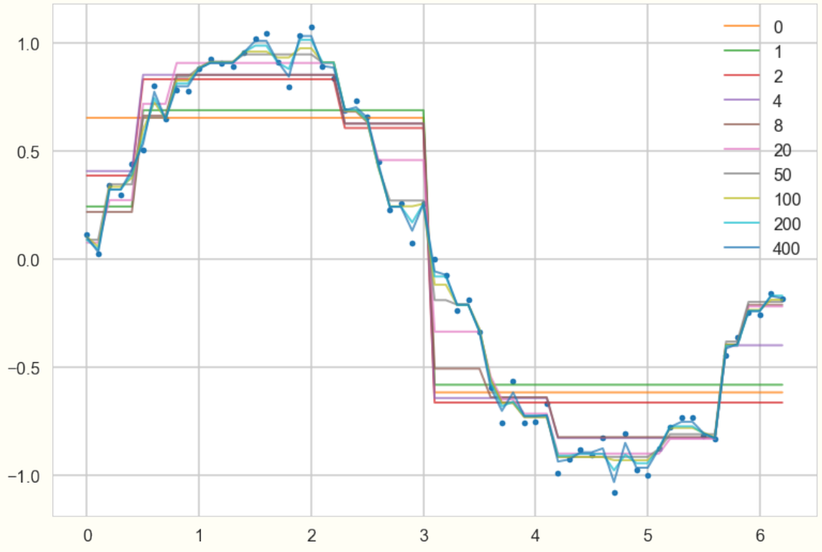
Python Environments

Hyper-parameter optimization

Eg, **Gradient boosting**: The basic idea is to fit the residuals of tree based regression models again and again. Peter Prettenhofer, who wrote sklearns GBRT implementation writes in his pydata14 talk:

I usually follow this recipe to tune the hyperparameters:

- Pick `n_estimators` as large as (computationally) possible (e.g. 3000)
- Tune `max_depth/min_samples_leaf`, `learning_rate`, and `max_features` via grid search
- A lower `learning_rate` requires a higher number of `n_estimators`. Thus increase `n_estimators` even more and tune `learning_rate` again holding the other params fixed.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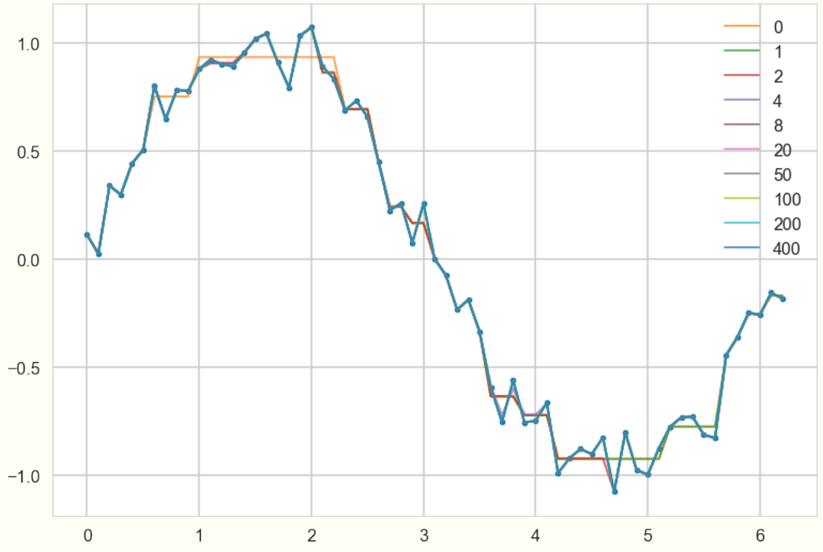
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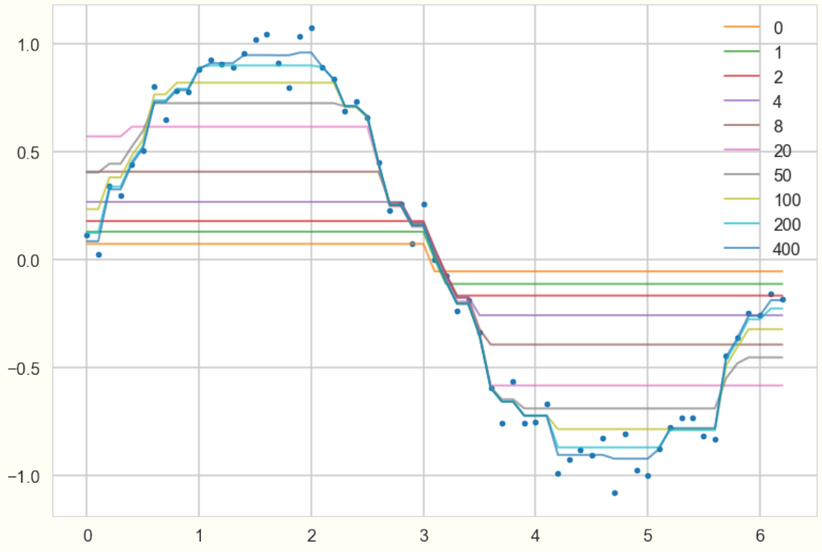
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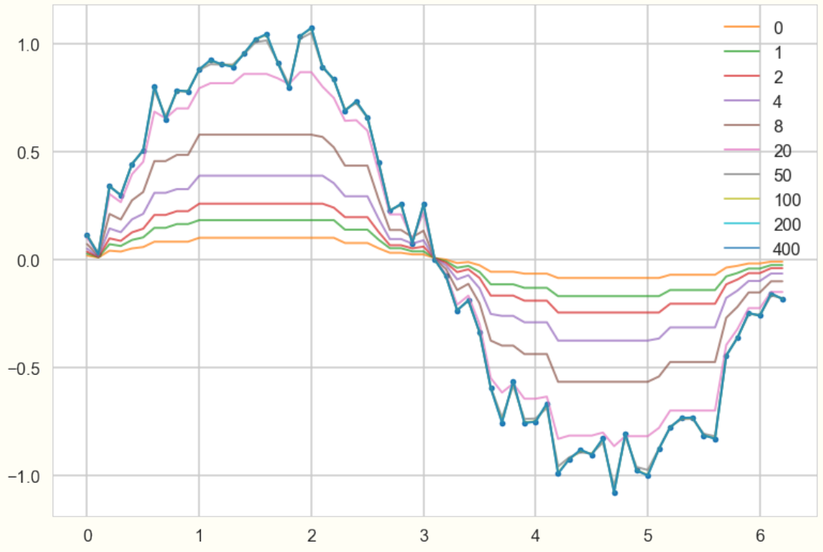
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Why is this bad? Or, why pipelines?

```
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)
```

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

Grid search on pipelines

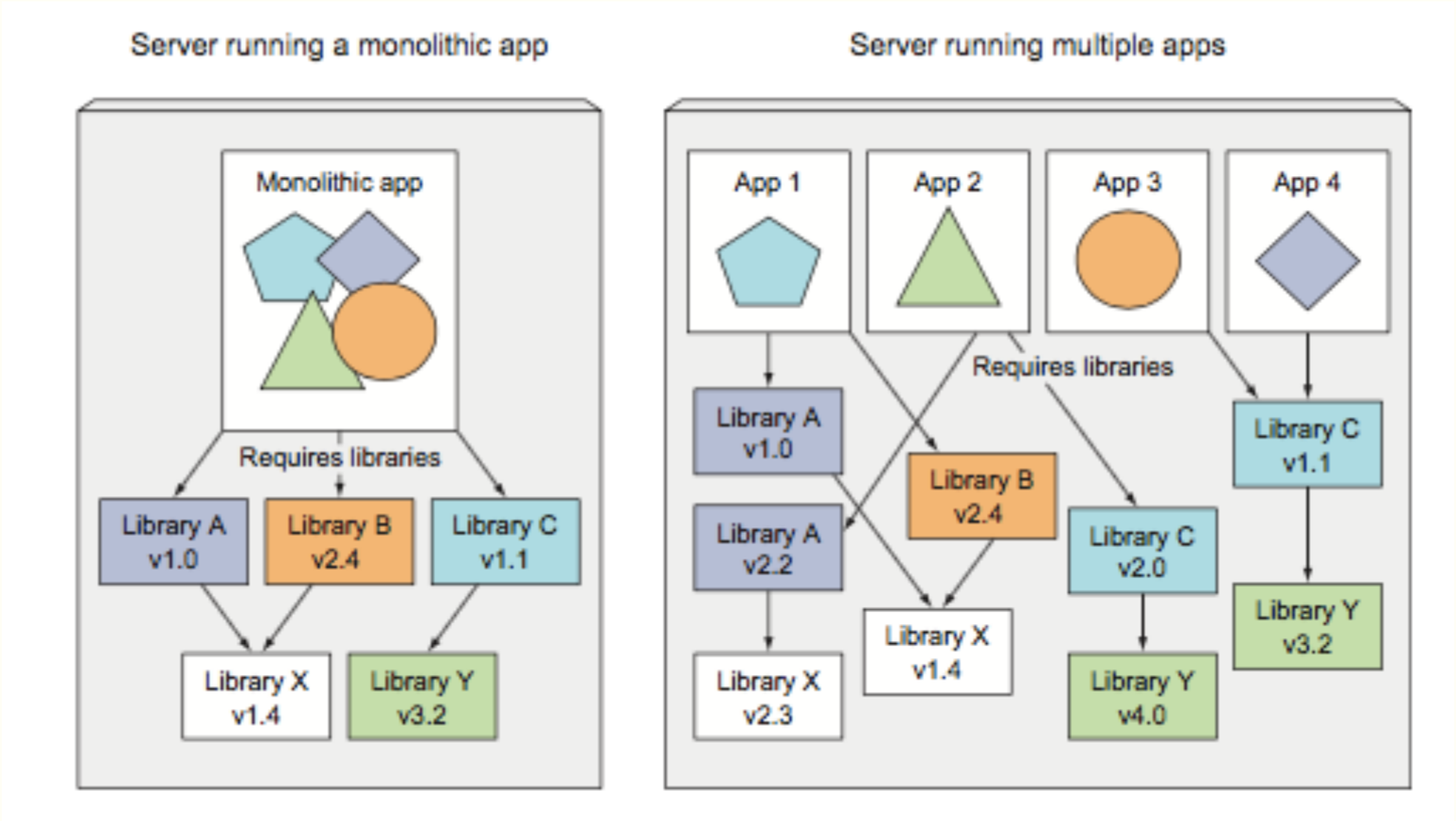
```
from sklearn.feature_extraction.text import CountVectorizer, TfidfTransformer
from sklearn.linear_model import SGDClassifier
from sklearn.pipeline import Pipeline
from sklearn.model_selection import GridSearchCV
from sklearn.datasets import fetch_20newsgroups

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())
```

ok, so you want to do this

PERFORMANTLY, AND REPRODUCIBLY

- same random seed
- same programming environment on multiple machines (ideally same version of OS/python-conda stack/BLAS libraries, etc)
- then run the same code with a different parameter combination on each machine
- deal with the possible loss of some machines in this computation (they die, you got an amazon spot instance..)
- combine all the data output from these runs to make hyperparameter choices

Programming environment: The multiple libraries problem



The solution

Virtual Environments

But first:

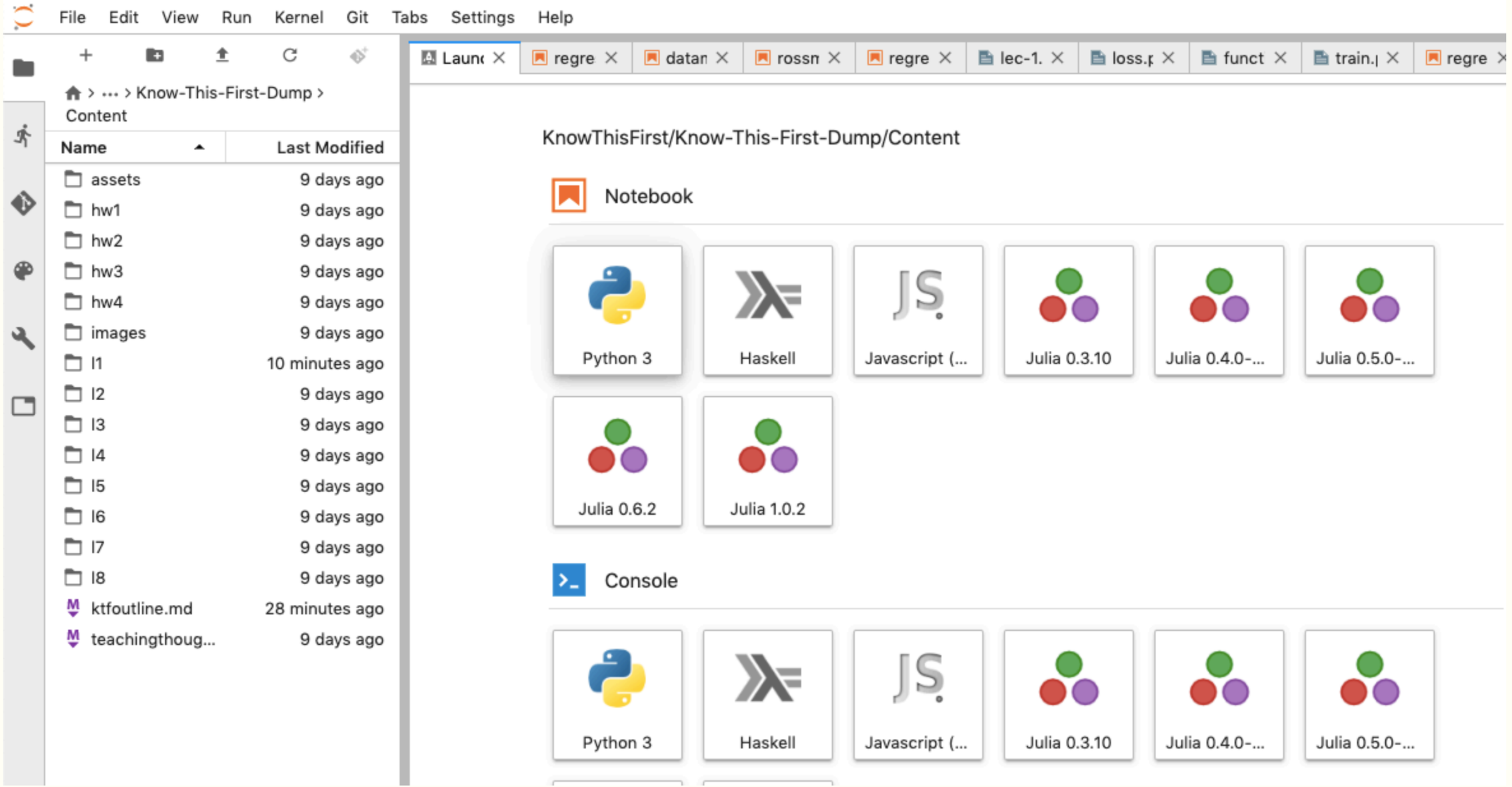
1. Setting up your Python Infrastructure

Installing Anaconda/Miniconda/Miniforge

- If you are completely new, you can use anaconda, and you get a nice graphical user interface
- if you have some command line experience, you might want to use Miniconda
- Install miniconda on non m1 platforms if you like, and you get access to Anaconda Inc's `default` channel
- But you can (must if commercial and you dont want to pay) also leverage the community driven `conda-forge` channel using miniforge
- Use miniforge on a m1 mac

How this workshop will run

- We are not going to bother with the initial anaconda/miniconda/miniforge installation: this will take too much time. If you dont have such a system, install it and let us know on the community forum. We can help you.
- Instead, ee have set up a `conda-forge` based Jupyterlab installation for you at: https://mybinder.org/v2/gh/univai-ghf/python-environments/HEAD. This uses the mybinder.org service. Click on the link to have a python environment set up for you in the cloud. You will get a web browser that looks like this: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Julia 0.4.0-...
Julia 0.5.0-...
Julia 0.6.2
Julia 1.0.2
Console
Python 3
Haskell
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Julia 0.3.10
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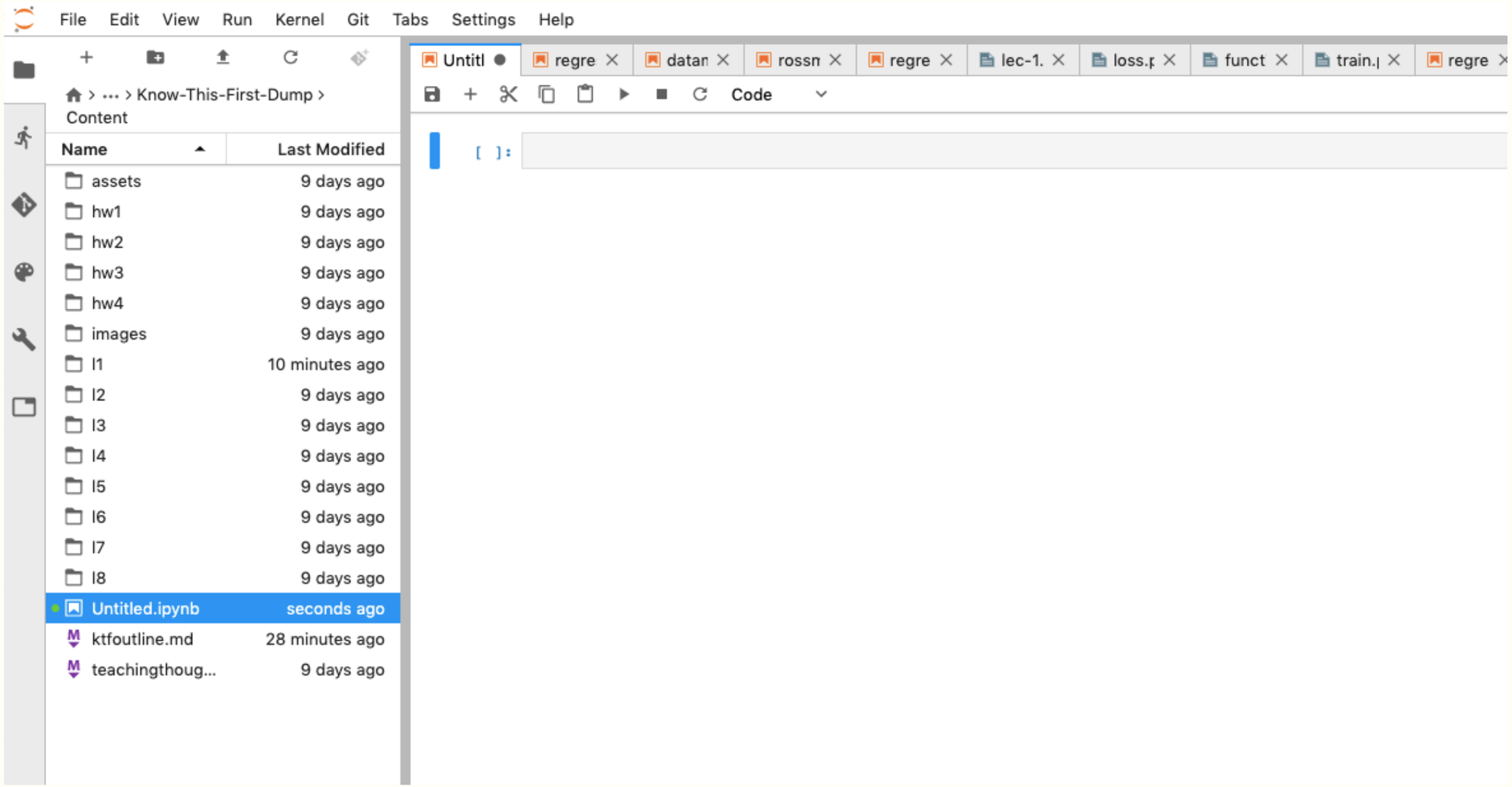
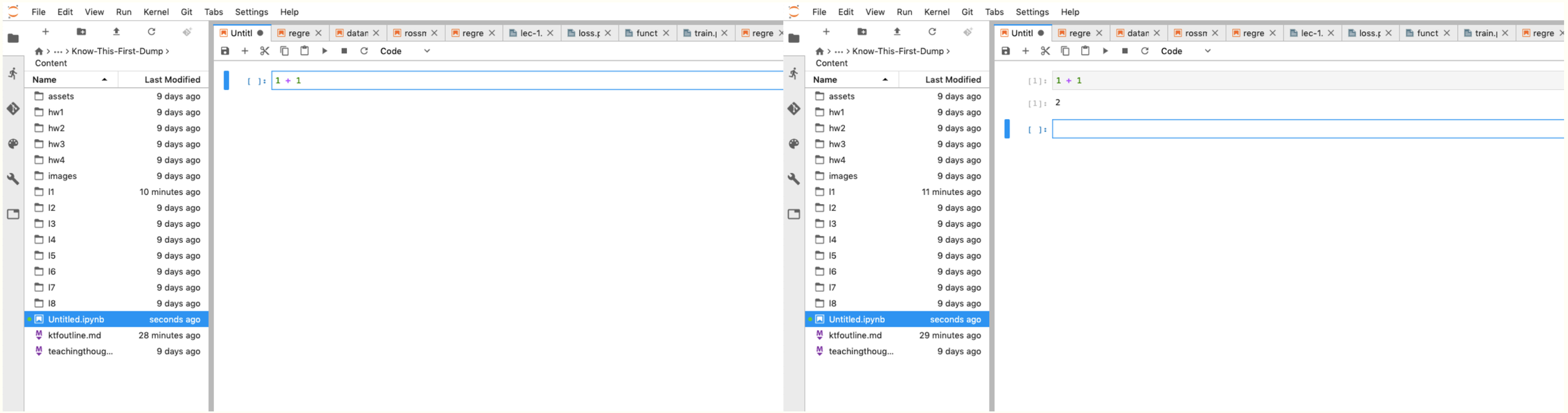
This screen is called the **Launcher**. Click on "Python" to get a new document window, called a **Jupyter Notebook** to this process.



You can now type in text boxes in the Jupyter Notebook, called **cells** in this new window. The left side is a file manager and is likely showing your home folder. This notebook is called `Untitled.ipynb`.

Type `1+1` in the text box and hit "Shift-Enter" or mouse-press the "Play icon" on the toolbar at the top.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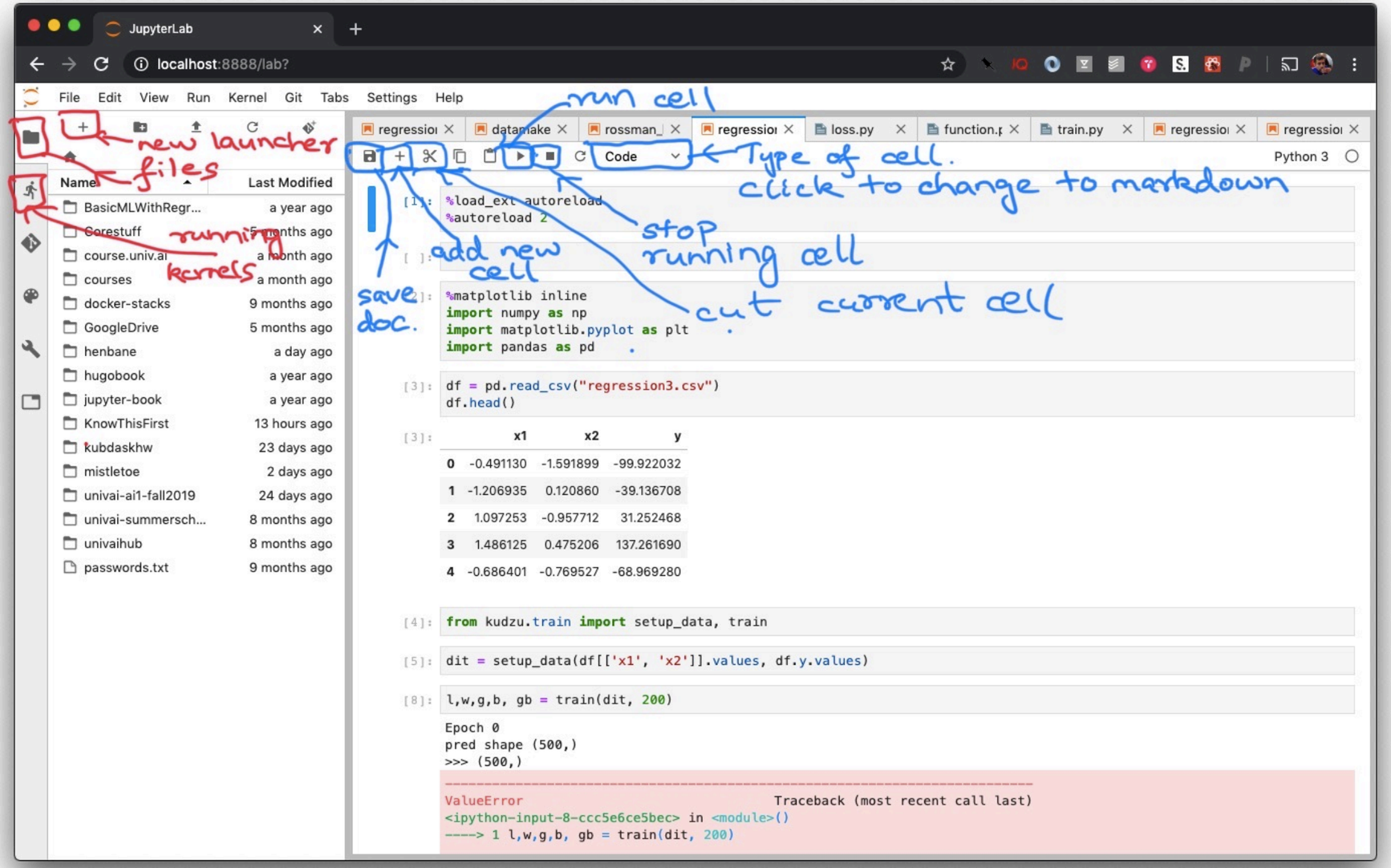
Jupyter cells have modes (and other GUI controls)

By default the cells are in `Code` mode. These can be changed to `Markdown` mode in the toolbar to enter text. The next picture shows some buttons and what they do.


JupyterLab
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course.univ.ai a month ago
courses a month ago
docker-stacks 9 months ago
GoogleDrive 5 months ago
henbane a day ago
hugobook a year ago
jupyter-book a year ago
KnowThisFirst 13 hours ago
kubdaskhw 23 days ago
mistletoe 2 days ago
univai-ai1-fall2019 24 days ago
univai-summersch... 8 months ago
univaihub 8 months ago
passwords.txt 9 months ago
%load_ext autoreload
%autoreload 2
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
df = pd.read_csv("regression3.csv")
df.head()
x1 x2 y
0 -0.491130 -1.591899 -99.922032
1 -1.206935 0.120860 -39.136708
2 1.097253 -0.957712 31.252468
3 1.486125 0.475206 137.261690
4 -0.686401 -0.769527 -68.969280
from kudzu.train import setup_data, train
dit = setup_data(df[['x1', 'x2']].values, df.y.values)
l,w,g,b, gb = train(dit, 200)
Epoch 0
pred shape (500,)
>>> (500,)
ValueError Traceback (most recent call last)
<ipython-input-8-ccc5e6ce5bec> in <module>()
----> 1 l,w,g,b, gb = train(dit, 200)

2. Setting up
Virtual Environments

What is a virtual environment?

- It's own set of packages that do not conflict with other sets of packages
- thus we can have competing packages with different dependency versions isolated from each other
- space is not wasted: packages can be installed into multiple environments if the dependencies are met

Creating a virtual environment

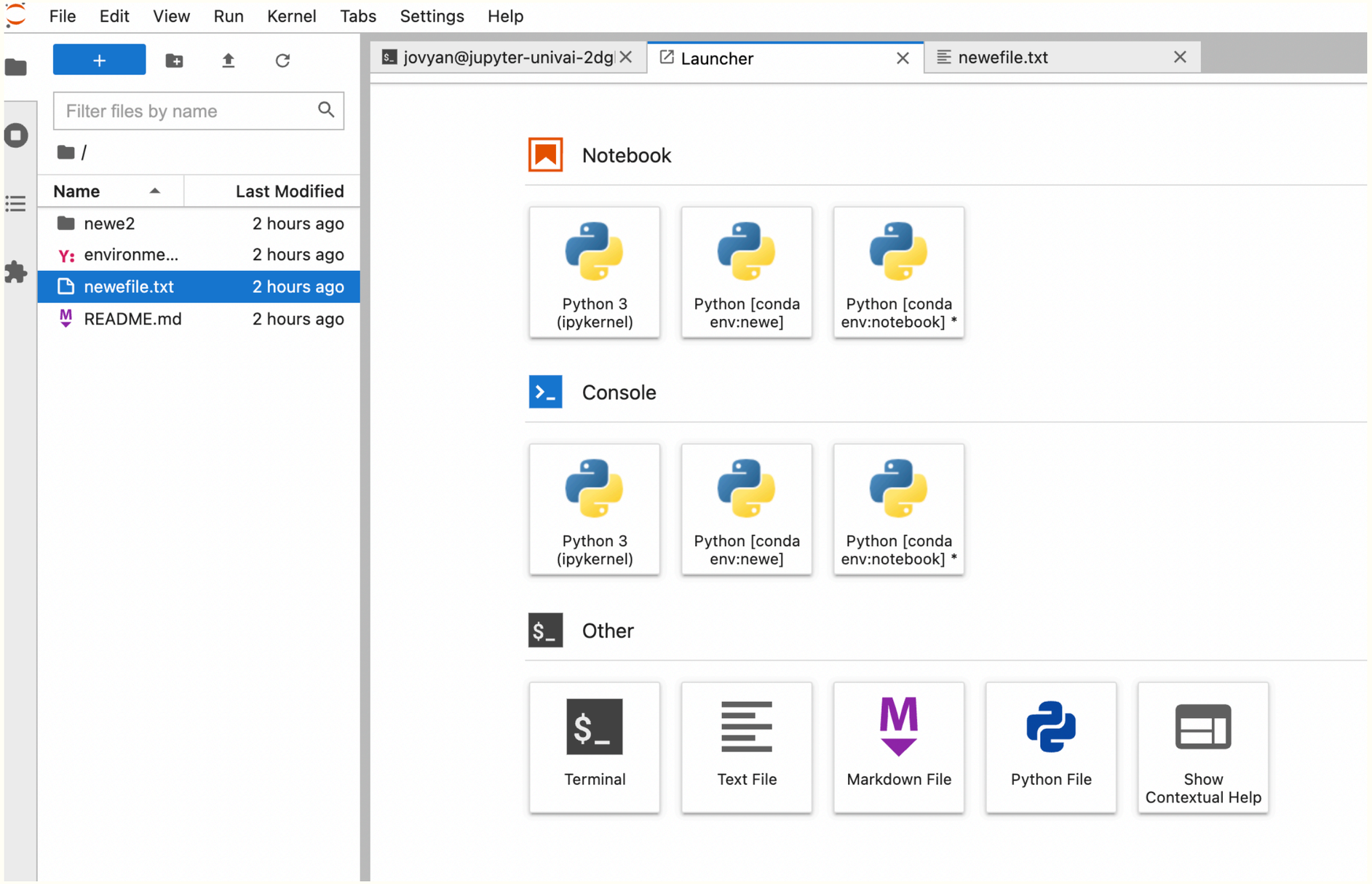
- `conda create --name environment-name [python=3.6]`
- `conda activate environment-name`
- `conda deactivate environment-name`
- `conda install <packagename>`

Eg:

```
conda create -n newe
conda activate newe
conda install numpy pandas ipykernel
conda deactivate newe
```

Making sure environments are available on jupyterlab

- in the base installation, make sure you `conda install nb_conda_kernels`.
- this will depend on how you installed the base. But run the above command is needed
- in our binder system, this is already installed.
- now in every new environment make sure you install `ipykernel`.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newefile.txt
Notebook
Python 3 (ipykernel)
Python [conda env:newe]
Python [conda env:notebook] *
Console
Python 3 (ipykernel)
Python [conda env:newe]
Python [conda env:notebook] *
Other
Terminal
Text File
Markdown File
Python File
Show Contextual Help

Capturing a virtual environment

`conda env export` will capture the exact dependencies. You can now redirect into a file, and use elsewhere on the same OS to recreate this environment.

The file is usually called `environment.yml`, so we do:

```
conda env export > environment.yml
```

If this file is in a particular folder, just type `conda env create` to create an environment with these packages.

Using environment.yml files

- you can write your own `environment.yml` file to be much less tied to specific package versions, unless needed.

For example, for an environment `newe2`, we create a folder `newe2`, and in that folder, we create a `environment.yml` with the contents:

```
name: newe2
channels:
- conda-forge
dependencies:
- ipykernel
- matplotlib
- pandas
- numpy
- scipy
- seaborn
- scikit-learn
- tensorflow
- keras
```

A conda env per project

- create a conda environment for each new project
- put an `environment.yml` in each project folder (like `newe2`) with a `name` line reflecting the folder name
- `conda|mamba env create` in project folder (like `newe2`)
- if not per project, at least have one for each new class, or class of projects
- environment for class of projects may grow organically, but capture its requirements from time-to-time.
- for example, on my dual-gpu machine, I have 3 separate environments for pytorch, tensorflow, and jax, as they even had slightly different CUDA requirements.

see here

Mamba

- mamba is a version of conda that works with conda but is faster.
- use `mamba` to create and/or install
- use `conda` to activate/deactivate
- See https://mamba.readthedocs.io/en/latest/user_guide/mamba.html
- on our binder environment I can issue `mamba env create`. Its faster. But then I must use `conda activate newe2` to startup the new environment
- by default conda will use both default and conda-forge channels, mamba will use conda-forge. I found keras currently only installable with mamba.

```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/)

More information

- https://carpentries-incubator.github.io/introduction-to-conda-for-data-scientists/
- https://goodresearch.dev/setup.html , which is part of the excellent book
- https://goodresearch.dev/index.html

3. Structure

The Importance of Structure

- one might as well use the one env per project ot set-of-projects structure to organize work
- it is really important to organize your data science work well
- a good tool for this is `cookiecutter`, which sets up a template folder structure for you. Install by `pip install cookiecutter` in your base.
- you install a cookiecutter by doing `cookiecutter source`.

Two nice cookiecutters

- https://github.com/patrickmineault/true-neutral-cookiecutter
- Install via: `cookiecutter gh:patrickmineault/true-neutral-cookiecutter`
- https://drivendata.github.io/cookiecutter-data-science/
- Install via: `cookiecutter gh:drivendata/cookiecutter-data-science`

True Neutral Cookiecutter

```
├── data
├── doc
├── results
├── scripts
├── src
│   └── __init__.py
├── tests
├── .gitignore
├── environment.yml
├── README.md
└── setup.py
```

An example

- We do: `cookiecutter gh:drivendata/cookiecutter-data-science`
- name the project perceptron
- create the conda environment:
- `conda create --name perceptron; conda activate perceptron; mamba install ipykernel numpy tensorflow keras` or do `mamba env create` with an appropriate environment file
- then do `pip install -e .` which creates the src directory loadable into python

Best practices for use

- now we can do development with both the notebook and files. In anotebook cell put the following to have the notebook automatically reload the file when it changes.

```
%load_ext autoreload
%autoreload 2
```

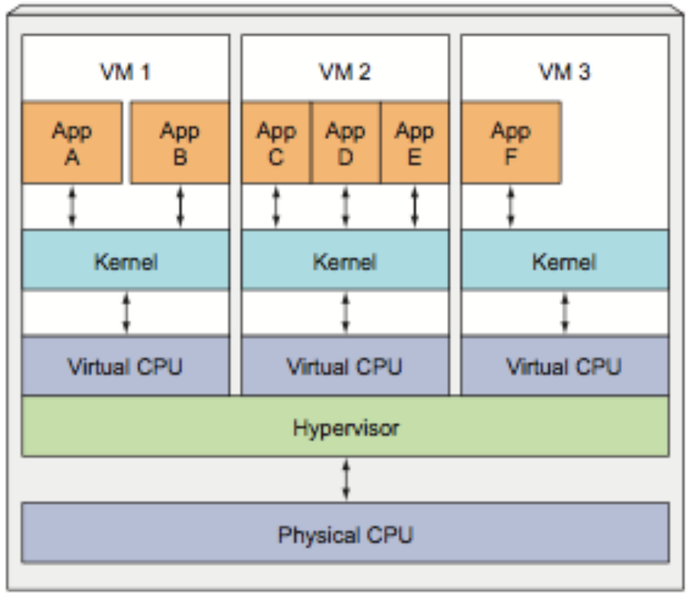
- refactor anything repeated multiple times to python files with functions in them. Notebooks should be very readable
- output all intermediate files into `data` or `results` while writing your pipelines: files from train test splits, parameter values and results, etc
- future you will than current you.

4. Extra

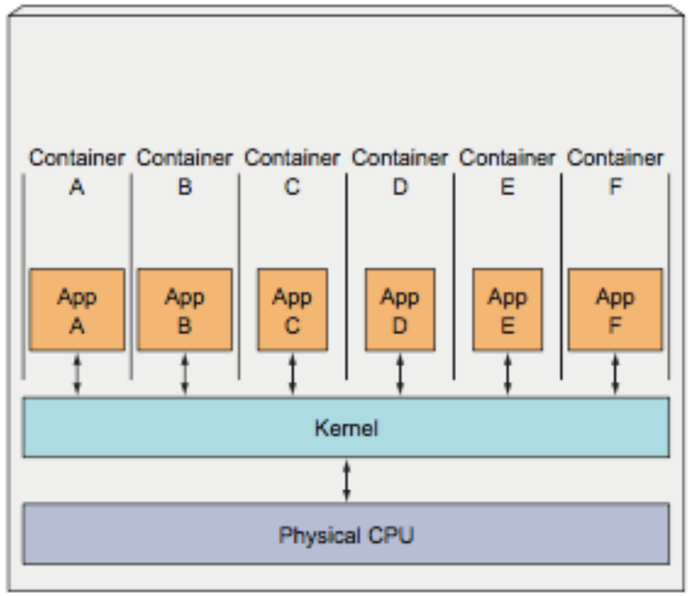
Going even further: Docker

- More than python libs
- C-library, BLAS, linux kernel, etc
- we could use virtual machines (VMs) like vmware/virtualbox/lvm
- but these are heavy duty, OS level "hypervisor"s
- more general, but resource hungry

Apps running in multiple VMs



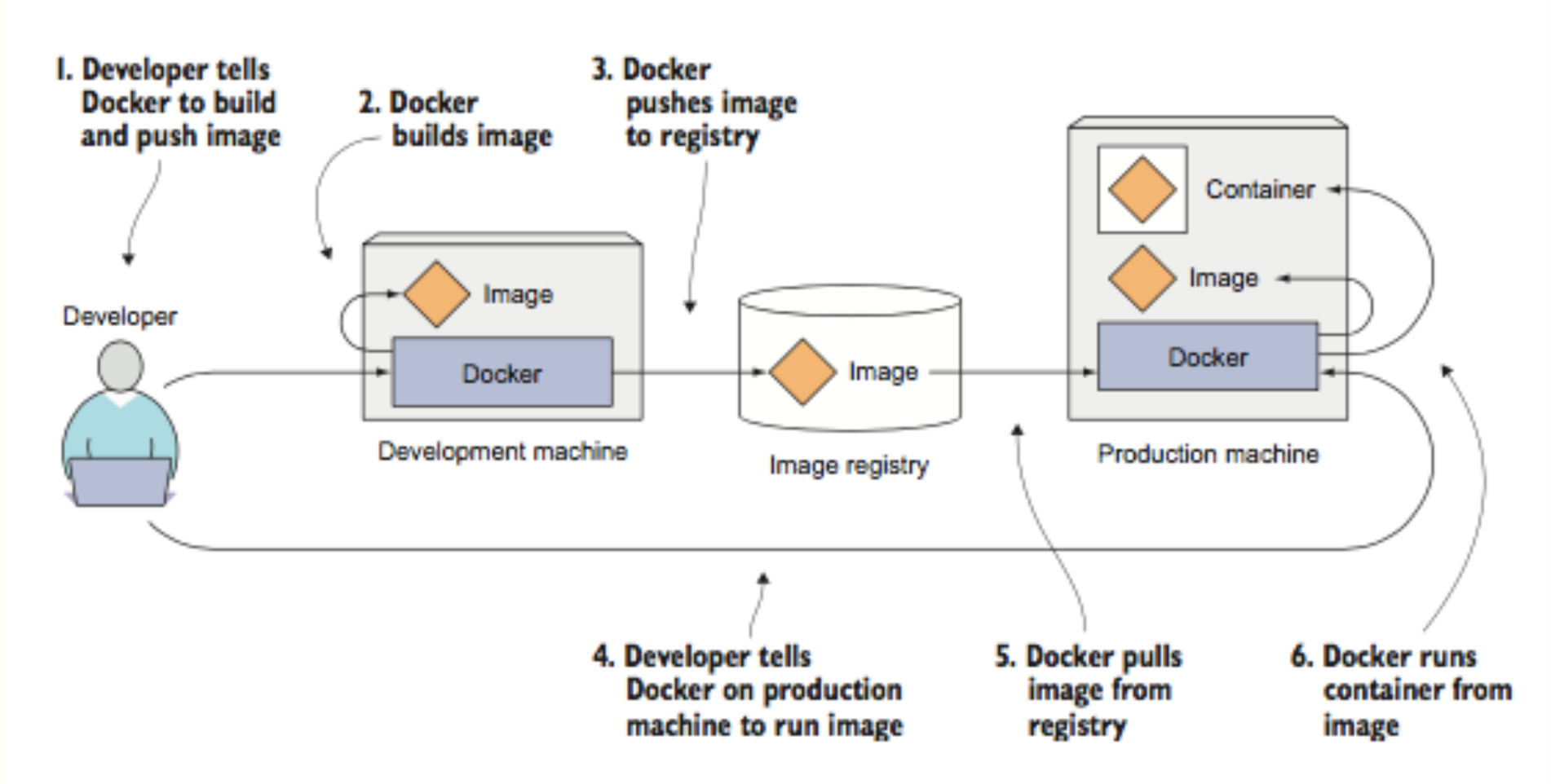
Apps running in isolated containers



Containers vs Virtual Machines

- 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, and on many cloud providers. They can also run on a host linux OS on bare metal

Docker Architecture



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
- side benefit: integration testing and testing for CI

An Example

base notebook -> minimal notebook -> scipy notebook -> tensorflow notebook

```
# 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
```

```
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*' \
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    '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 && ...
```

```
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
```

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
- built repo's can be used with multiple software such as jupyterhub/dask/kubernetes, etc