TensorFlow at Scale

MPI, RDMA and All That

Thorsten Kurth, Mikhail Smorkalov, Peter Mendygral, Srinivas Sridharan, Amrita Mathuriya

CUG18
Stockholm, Sweden
Motivation for Scalable Deep Learning

- rapid prototyping/model evaluation
- problem scale
- volume of scientific datasets can be large
- scientific datasets can be complex (multivariate, high-dimensional)
- machine learning models become bigger (model parallelism)

http://tjmachinelearning.com/lectures/deep/deepnn.html
Data Parallel Training

- applies to Stochastic Gradient Descent-type algorithms
- each node takes part of the data and computes model updates independently without communication
- these updates are then collectively summed and applied to the local model

From Pradeep Dubey, “Scaling to Meet the Growing Needs of Artificial Intelligence (AI), IDF 2016
TensorFlow

- high-productivity deep learning framework
- uses Python functions with optimized backends (MKL-DNN, cuDNN)
- user defines graph and executes it in a `tf.Session`
- enables users to write efficient dl code for cutting edge hardware without knowledge about performance-oriented programming

```python
import tensorflow as tf
import numpy as np

# Parameters
learning_rate = 0.01
training_epochs = 1000
display_step = 50

# Training Data
train_X = np.asarray([3.3, 4.4, 5.5, 6.71, 6.93, 4.16, 9.779, 6.182, 7.59, 2.167, 7.042, 10.791, 5.313, 7.997, 5.654, 9.27, 3.1])
train_Y = np.asarray([1.7, 2.76, 2.09, 3.19, 1.694, 1.573, 3.366, 2.596, 2.53, 1.221, 2.827, 3.465, 1.65, 2.904, 2.42, 2.94, 1.3])
n_samples = train_X.shape[0]

# tf Graph Input
X = tf.placeholder("float")
Y = tf.placeholder("float")

# Set model weights
W = tf.Variable(rng.randn(), name="weight")
b = tf.Variable(rng.randn(), name="bias")

# Construct a linear model
pred = tf.add(tf.multiply(X, W), b)

# Mean squared error
cost = tf.reduce_sum(tf.pow(pred - Y, 2))/(2*n_samples)

# Gradient descent
optimizer = tf.train.GradientDescentOptimizer(learning_rate).minimize(cost)

# Initialize the variables (i.e. assign their default value)
init = tf.global_variables_initializer()

# Start training
with tf.Session() as sess:
    sess.run(init)
    for epoch in range(training_epochs):
        for (x, y) in zip(train_X, train_Y):
            sess.run(optimizer, feed_dict={X: x, Y: y})
```
Distributed Training in TensorFlow

- TensorFlow natively supports Google RPC
  
  **pros**: asynchronous, multi-platform, resilient, integrated

  **cons**: not made for HPC, slow, server-client model, initialization on HPC systems painful

  **solution**: use custom TensorFlow ops hook to hook-in *your own* framework

https://www.theregister.co.uk/2015/10/27/another_go_at_remote_objects_google_grpc_hits_beta/

A. Mathuriya, et.al.: Scaling GRPC Tensorflow on 512 nodes of Cori Supercomputer
Horovod(-MPI)

- plugin developed by Uber
- works with TensorFlow and Keras (higher level TF abstraction)
- couples communication background thread asynchronously into executed TensorFlow graph
- communication performed using MPI intrinsics (Send/Recv/Bcast/Allreduce)
- works on all platforms with MPI
- can be mixed and matched with mpi4py

```python
import tensorflow as tf
import numpy
import horovod.tensorflow as hvd

hvd.init()

# Parameters

# tf Graph Input
X = tf.placeholder("float")
Y = tf.placeholder("float")

# Set model weights
W = tf.Variable(rng.randn(), name="weight")
b = tf.Variable(rng.randn(), name="bias")

# Construct a linear model
pred = tf.add(tf.multiply(X, W), b)

# Mean squared error
cost = tf.reduce_sum(tf.pow(pred-Y, 2))/(2*n_samples)

# Gradient descent
global_step = tf.train.get_or_create_global_step()
optimizer = tf.train.GradientDescentOptimizer(learning_rate)
optimizer = hvd.DistributedOptimizer(optimizer)
 optimizer = optimizer.minimize(cost, global_step=global_step)

# Initialize the variables (i.e. assign their default value)
init = tf.global_variables_initializer()
bcast = hvd.broadcast_global_variables(0)

# Start training
with tf.train.MonitoredTrainingSession() as sess:
    sess.run(init)
sess.run(bcast)

    # Fit all training data
    for epoch in range(training_epochs):
        for (x, y) in zip(train_X, train_Y):
            sess.run(optimizer, feed_dict={X: x, Y: y})
```
Horovod(-MPI)

- plugin developed by Uber
- works with TensorFlow and Keras (higher level TF abstraction)
- couples communication background thread asynchronously into executed TensorFlow graph
- communication performed using MPI intrinsics (Send/Recv/Bcast/Allreduce)
- works on all platforms with MPI
- can be mixed and matched with mpi4py

```python
import tensorflow as tf
import numpy as np
import horovod.tensorflow as hvd

hvd.init()
# Parameters
...
# tf Graph Input
X = tf.placeholder("float")
Y = tf.placeholder("float")
# Set model weights
W = tf.Variable(rng.randn(), name=\"weight\")
b = tf.Variable(rng.randn(), name=\"bias\")
# Construct a linear model
pred = tf.add(tf.multiply(X, W), b)
# Mean squared error
cost = tf.reduce_sum(tf.pow(pred-Y, 2))/(2*n_samples)
# Gradient descent
global_step = tf.train.get_or_create_global_step()  # Global step
optimizer = tf.train.GradientDescentOptimizer(learning_rate)
optimizer = hvd.DistributedOptimizer(optimizer)
optimizer = optimizer.minimize(cost, global_step=global_step)
# Initialize the variables (i.e. assign their default value)
init = tf.global_variables_initializer()
bcast = hvd.broadcast_global_variables(0)
# Start training
with tf.train.MonitoredTrainingSession() as sess:
sess.run(init)
sess.run(bcast)
# Fit all training data
for epoch in range(training_epochs):
    for (x, y) in zip(train_X, train_Y):
        sess.run(optimizer, feed_dict={X: x, Y: y})
```

limited changes to source code
Other Horovod Variants

• Horovod-MLSL by Intel
  • uses MLSL instead of MPI
  • wrappers are source code compatible with Horovod-MPI
  • can employ more than one BG process to progress communication
  • on machines without MPI_Comm_spawn() support, MLSL servers need to be launched manually

• Horovod-NCCL
  • uses nvidia NCCL 2 for GPU2GPU communication and efficient collectives
  • aims at improving performance for HPC systems with fat (multi-GPU) nodes
CPE ML Plugin

- plugin similar to Horovod
- different syntax
- more LOC need to be changed
- support for other frameworks than TensorFlow
- support for sophisticated features such as pipelining, multi-threaded communication, solver cool-down
- only available on Cray hardware

```python
import tensorflow as tf
import numpy as np
import ml_comm as mc

mc.init(1, 1, 5*1024*1024, "tensorflow")

# Parameters
...

# tf Graph Input
X = tf.placeholder("float")
Y = tf.placeholder("float")

# Set model weights
W = tf.Variable(rng.randn(), name="weight")
b = tf.Variable(rng.randn(), name="bias")

# Construct a linear model
pred = tf.add(tf.multiply(X, W), b)

# Mean squared error
cost = tf.reduce_sum(tf.pow(pred - Y, 2))/(2*n_samples)

# Gradient descent
global_step = tf.train.get_or_create_global_step()
optimizer = tf.train.GradientDescentOptimizer(learning_rate)

# Split global and local reduction
grads_and_vars = optimizer.compute_gradients(cost)
grads = mc.gradients([gv[0] for gv in grads_and_vars], 0)
gs_and_vs = [(g,v) for (_,v), g in zip(grads_and_vars, grads)]
optimizer = optimizer.apply_gradients(gs_and_vs, global_step=global_step)

# Initialise the variables (i.e. assign their default value)
init = tf.global_variables_initializer()
bcast = ...

# Start training
...
```
HPC Systems

- Cori-KNL (NERSC, XC40)
  - 9688 Intel Xeon Phi 7250 (KNL)
  - 68 cores@1.4Ghz, AVX512
  - 96GB DDR and 16GB on-package MCDRAM
- Piz Daint (CSCS, XC50)
  - 5320 CPU+GPU
  - Xeon E5-2695v3 and Tesla P100
  - 64 GB DDR, 16GB HBM2
Deep Learning Models

- HEP-CNN
  - binary collider event-classification
  - 7-layer CNN
  - lightweight: sparse or small layers only
- CosmoGAN
  - generates cosmology mass-maps
  - 2x5-layer DC-GAN
  - underlying architecture for other scientific GAN use-cases at NERSC
Strong Scaling on Cori

- scale from 1 node w/ batch-size 64 to 64 nodes w/ batch-size 1
- efficient performance scaling stops around 8 or 16 nodes for all frameworks
- can be applied for small-scale parallelization w/o as it requires no additional HPO
- not the favorable mode to scale deep learning training

CosmoGAN
Weak Scaling CosmoGAN

- good scaling efficiency of all frameworks
- Horovod-MPI: high variability but outperforms CPE ML on Piz Daint (better overlap, more threads might help)
Weak Scaling HEP-CNN

- network latency and jitter sensitive, ~40 ms (FW+BW)/sample (KNL)
- on Cori similar efficiency for all frameworks, on Piz Daint CPE significantly better than Horovod-MPI
Convergence (Time to Solution)

- result with plain ADAM optimizer
Conclusion

• scalable deep learning solutions can be implemented in high productivity frameworks such as TensorFlow

• all tested frameworks integrate beautifully into TensorFlow and outperform GRPC

• performance: Horovod-MLSL, CPE ML Plugin

• portability: Horovod-MPI, Horovod-MLSL

• fat nodes? try Horovod-NCCCL but has some limitations still

• missing in all frameworks: hooks for model parallelism