Reproducible Machine Learning

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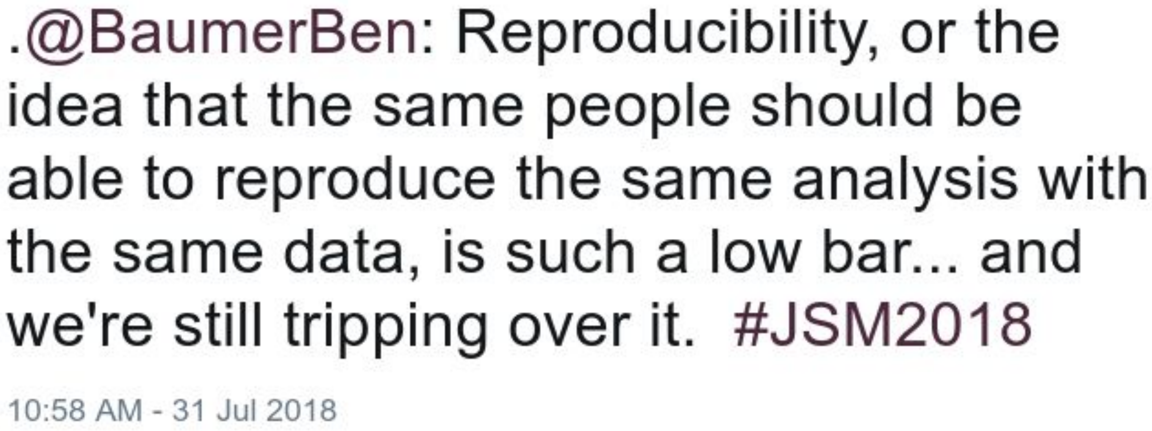
@rctatman

kaggle™



.@BaumerBen: Reproducibility, or the idea that the same people should be able to reproduce the same analysis with the same data, is such a low bar... and we're still tripping over it. #JSM2018

10:58 AM - 31 Jul 2018

Why should you care about reproducibility?

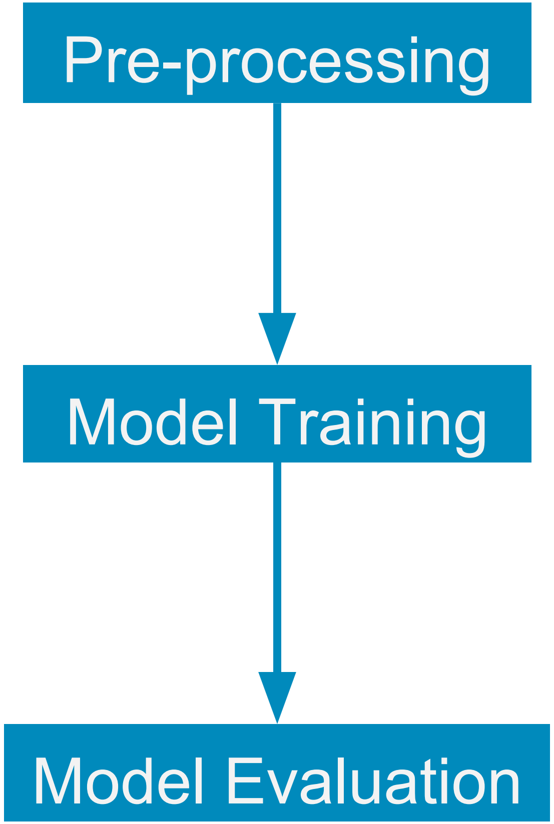
Because the person most likely to need to reproduce your work… is you.

code + data + environment =
reproducible machine learning

code + data + environment + some ML-specific stuff =
reproducible machine learning

Levelling up reproducibility

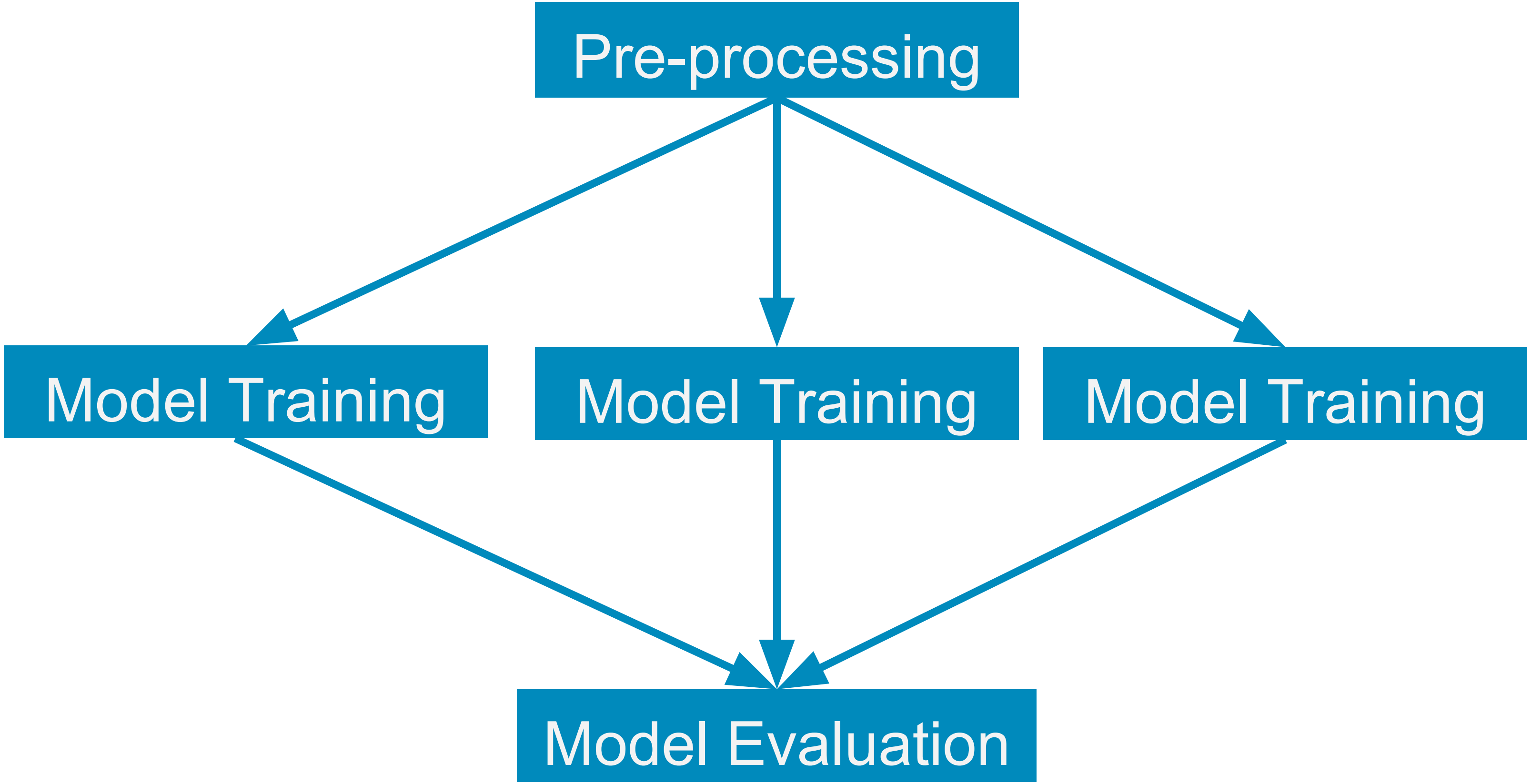
1. Code
   a. Structuring your project
   b. Stochastic -> static
2. Data
3. Environment

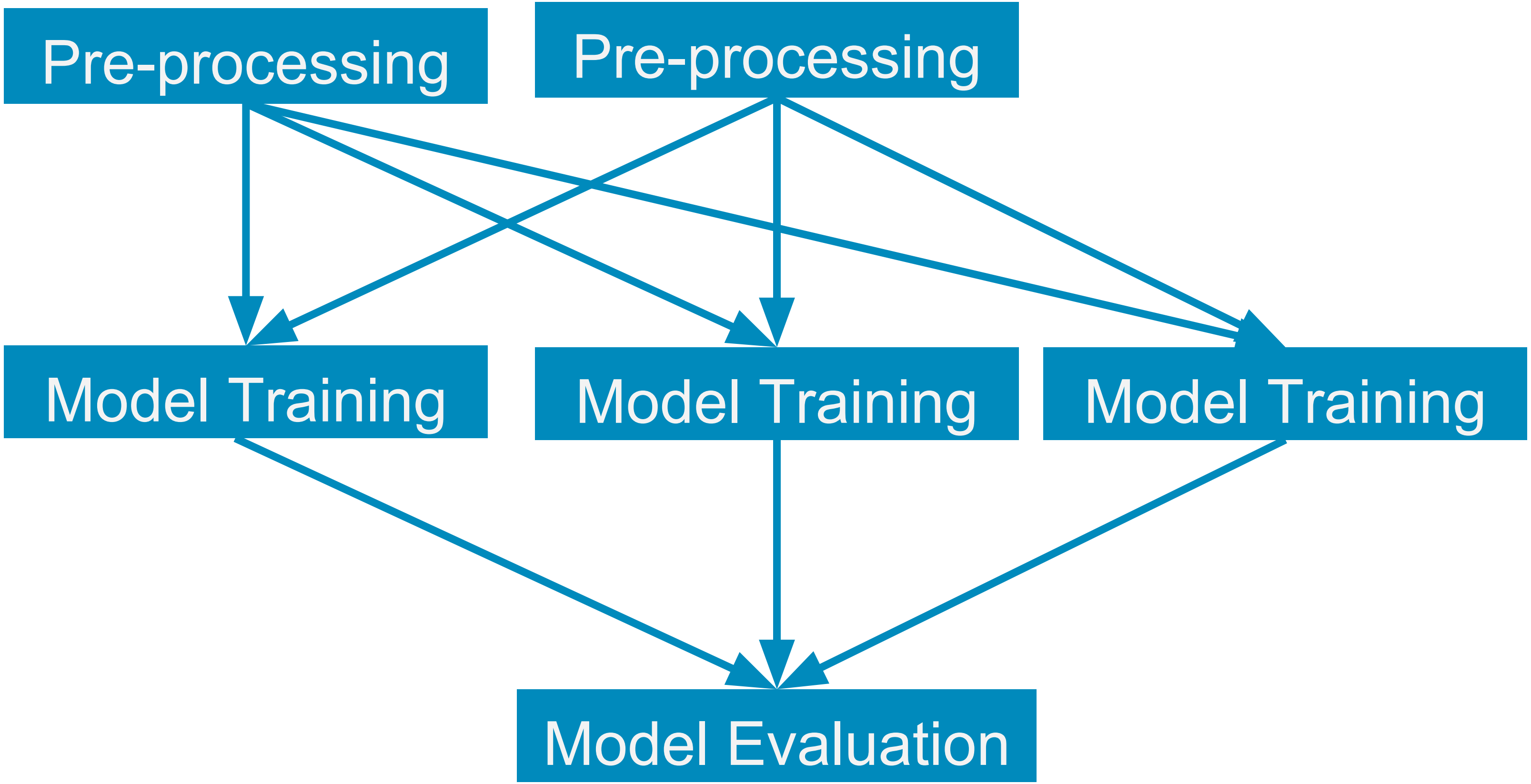


Pre-processing

Model Training

Model Evaluation


Pre-processing
Model Training
Model Training
Model Training
Model Evaluation



Pre-processing

Pre-processing

Model Training

Model Training

Model Training

Model Evaluation

Stochastic -> Static

Help! I'm getting different results with the same code!

Most machine learning methods rely on some sort of pseudorandomness for things like:

- Weight initialization
- Dropout
- Subsetting/shuffling for mini-batches
- Training/testing/validation split

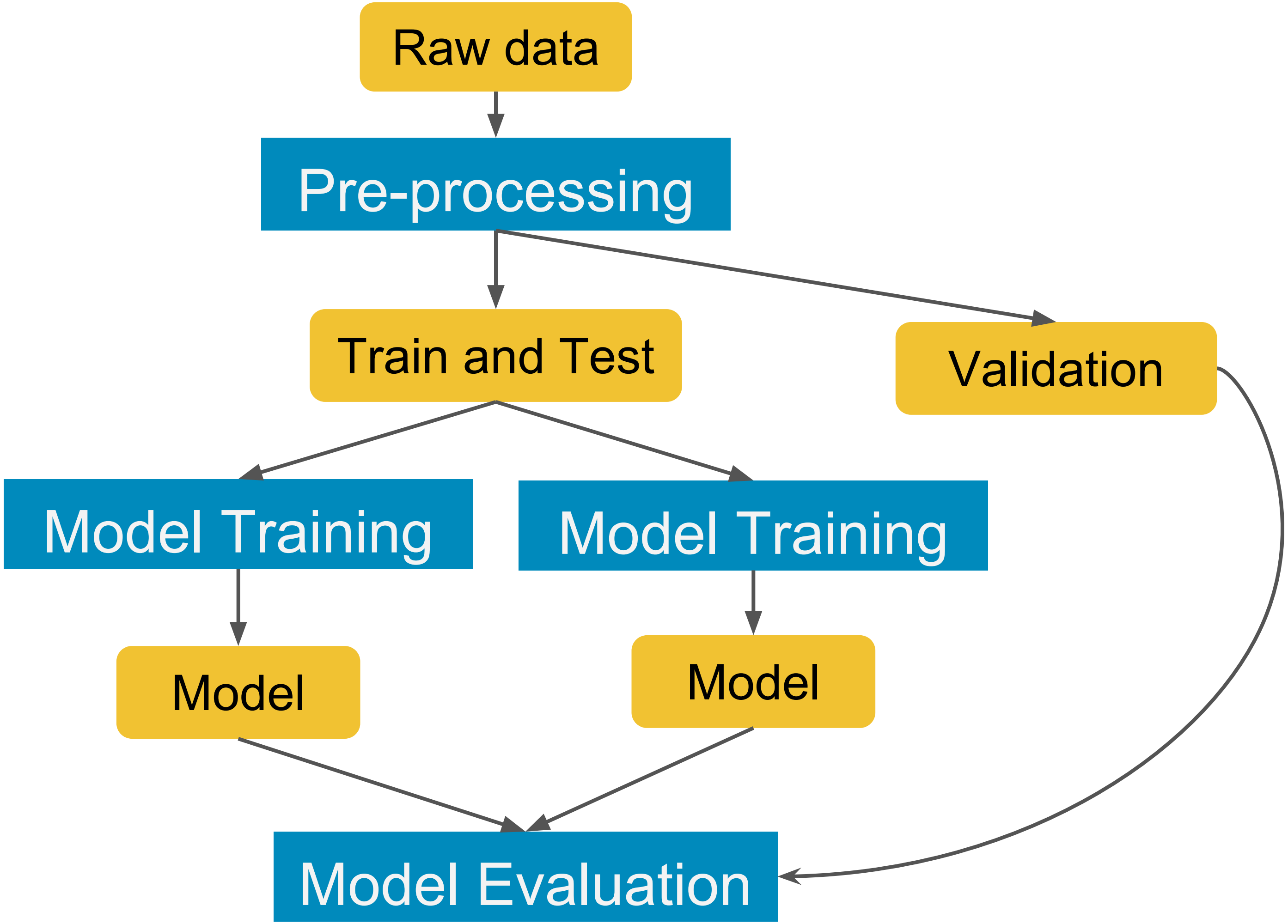
Stochastic -> Static

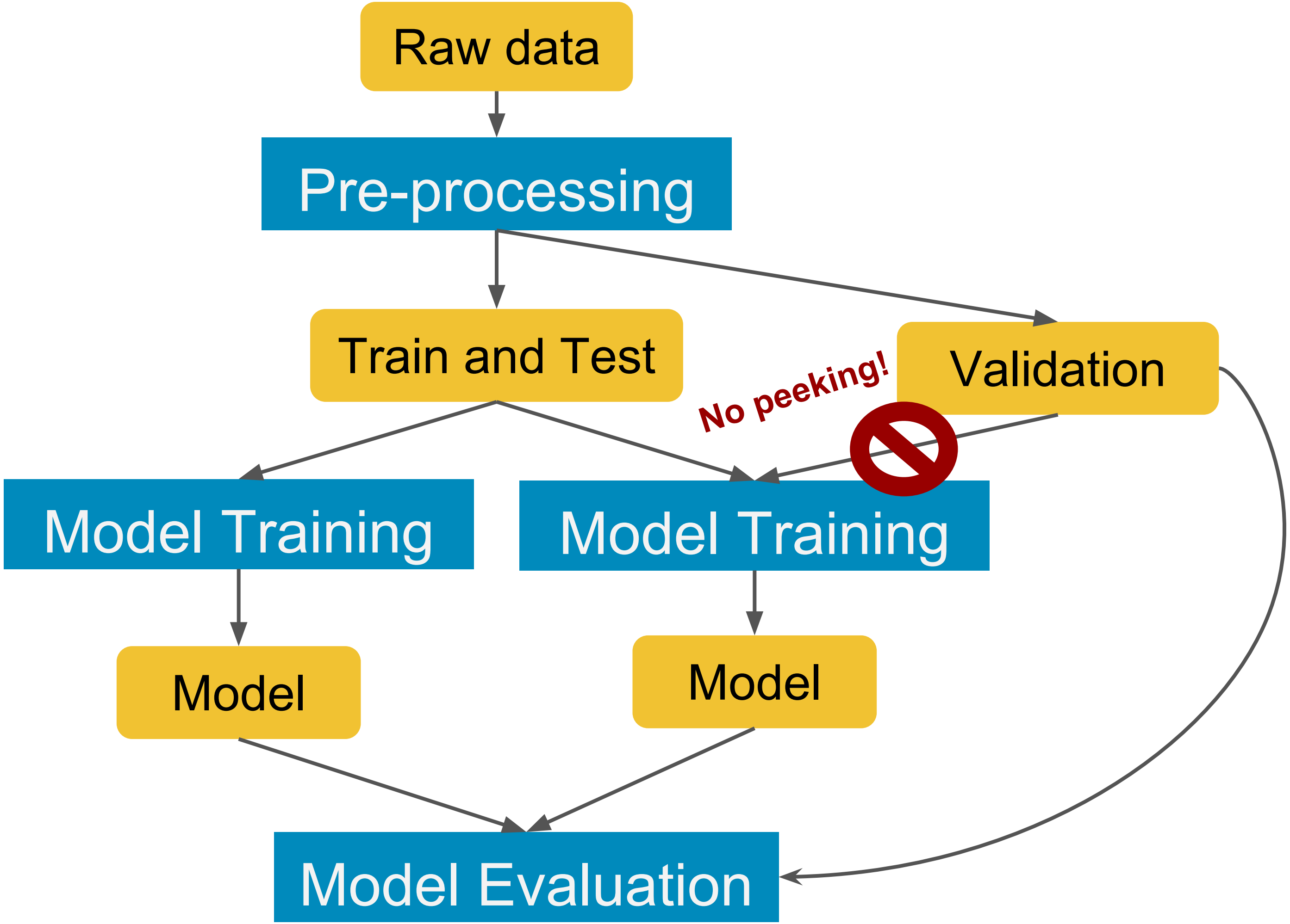
In order to get the same results more than once, you need to make sure to set *all* the random number generators (RNGs) your code depends on.

- Numpy & Keras:
  - np.random.seed(42) (<- will bork on multi-threading)
- Tensorflow:
  - tf.set_random_seed(42)
- Anything that uses hash randomization (like Theano):
  - PYTHONHASHSEED=0 (<- this can be a security risk so don’t do it by default)
- cuDNN
  - ¯_(ツ)_/¯
  - Some routines (like backward pass & backward pooling) do not guarantee reproducibility because they use atomic operations

Levelling up reproducibility

1. Code
2. **Data**
   a. **What should you be saving?**
   b. **Always work from a copy**
   c. **Version your data**
3. Environment


Raw data
Pre-processing
Train and Test
Validation
Model Training
Model Training
Model
Model
Model Evaluation


Raw data
Pre-processing
Train and Test
Validation
No peeking!
Model Training
Model Training
Model
Model
Model Evaluation

Always work from a copy of your data

Keep a seperate copy of your raw data that you never, ever touch. Work from copies of it.

Versioning, not just for code anymore!

- If you’re already using version control & have small/medium data, add your data files to the system you use for your code
- For databases, there are many version control options (versionSQL, DBmaestro, etc.)
- For streaming data, save & work from a specific time span

Levelling up reproducibility

1. Code
2. Data
3. **Environment**

You can think of reproducibility as a scale:
The longer it takes to reproduce a project,
the less reproducible it is.

Sharing your environment

Your environment includes:

- All dependencies, including versions and subversions
- Your file system
- Your OS
- (In some cases) hardware

Options for sharing your environment:

- Containers (like Docker)
- Virtual machines
- Hosted environments

Sharing your environment: Containers

Benefits:

- Contains data, code, file systems, dependencies
- Portable
- Lightweight

Drawbacks:

- Uses the host OS, can be dicey cross-platform
- Can take a while to get set up

Sharing your environment: Virtual machines

Benefits:

- Contains data, code, file systems, dependencies and OS
- Portable, even between platforms

Drawbacks:

- Larger/slower to get started than containers
- Can take a while to get set up

Sharing your environment: Hosted environments

Benefits:

- Very fast set-up
- Extremely easy to share (in many cases just copying & pasting a link)

Drawbacks:

- Less control over environment
- May not be feasible for security/privacy reasons

Name	Price	Languages	GPU	Data hosting	Specs (Free tier)
Kaggle Kernels	Free	Python 3, R	Yes	Yes	GPU: 1xTesla K80 (6 hr/run) RAM: 16 GB Disk: 5 GB
Google Colaboratory	Free	Python 2 & 3	Yes	No	GPU: 1xTesla K80 (12 hr/run) RAM: ~12.6 GB Available Disk: ~33 GB Available
Azure Notebooks	Free	Python 2 & 3, R, F#	No	Yes	4G memory limit & 1G data limit
Amazon SageMaker	Varies, 2 month free trial	Python 2 & 3	Yes	No	250 hours/month of t2.medium notebook 50 hours/month of m4.xlarge 125 hours/month of m4.xlarge
IBM Watson Studio	Varies, limited free tier	Python, R, Scala	Yes	Yes	1 vCPU and 4 GB RAM, 50 hours run-time per month
Codalab	Free	Any	Yes	Yes	non-GPU machine has 4 cores and 14 GB of memory, and each GPU machine has 6 cores and 56 GB of memory
MyBinder	Free	Python 2 & 3, R, Julia	No	No	CPU: x86-64 RAM: ~13 GB (est) Disk: ~100 GB (est)

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Amazon SageMaker	Varies, 2 month free trial	Python 2			m 125
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Hosting services change their services from time to time, so be sure to double check the before starting your project!

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Slides:

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