delayed
from sklearn.datasets import make_blobs
import numpy as np
from dask_ml.cluster import KMeans

n_centers = 12
n_features = 20
X_small, y_small = make_blobs(n_samples=1000, centers=n_centers, n_features=n_features, random_state=0)
centers = np.zeros((n_centers, n_features))
for i in range(n_centers):
    centers[i] = X_small[y_small == i].mean(0)
print(centers)

from dask.distributed import Client

# Setup a local cluster.
# By default this sets up 1 worker per core
if __name__=='__main__':
    client = Client()
    print(client.cluster)
    n_samples_per_block = 20000 # 0
    n_blocks = 500
    delayeds = [dask.delayed(make_blobs)(n_samples=n_samples_per_block,
                                        centers=centers,
                                        n_features=n_features,
                                        random_state=i)[0] for i in range(n_blocks)]
    arrays = [da.from_delayed(obj, shape=(n_samples_per_block, n_features), dtype=X_small.dtype) for obj in delayeds]
    X = da.concatenate(arrays)
    print(X.nbytes / 1e9)
    X = X.persist() #actually run the stuff

    clf = KMeans(init_max_iter=3, oversampling_factor=10)
    clf.fit(X)
    print(clf.labels_[:10].compute()) #actually run the stuff
```

- we've seen the use of `dask.distributed`
- but we have run it locally. ideally we want to run on a cloud-provisioned cluster
- and we'd like this cluster to be self-repairing
- and then we'd like our code to respond to failures.
- and expand onto more machines if we need them

We need a cluster manager.

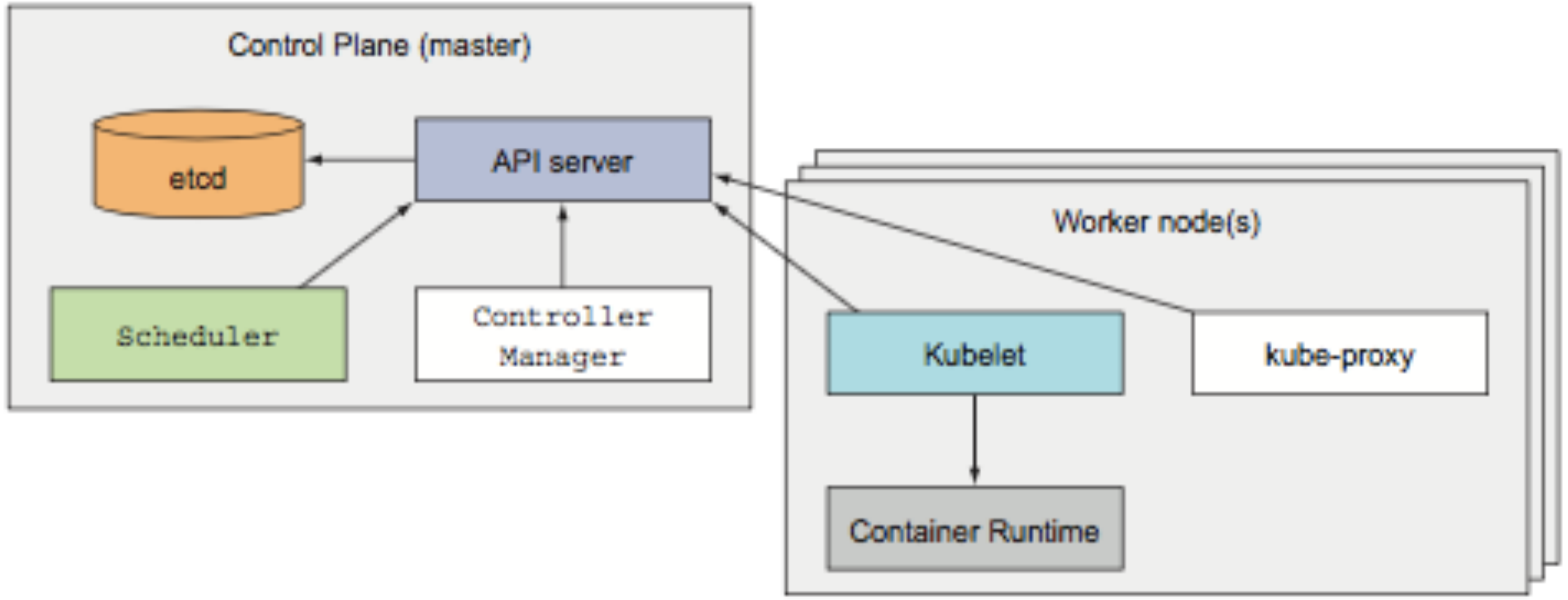

App descriptor
Tens or thousands of worker nodes exposed as a single deployment platform
Developer
1x
5x
2x
Kubernetes master

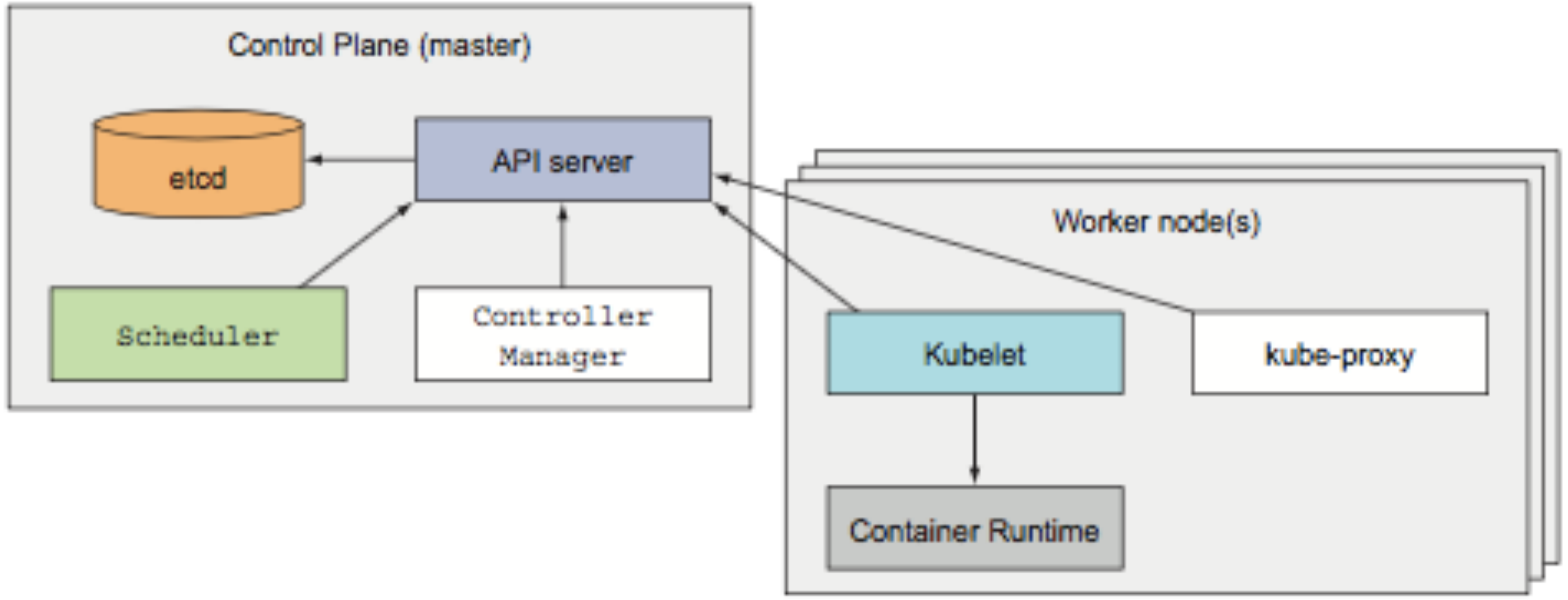
Enter Kubernetes

- OS for the cluster
- provides service discovery, scaling, load-balancing, self-healing, leader election
- think of applications as stateless, and movable from one machine to another to enable better resource utilization
- thus does not cover mutable databases which must remain outside the cluster
- there is a controlling master node, and worker nodes

master node:

- API server, communicated with my control-plane components and you (using `kubectl`)
- Scheduler, assigns a worker node to each application
- Controller Manager, performs cluster-level functions, such as replicating components, keeping track of worker nodes, handling node failures
- etcd, a reliable distributed data store that persistently stores the cluster configuration.

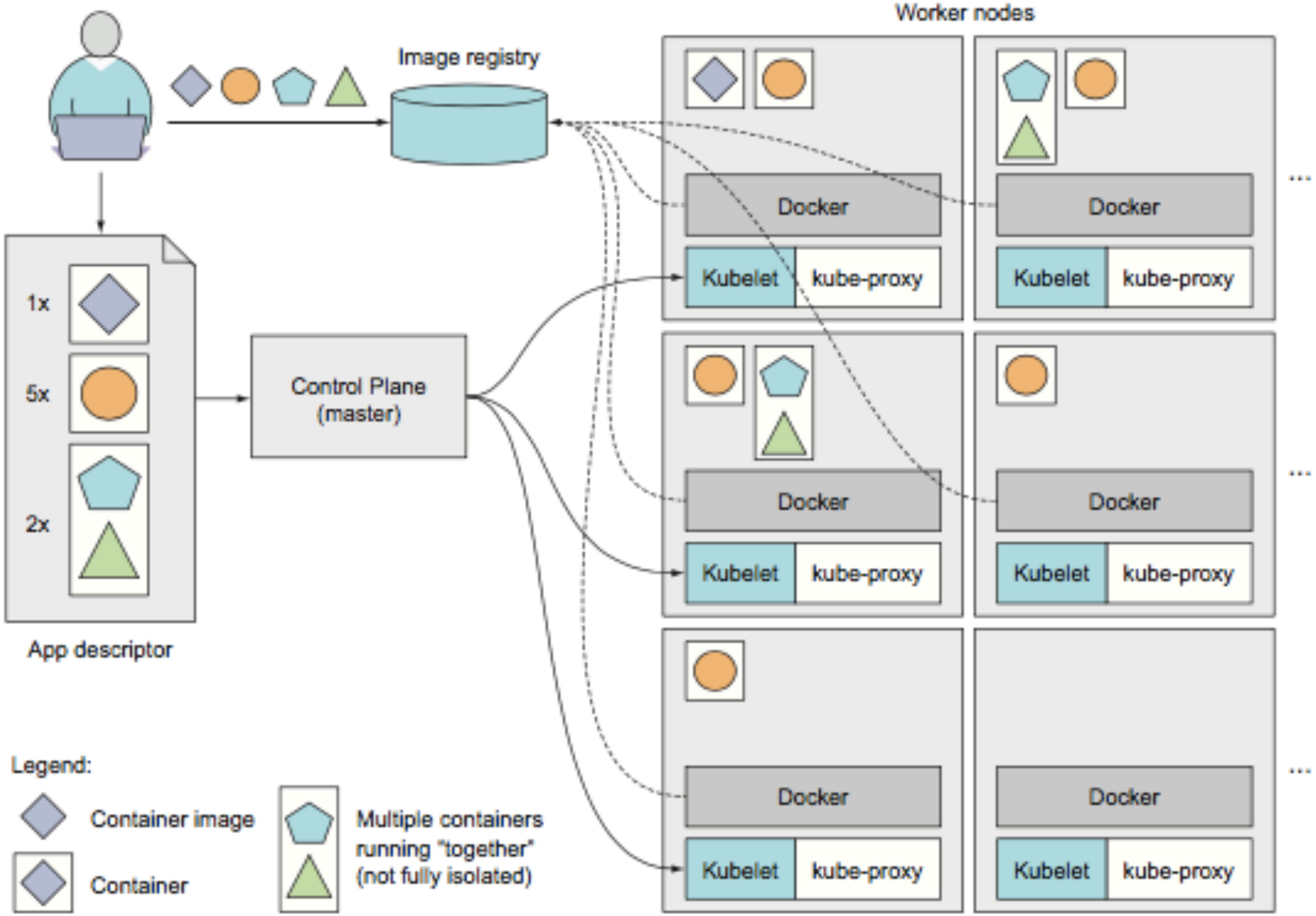




worker node:

- Docker, to run your containers
- you package your apps components into 1 or more docker images, and push them to a registry
- Kubelet, which talks to the API server and manages containers on its node
- kube-proxy, which load-balances network traffic between application components

- To run an application in Kubernetes, you post a description of your app to the Kubernetes API server.
- people have created canned "descriptions" for multi-component software, which you can reuse. These use a "package manager" called `helm`, and its what is used to install dask and jupyterhub on a cluster
- description includes info on component images, their relationship, which ones need co-location, and how many replicas
- internal or external network services are also described. A lookup service is provided, and a given service is exposed at a particular ip address. kube-proxy makes sure connec- tions to the service are load balanced
- master continuously makes sure that the deployed state of the application matches description


Worker nodes
Image registry
1x
5x
2x
App descriptor
Control Plane
(master)
Docker
Kubelet
kube-proxy
...
Legend:
Container image
Container
Multiple containers
running "together"
(not fully isolated)

Example: website with 3 replicas

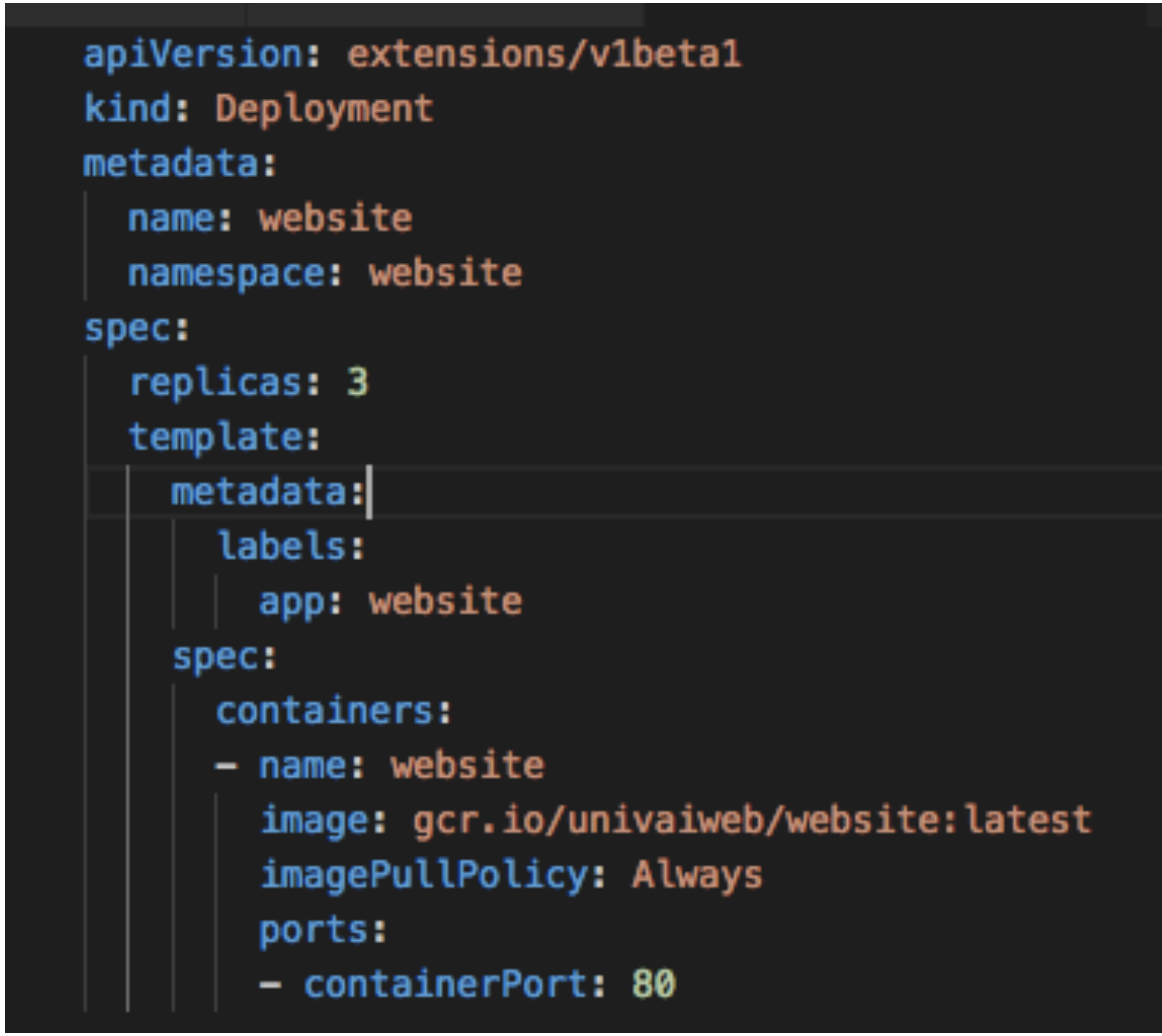
Image:

```
FROM nginx:stable-alpine
COPY  site/ /usr/share/nginx/html/
EXPOSE 80
```

Namespace:

```
apiVersion: v1
kind: Namespace
metadata:
  name: website
```

deployment.yaml ->

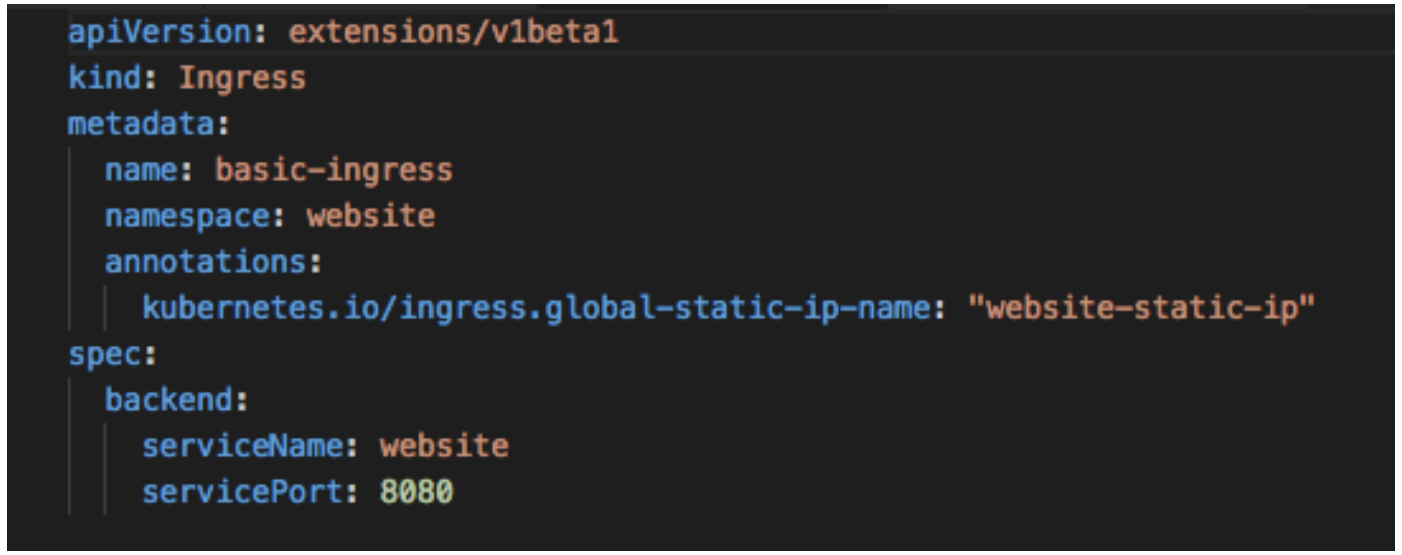


```
apiVersion: extensions/v1beta1
kind: Deployment
metadata:
  name: website
  namespace: website
spec:
  replicas: 3
  template:
    metadata:
      labels:
        app: website
    spec:
      containers:
      - name: website
        image: gcr.io/univaiweb/website:latest
        imagePullPolicy: Always
        ports:
        - containerPort: 80
```

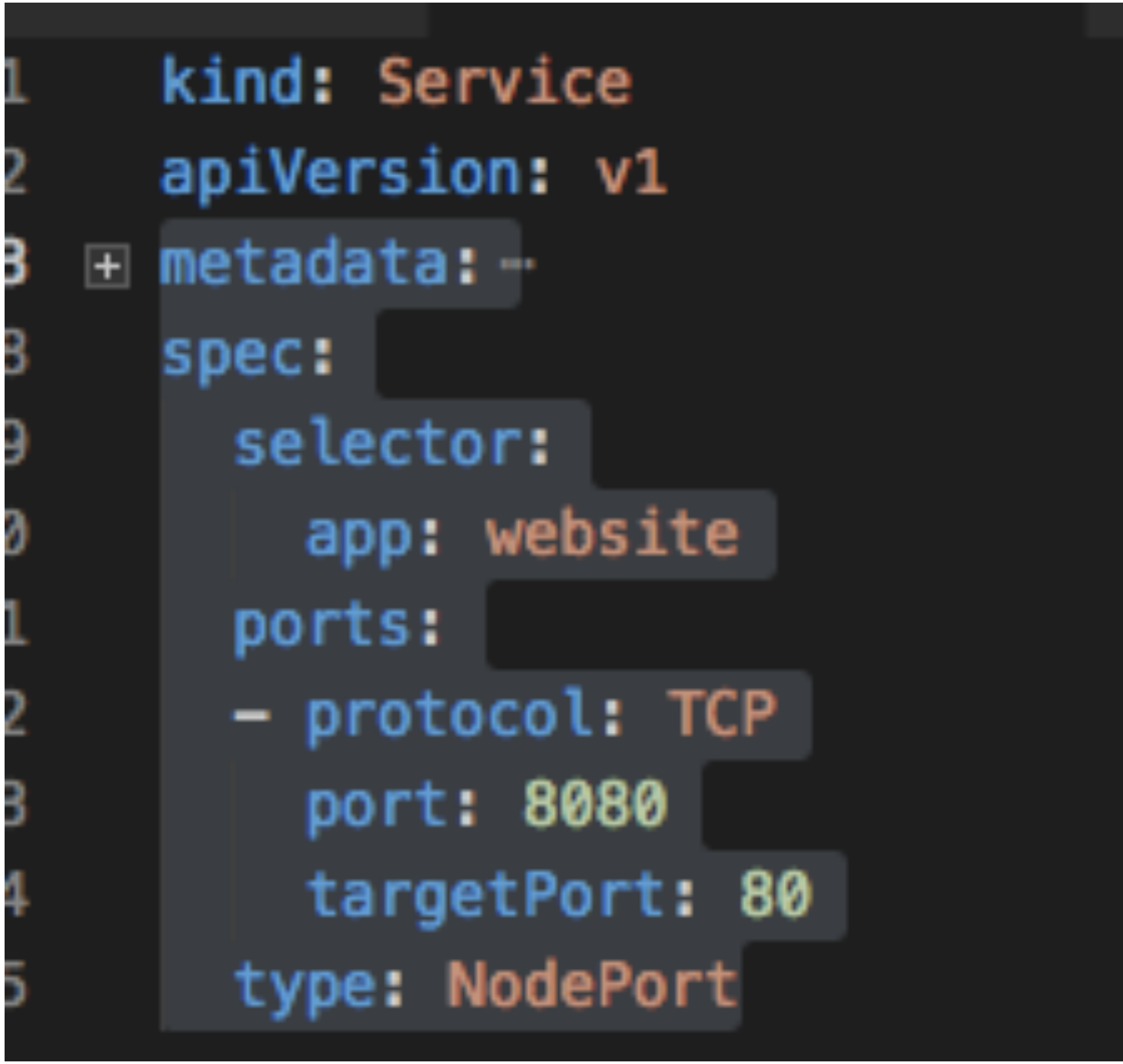
Networking

right: internal networking

below: external ingress



```
apiVersion: extensions/v1beta1
kind: Ingress
metadata:
  name: basic-ingress
  namespace: website
  annotations:
    kubernetes.io/ingress.global-static-ip-name: "website-static-ip"
spec:
  backend:
    serviceName: website
    servicePort: 8080
```



```
kind: Service
apiVersion: v1
metadata:
spec:
  selector:
    app: website
  ports:
  - protocol: TCP
    port: 8080
    targetPort: 80
  type: NodePort
```

Dask cloud deployment

Kubernetes is recommended

This can be done on your local machine using Minikube or on any of the 3 major cloud prociders, Azure, GCP, or AWS.

1. set up a Kubernetes cluster
2. Next you will set up Helm, which is a package maner for Kubernetes which works simply by filling templated yaml files with variables also stored in another yaml file `values.yaml`.
3. Finally you will install dask. First `helm repo update` and then `helm install stable/dask`.

See https://docs.dask.org/en/latest/setup/kubernetes-helm.html for all the details.

Deep Learning on the cloud

- tensorflow can be put on the cloud using `tf.distributed` of `kubeflow`
- parallelism can be trivially used at prediction time--you just need to distribute your weights
- as in our keras example you might have grid optimization
- but it would seem SGD is sequential
- can train it asynchronously using parameter servers. use `tf.distributed`.
- for training as well as serving