EUDAT Collaborative Data Infrastructure

PRACE

Introduction to Keras TensorFlow

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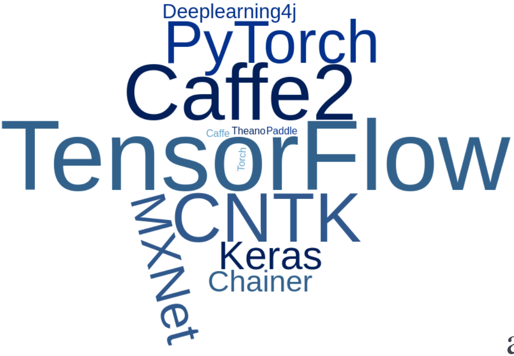
Deep learning frameworks



and others

https://skymind.ai/wiki/comparison-frameworks-dl4j-tensorflow-pytorch

TensorFlow

- Google Brain's second generation machine learning system

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- computations are expressed as stateful data-flow graphs

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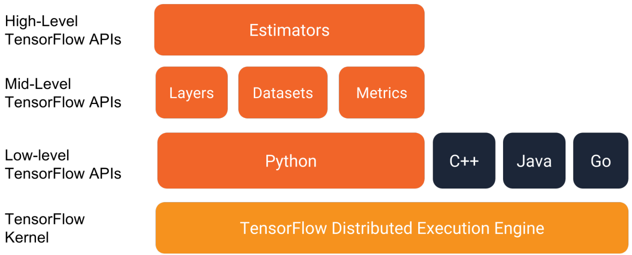
- Apache 2.0 open-source license

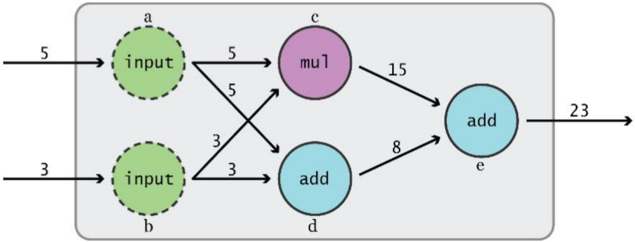
Tensorflow

- Tensorflow is a computational framework for building machine learning models
  - High-level, object-oriented API (tf.estimator)
  - Libraries for common model components (tf.layers/tf.losses/tf.metrics)
  - Lower-level APIs (TensorFlow)



TensorFlow dataflow graph

- TensorFlow 1 separates definition of computations from their execution
  - Phase 1: assemble a graph
  - Phase 2: use a session to execute operations in the graph.
- not true in eager mode (default in TensorFlow 2)



Introduction

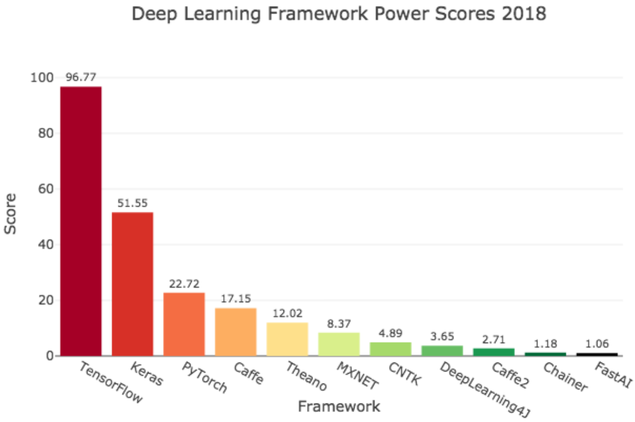
Keras

Distributed Deep Learning

Keras

- Keras is a high-level neural networks API, written in Python, developed with a focus on enabling fast experimentation.
- Keras offers a consistent and simple API, which minimizes the number of user actions required for common use cases, and provides clear and actionable feedback upon user error.
- Keras is capable of running on top of many deep learning backends such as TensorFlow, CNTK, or Theano. This capability allows Keras model to be portable across all these backends.
- Kesas is one of the most used Deep Learning Framework used by researchers, and is now part of the official TensorFlow Higher Level API as tf.keras
- Keras models can be trained on CPUs, Xeon Phi, Google TPUs and any GPU or OpenCL-enabled GPU like device.
- Keras is the TensorFlow's high-level API for building and training deep learning models.

Keras



Deep Learning Framework Power Scores 2018
Score
100
80
60
40
20
0
96.77
51.55
22.72
17.15
12.02
8.37
4.89
3.65
2.71
1.18
1.06
TensorFlow
Keras
PyTorch
Caffe
Theano
MXNET
CNTK
DeepLearning4J
Caffe2
Chainer
FastAI
Framework

Building models with Keras

- The core data structure of Keras is the Model which is basically a container of one or more Layers.
- There are two main types of models available in Keras: the Sequential model and the Model class, the latter used to create advanced models.
- The simplest type of model is the Sequential model, which is a linear stack of layers. Each layer is added to the model using the .add() method of the Sequential model object.
- The model needs to know what input shape it should expect. The first layer in a Sequential model (and only the first) needs to receive information about its input shape, specifing the input_shape argument. The following layers can do automatic shape inference from the shape of its predecessor layer.

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Model build

```
import tensorflow as tf
from tensorflow import keras

from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Activation

model = Sequential()
# Adds to the model a densely-connected
# layer with 32 units with input shape 16:
model.add(Dense(32, input_shape=(16,)))
# Adds another layer with 16 units,
# each connected to 32 outputs of previous layer
model.add(Dense(16))
# Last layer with 8 units,
# each connected to 16 outputs of previous layer
model.add(Dense(8, activation='softmax'))
```

Activation functions

- The activation argument specifies the activation function for the current layer. By default, no activation is applied.
- The softmax activation function normalize the output to a probability distribution. Is commonly used in the last layer of a model. To select a single output in a classification problem the most probable one can be selected.
- The ReLU (Rectified Linear Unit), $\max(0,x)$, is commonly used as activation function for the hidden layers.
- Many other activation functions are available or easily defined as well as layer types.

Model compile

- Once the model is built, the learning process is configured by calling the compile method. The compile phase is required to configure the following (mandatory) elements of the model:
  - optimizer: this object specifies the optimization algorithm which adapt the weights of the layers during the training procedure;
  - loss: this object specifies the function to minimize during the optimization;
  - metrics: [optional] this objects measure the performance of your model and is used to monitor the training

```
# Configure the model for mean-squared error regression.
model.compile(optimizer='sgd', # stochastic gradient descent
loss='mse', # mean squared error
metrics=['accuracy']) # an optional list of metrics
```

Model compile

- Once the model is compiled, we can check its status using the summary and get precious information on model composition, layer connections and number of parameters.

```
model.summary()

_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense (Dense)                (None, 32)                544
_________________________________________________________________
dense_1 (Dense)              (None, 16)                528
_________________________________________________________________
dense_2 (Dense)              (None, 8)                 136
=================================================================
Total params: 1,208
Trainable params: 1,208
Non-trainable params: 0
_________________________________________________________________
```

Model training

- The .fit method trains the model against a set of training data, and reports loss and accuracy useful to monitor the training process.

```
import numpy as np

# generate synthetic training dataset
x_train = np.random.random((1000, 16))
y_train = np.random.random((1000, 8))

# generate synthetic validation data
x_valid = np.random.random((100, 16))
y_valid = np.random.random((100, 8))

# fit the model using training dataset
# over 10 epochs of 32 batch size each
# report training progress against validation data
model.fit(x=x_train, y=y_train,
          batch_size=32, epochs=10,
          validation_data=(x_valid, y_valid))
```

Model evaluation and prediction

- Once the training process has completed, the model can be evaluated against the validation dataset. The evaluate method returns the loss value and, if the model was compiled providing also a metrics argument, the metric values.

```
model.evaluate(x_valid, y_valid, batch_size=32)
```

- The predict method can finally be used to make inference on new data

```
model.predict(x_valid, batch_size=128)
```

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Model saving and restore

- A trained model can be saved and stored to a file for later retreival. This allows you to checkpoint a model and resume training later without rebuiling and training from scratch.
- Files are saved in HDF5 format, with all weight values, model's configuration and even the optimizer's configuration.

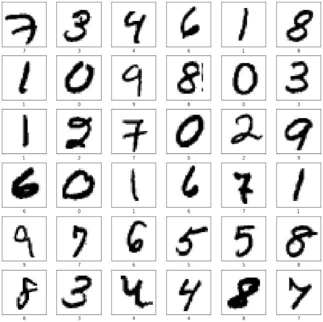
```
save_model_path='saved/intro_model'
model.save(filepath=save_model_path, include_optimizer=True)
```

```
model = tf.keras.models.load_model(filepath=save_model_path)
```

Try it out

The MINIST dataset

- The MNIST data set is a standard set of handwritten numerical digits from 0 to 9 which is commonly used as the "Hello World" test for Deep Learning classification problem.
- Each sample is a 28×28 grayscale image.



Loading MNIST

- Keras comes with many dataset built in and automatically splits the data into a training and validation set.

```
(x_train, y_train), (x_test, y_test) = tf.keras.datasets.mnist.
    load_data()
```

Defining a model

```
model.add(tf.keras.layers.Conv2D(filters=64, kernel_size=2, padding='
    same', activation='relu', input_shape=(??,??,?)))
model.add(tf.keras.layers.MaxPooling2D(pool_size=2))
model.add(tf.keras.layers.Dropout(0.3))
model.add(tf.keras.layers.Conv2D(filters=32, kernel_size=2, padding='
    same', activation='relu'))
model.add(tf.keras.layers.MaxPooling2D(pool_size=2))
model.add(tf.keras.layers.Dropout(0.3))
model.add(tf.keras.layers.Flatten())
model.add(tf.keras.layers.Dense(256, activation='relu'))
model.add(tf.keras.layers.Dropout(0.5))
model.add(tf.keras.layers.Dense(?, activation='softmax'))
```

Compiling and Training

- The categorical cross entropy, $-\sum p(x)q(x)$, with p the true distribution and q the expected one.
- Adam is adaptive learning rate optimization algorithm.

```
model.compile(loss='categorical_crossentropy',
              optimizer='adam',
              metrics=['accuracy'])
```

```
model.fit(x_train,
          y_train,
          batch_size=64,
          epochs=10,
          validation_data=(x_valid, y_valid),
          )
```

- Try it out

Callbacks

- What if we want to stop if accuracy is > 0.01 ?
- define a callback

```
class myCallback(keras.callbacks.Callback)
    def on_epoch_end(self,epoch,logs={}):
        if(logs.get('acc')>0.01):
            print("\nAccuracy exceeds threshold, Stop train!")
            self.model.stop_training =True
```

- the install it

```
mycallbacks=myCallBack()
model.fit(train_images,train_labels,epoch=100,callbacks=[mycallbacks
     ])
```

Callbacks

- Keras provides some predefined callbacks to feed in, among them for example:
  - **TerminateOnNaN()**: that terminates training when a NaN loss is encountered
  - **ProgbarLogger()**: that prints metrics to stdout
  - **ModelCheckpoint(filepath)**: that save the model after every epoch
  - **EarlyStopping**: which stop training when a monitored quantity has stopped improving
  - **LambdaCallback**: for creating simple, custom callbacks on-the-fly
- You can select one or more callback and pass them as a list to the callback argument of the fit method.
- You can also create a callback object from scratch, customizing its behaviour overloading the base methods of the Callback Keras class:
  - **on_epoch_begin** and **on_epoch_end**
  - **on_batch_begin** and **on_batch_end**
  - **on_train_begin** and **on_train_end**
- A callback has access to its associated model through the class property self.model, so that you can monitor and access many of the quantities which are in the optimization process.

Introduction

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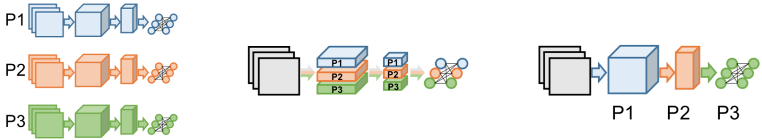
Distributed Deep Learning

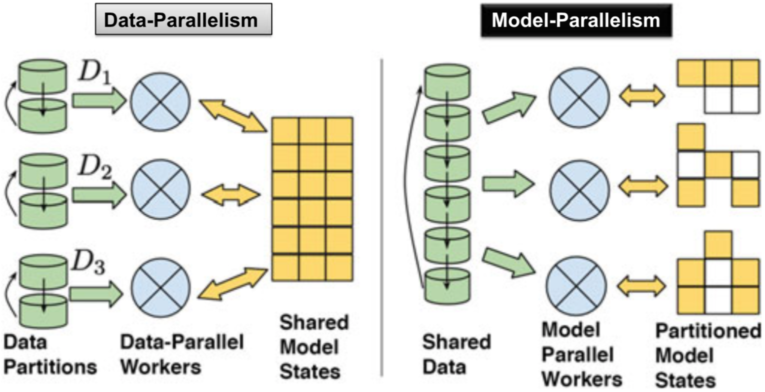
Neural Network concurrency



(a) Data Parallelism (b) Model Parallelism (c) Layer Pipelining

Tal Ben-Nun and Torsten Hoefler, Demystifying Parallel and Distributed Deep Learning: An In-Depth Concurrency Analysis, 2018

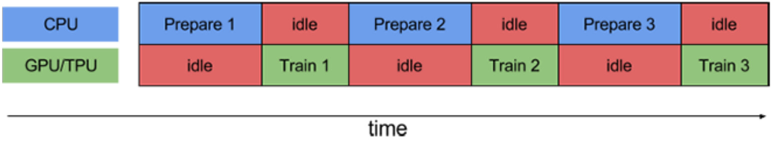
Data Parallelism vs Model Parallelism

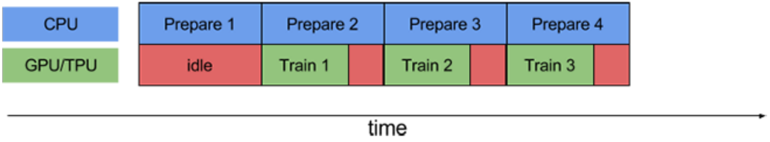


Hardware and Libraries

- It is not only a matter of computational power:
  - CPU (MKL-DNN)
  - GPU (cuDNN)
  - FPGA
  - TPU
- Input/Output
  - SSD
  - Parallel file system (if you run in parallel)
- Communication and interconnection too, if you are running in distributed mode
  - MPI
  - gRPC + verbs (RDMA)
  - NCCL

Data Input Pipeline





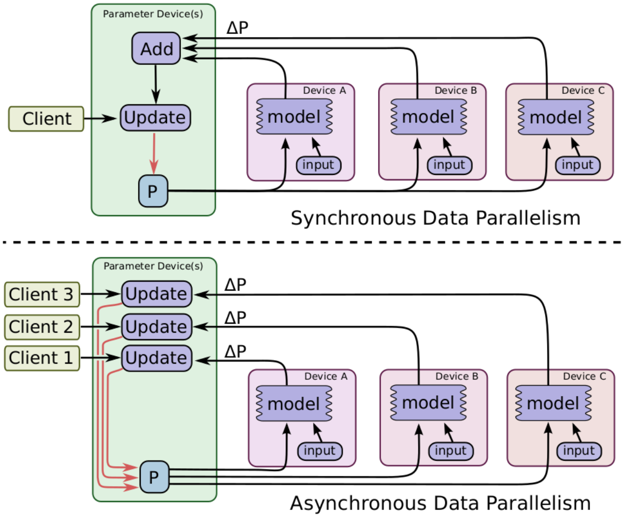
CPU optimizations

- Built from source with all of the instructions supported by the target CPU and the MKL-DNN option for Intel® CPU.
- Adjust thread pools
  - *intra_op_parallelism_threads*: Nodes that can use multiple threads to parallelize their execution will schedule the individual pieces into this pool. (*OMP_NUM_THREADS*)
  - *inter_op_parallelism_threads*: All ready nodes are scheduled in this pool

```
config = tf.ConfigProto()
config.intra_op_parallelism_threads = 44
config.inter_op_parallelism_threads = 44
tf.session(config=config)
```

- The MKL is optimized for NCHW (default NHWC) data format and use the following variables to tune performance: *KMP_BLOCKTIME*, *KMP_AFFINITY*, *OMP_NUM_THREADS*

Synchronous and asynchronous data parallel training



Keras GPUs Parallel Model

```
model = keras.Sequential()
...
gpus=4
parallel_model = keras.utils.multi_gpu_model(model, gpus=gpus)

parallel_model.compile(loss='categorical_crossentropy',
             optimizer='adam',
             metrics=['accuracy'])

parallel_model.fit(x_train,
         y_train,
         batch_size=batch_size,
         epochs=epochs,
         validation_data=(x_valid, y_valid),
         )
```

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Keras + Uber/Horovod

```
...
import horovod.tensorflow.keras as hvd
...
#Horovod: initialize Horovod.
hvd.init()

opt = tf.keras.optimizers.Adam(0.001 * hvd.size())
opt = hvd.DistributedOptimizer(opt)

model.compile(loss='categorical_crossentropy',
              optimizer=opt,
              metrics=['accuracy'])

callbacks = [
    # Horovod: broadcast initial variable states from rank 0 to all
         other processes.
    hvd.callbacks.BroadcastGlobalVariablesCallback(0),
]

model.fit(x_train,
         y_train,
         batch_size=batch_size,
         callbacks=callbacks,
         epochs=epochs,
         validation_data=(x_valid, y_valid)
         )
```

Hands-on

- Use $keras - mnist.py$
- Define the input shape in the first layer and the output shape in the last layer
- Run it and play with hyperpameters

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- Use *keras – mnist.py*
- Define the input shape in the first layer and the output shape in the last layer
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- Use *keras – mnist – mgpu.py*
- Try the multi GPU on Galileo. Play with the number of GPU and the hyperparameter (*batchsize* and *epochs*)

Hands-on

- Use $keras-mnist.py$
- Define the input shape in the first layer and the output shape in the last layer
- Run it and play with hyperpameters
- Use $keras-mnist-mgpu.py$
- Try the multi GPU on Galileo. Play with the number of GPU and the hyperparameter ($batchsize$ and $epochs$)
- Use $keras-mnist-hvd.py$. Play with the number of GPU, the number of nodes and the hyperparameters ($batchsize$ and $epochs$)

Other References

- Horovod
- NCCL
- MNIST
- CIFAR datasets
- Deeplearning.ai youtube channel