Scaling Deep Learning Training

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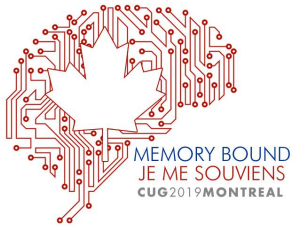
Data Analytics Tutorial
CUG19 – Montreal, Canada

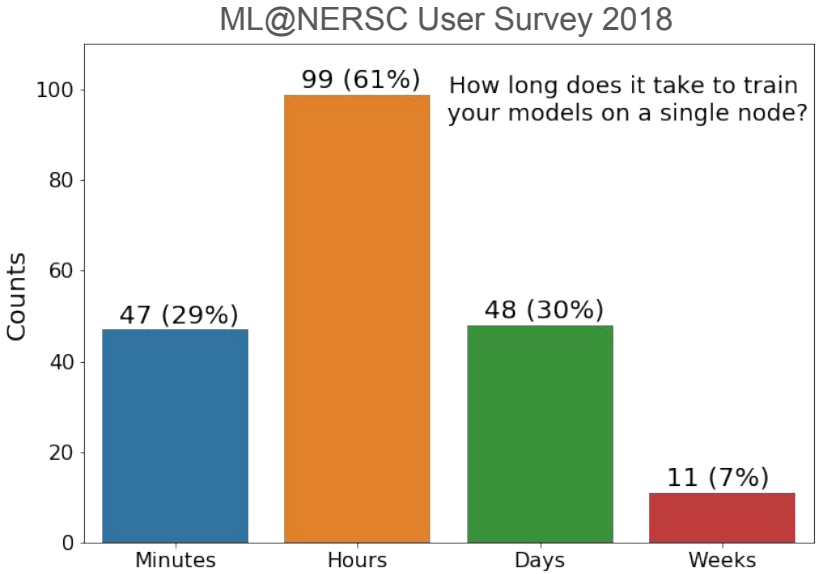


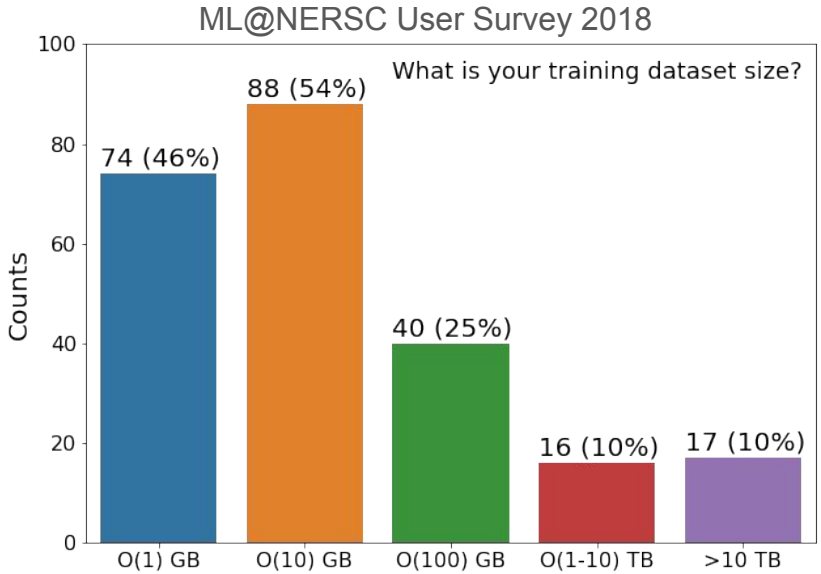
Overview

- Foundations of Distributed Training
  - motivation
  - training parallelization strategies
  - large batch training
    - learning rate scaling
    - batch size scaling
    - generalization gap

- Hands-On
  - dataset introduction
  - Horovod and CPE ML
  - Some remarks for improving accuracy
  - play around…

Why do we need to scale deep learning applications?

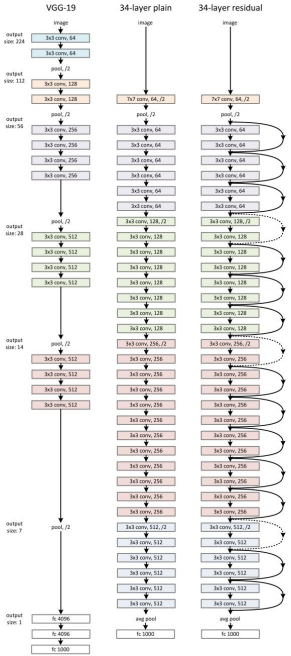


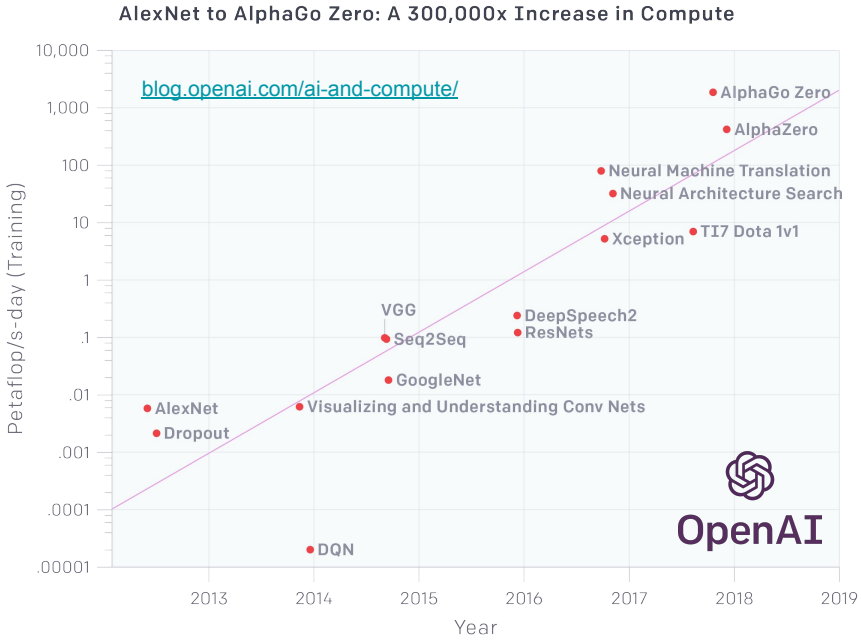


- Rapid prototyping/model evaluation
- Problem scale

- Volume of scientific datasets can be large
- Scientific datasets can be complex (multivariate, high dimensional)

Why do we need to scale deep learning applications?

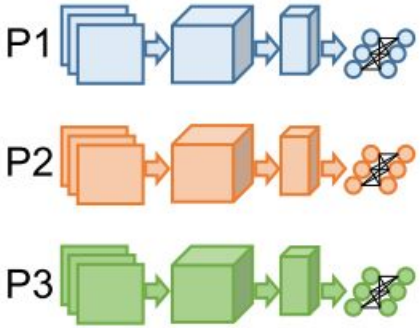




Models get bigger and more compute intensive as they tackle more complex tasks

"... total amount of compute, in petaflop/s-days, that was used to train selected results ... A petaflop/s-day (pfs-day) = ... 10^{15} neural net operations per second for one day, or a total of about 10^{20} operations." -- OpenAI Blog

Parallelism strategies

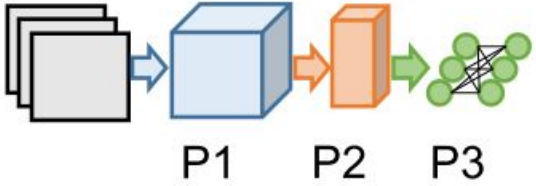


Data Parallelism

Distribute input samples.

Model Parallelism

Distribute network structure (layers).



Layer Pipelining

Partition by layer.

Fig. credit: Ben-Nun and Hoefler arXiv:1802.09941

Data parallelism, synchronous Updates

Gradients are computed locally and summed across nodes. Updates are propagated to all nodes

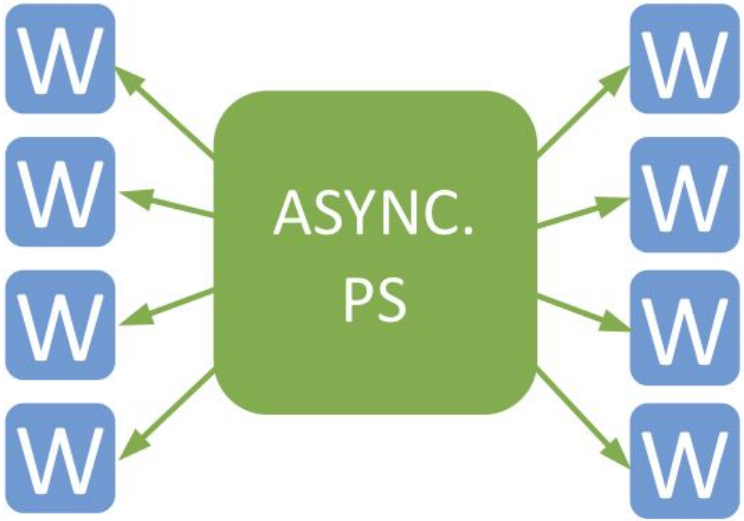
- stable convergence
- scaling is not optimal because all nodes have to wait for reduction to complete
- global (effective) batch size grows with number of nodes

Synchronous SGD, decentralized

Data parallelism, asynchronous Updates

Gradients are sent to parameters server. Parameters servers incorporates gradients into model as they arrive and sends back the updated model

- nodes don't wait (perfect scaling)
- resilient
- stale gradients impact convergence rate (depends on #workers)
- parameter server is a bottleneck

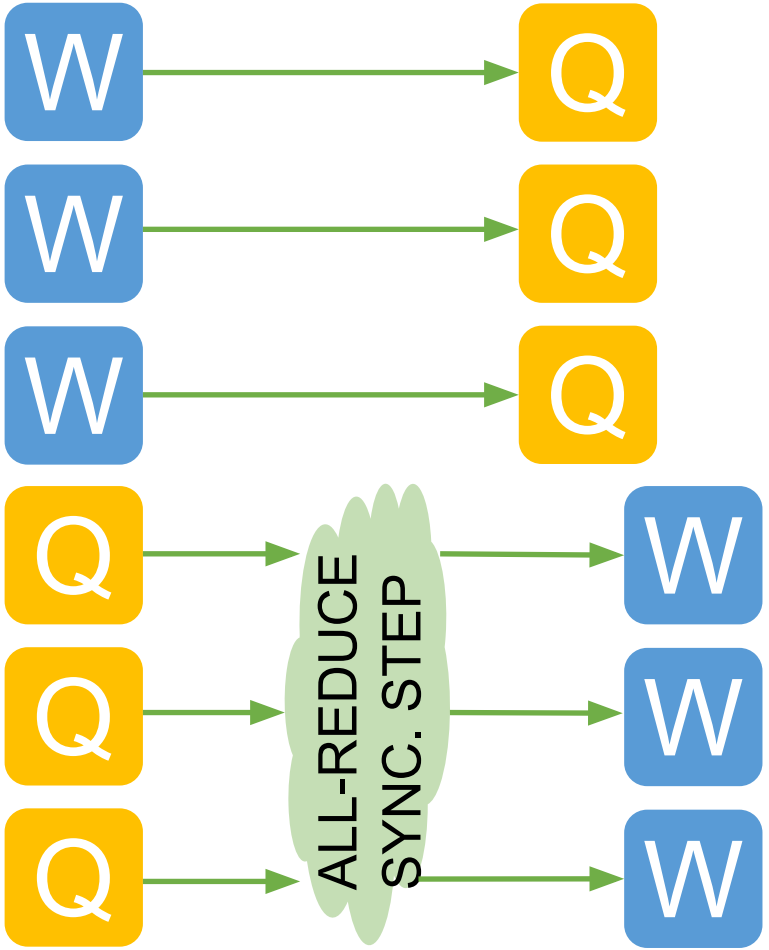


Asynchronous SGD, parameter-server

Data parallelism, stale-synchronous Updates (pipelining)

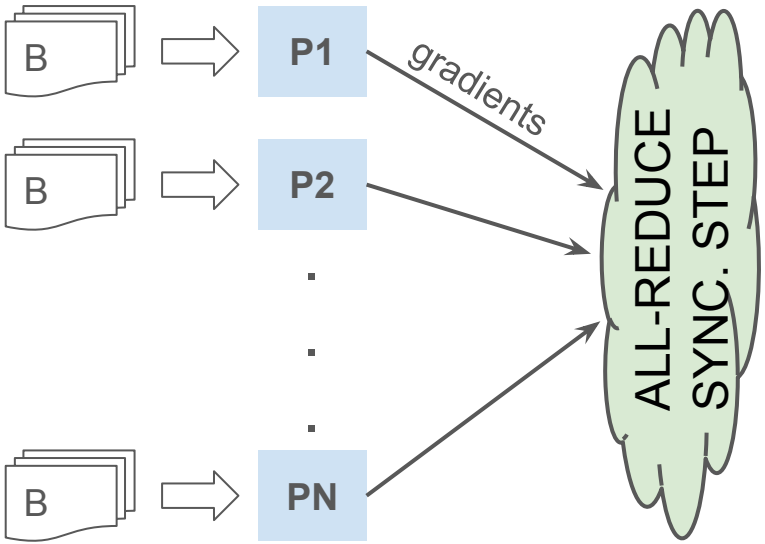
Current gradients are computed and pushed into queue while at the same time, older gradients are popped from the queue and reduced across all the nodes synchronously.

- better scaling than fully synchronous (especially on heterogeneous systems)
- not as *extreme* as fully asynchronous
- convergence can be negatively impacted if *lag* (=number of steps between reduced and current gradients) is large
- not resilient but smoothens runtime variability



Large-Batch Training (LBT), synchronous weak scaling

- applies to SGD-type algorithms
  - data batch per node. Model updates are computed independently
  - updates are collectively summed and applied to the local model

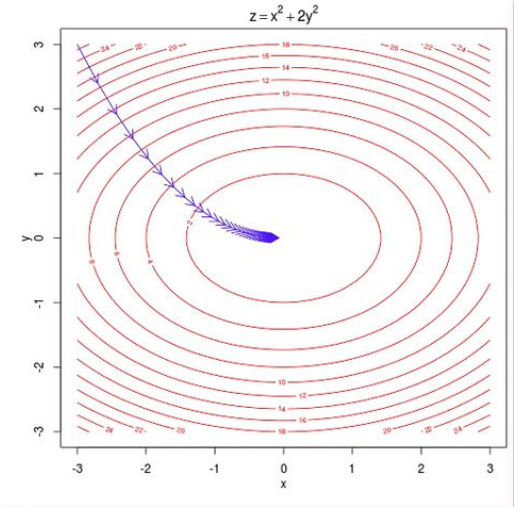


Local batch-size = B

Global batch-size = N * B

Stochastic Gradient Descent (SGD)

$$w_{t+1} \leftarrow w_t - \frac{\eta}{B} \sum_{i=1}^{B} \nabla L(x_i, w_t)$$



N is total sample size

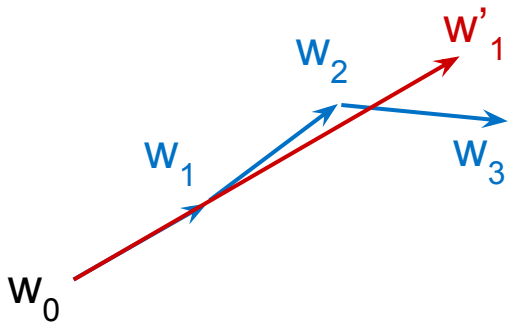
B is batch-size

η is learning rate

Δw is the parameter update in one gradient descent step

Linear learning-rate scaling

$$\eta \rightarrow N * \eta$$

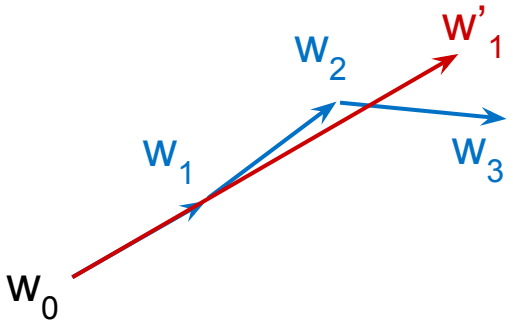


Upper: 3 SGD steps w. learning-rate = η
Lower: 1 SGD step w. learning-rate = 3 * η

Linear learning-rate scaling

$$w_{t+1} \leftarrow w_t - \frac{\eta}{B}\left(\sum_{i=1}^{B} \nabla L(x_i, w_t) + \sum_{j=1}^{B} \nabla L(x_j, w_{t+1})\right)$$

$$w_{t+1} \leftarrow w_t - \frac{\eta_2}{2B} \sum_{i=1}^{2B} \nabla L(x_i, w_t)$$



Where:

$$\eta_2 = 2 * \eta$$

Upper: 3 SGD steps w. learning-rate = η

Lower: 1 SGD step w. learning-rate = 3 * η

Assumption:

$$\nabla L(x_j, w_{t+1}) \approx L(x_j, w_t)$$

Sqrt learning-rate scaling

$\eta \rightarrow \text{sqrt}(N) * \eta$

Motivated by the observation that the variance of the gradient scales with 1/batch-size:

$$\text{cov}\left(\Delta w, \Delta w\right) \approx \frac{\eta^2}{B}\left(\frac{1}{N}\sum_{i=1}^{N} \mathbf{g_i}\,\mathbf{g_i^T}\right)$$

Learning-rate scaling

In practice, we see anywhere between sub-sqrt (e.g.You et al. arXiv:1708.03888) to linear scaling (e.g. Goyal et al. arXiv:1706.02677)

Recent OpenAI (arXiv:1812.06162) study has illuminated the dependence of optimal learning-rate on batchsize:

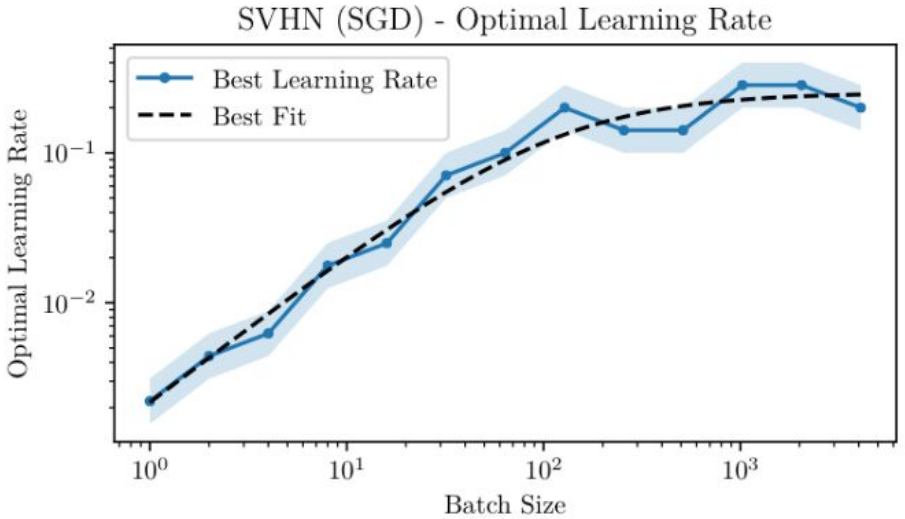


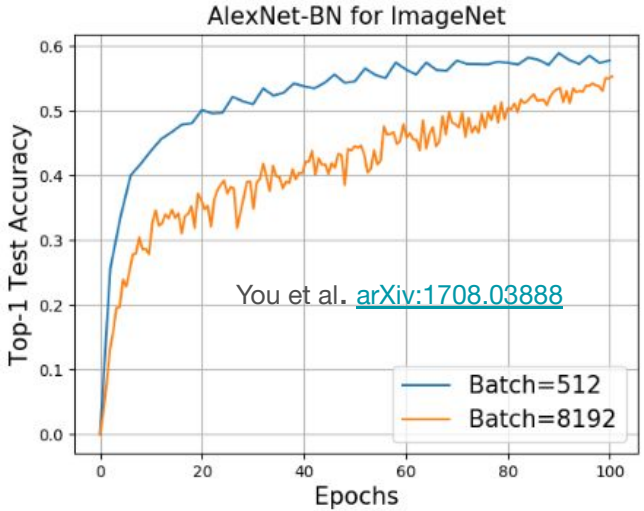
Fig. McCandlish, Kaplan and Amodei arXiv:1812.06162

Challenges with Large Batch Training

- Training with large learning rates is not stable in the initial stages of the training

  $\nabla L(w_{t+1}) \approx \nabla L(w_t)$ assumption breaks when parameters are changing rapidly

- A generalization gap appears: networks trained with small batches tend to optimize and generalize better



AlexNet You et al. arXiv:1708.03888

Batch	Base LR	accuracy,%
512	**0.02**	**60.2**
4096	0.16	58.1
4096	**0.18**	**58.9**
4096	0.21	58.5
4096	0.30	57.1
8192	0.23	57.6
8192	**0.30**	**58.0**
8192	0.32	57.7
8192	0.41	56.5

Challenges with Large Batch Training

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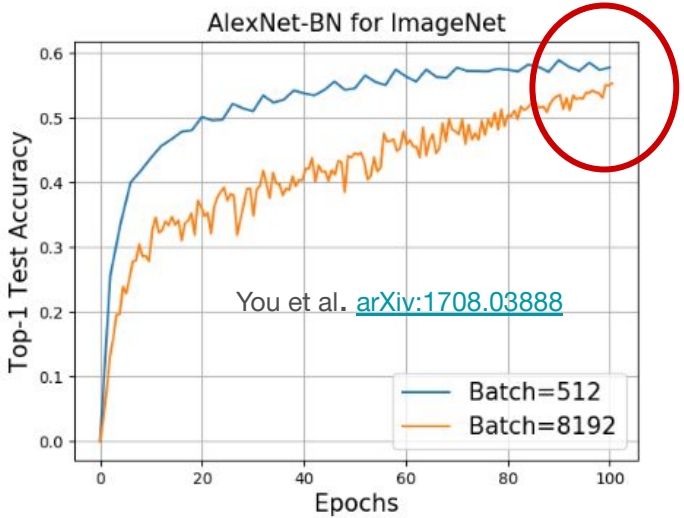
Scaling generalization gap



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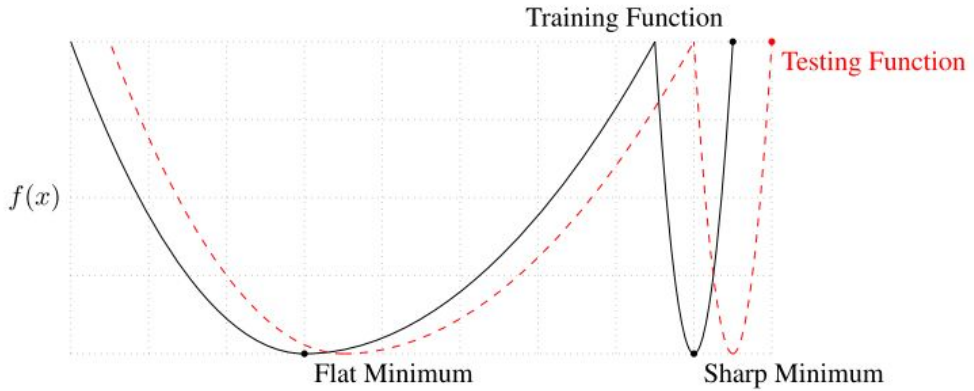
Explaining the generalization gap?

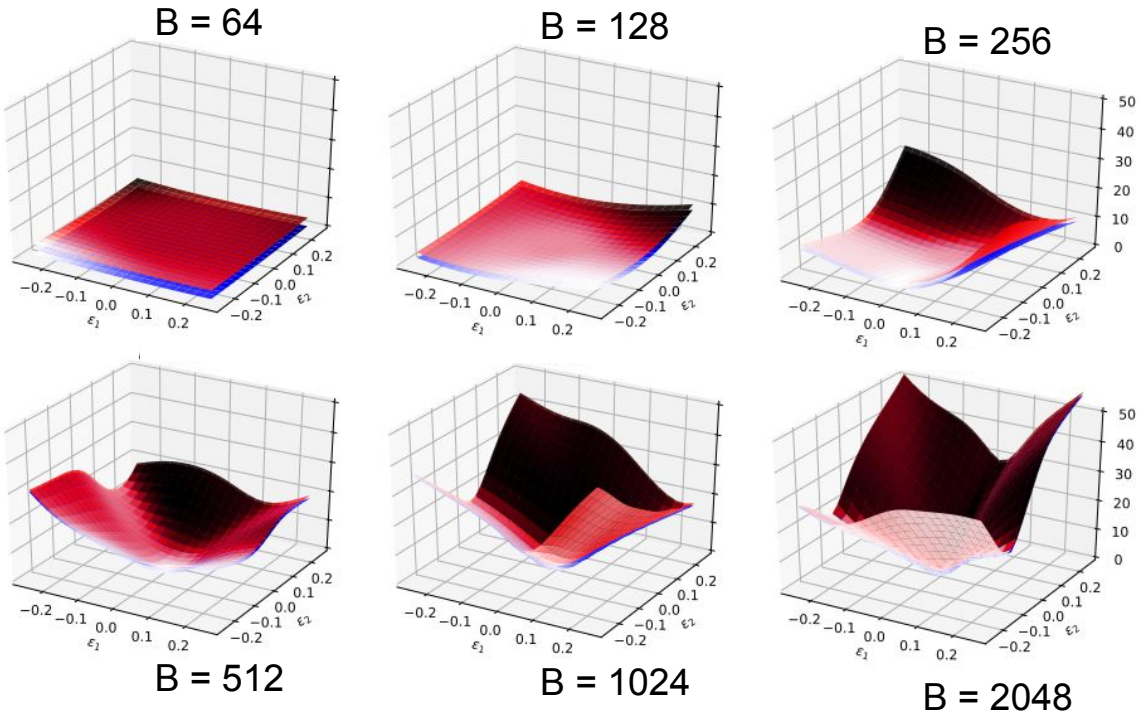
"*... large-batch … converge to sharp minimizers of the training function … In contrast, small-batch methods converge to flat minimizers*" -- Keskar et al, arXiv:1609.04836



Conceptual sketch of sharp and flat minimas of a loss function

Fig. credit: Keskar et al, arXiv:1609.04836

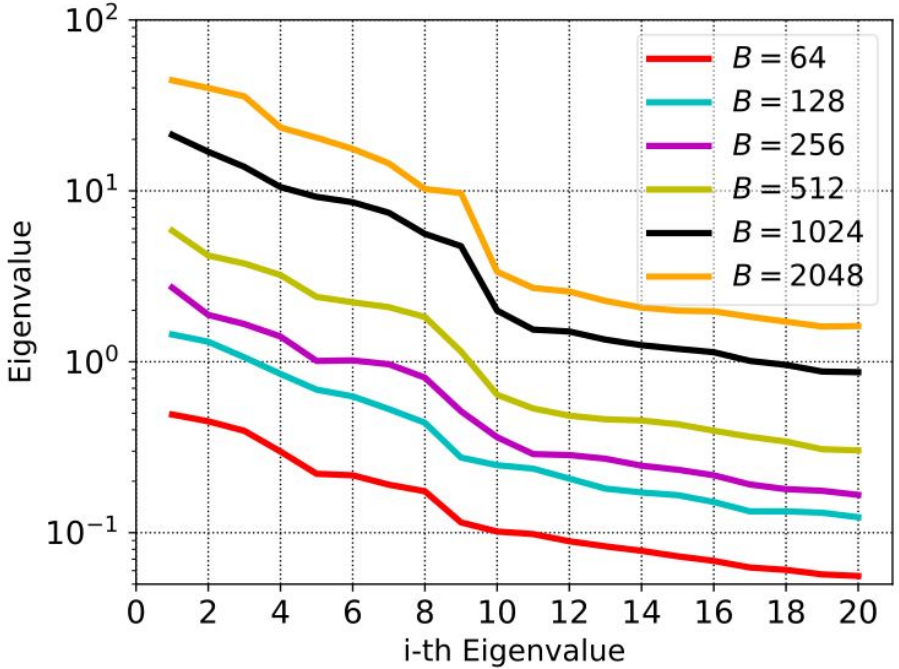
Explaining the generalization gap?



Loss at the end of training CIFAR-10 (axes are dominant eigenvectors of the Hessian)

Z. Yao et al. arXiv:1802.08241

Explaining the generalization gap?



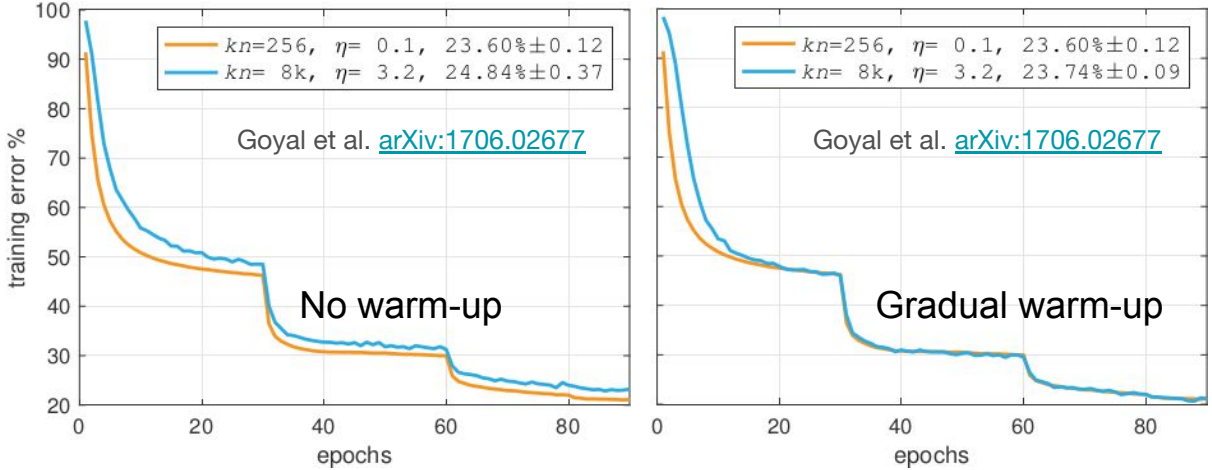
Hessian top-20 eigenvalues. Larger batchsize converge to points with higher spectrum.

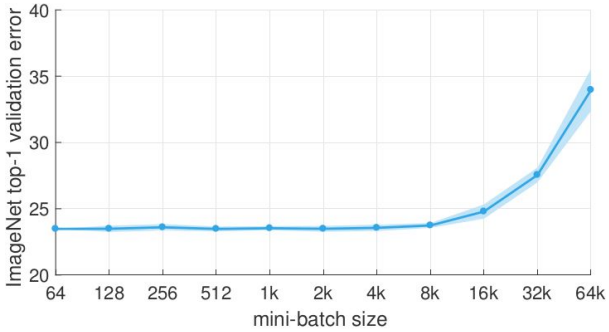
Z. Yao et al. arXiv:1802.08241

ResNet-50 ImageNet in 1 hour

FaceBook scaling result in 2017, batch-size=8k (using 256 GPUs):

- **Linear learning-rate warm-up** over 5 epochs to target rate
- **Linear scaling of learning-rate** (N * η) followed by original decay schedule
- The paper also clarifies subtleties and common pitfalls in distributed training

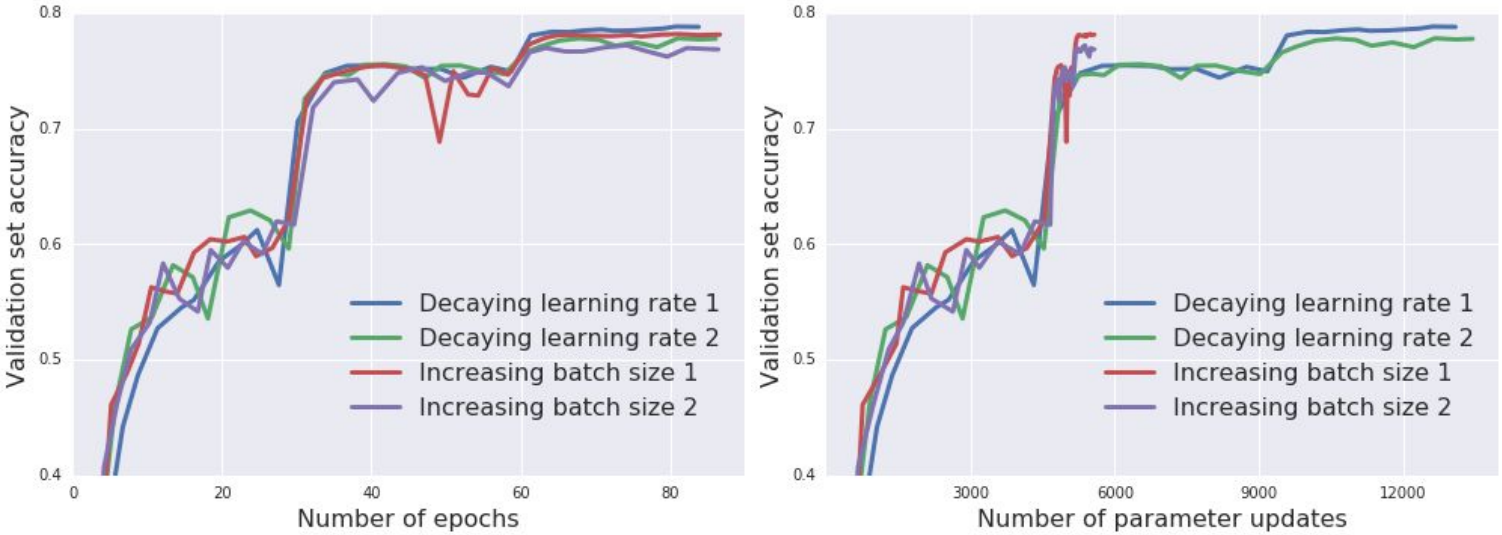




This scheme breaks down beyond batch-size = 8k for ResNet on ImageNet

Don’t decay the learning-rate, increase batch-size

Smith et al. arXiv:1711.00489 use batch-size scaling to train on ImageNet in 2500 parameter updates. Starting at batch-size 8k and scaling to 80k!

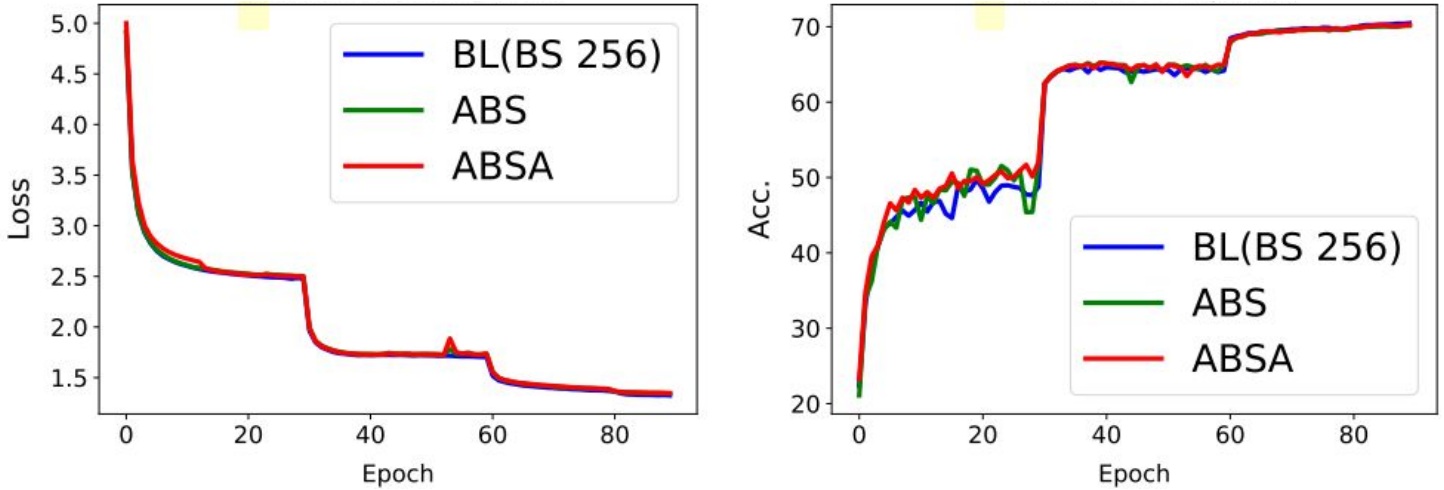


Inception-ResNet-V2 on ImageNet. Multiple runs to illustrate variance.

Adaptive batch-size scaling with 2nd-order information (ABSA)

Z. Yao et al. arXiv:1810.01021 close the generalization gap for a wide range of architectures on image classification tasks, using

- 2nd-order info. (~ loss surface curvature) to adaptively increase the batch-size
- adversarial training to regularize against *sharp-minima*



ABS and ABSA with ResNet-18 on ImageNet dataset with up to 16k batch-size

ImageNet/ResNet-50 Training in 224 Seconds

Hiroaki Mikami, Hisahiro Suganuma, Pongsakorn U-chupala,
Yoshiki Tanaka and Yuichi Kageyama
Sony Corporation
{Hiroaki.Mikami, Hisahiro.Suganuma, Pongsakorn.Uchupala,
Yoshiki.Tanaka, Yuichi.Kageyama}@sony.com

Abstract

Scaling the distributed deep learning to a massive GPU cluster level is challenging due to the instability of the large mini-batch training and the overhead of the gradient synchronization. We address the instability of the large mini-batch training with batch size control. We address the overhead of the gradient synchronization with 2D-Torus all-reduce. Specifically, 2D-Torus all-reduce arranges GPUs in a logical 2D grid and performs a series of collective operation in different orientations. These two techniques are implemented with Neural Network Libraries (NNL)[1] . We have successfully trained ImageNet/ResNet-50 in 224 seconds without significant accuracy loss on ABCI[2] cluster.

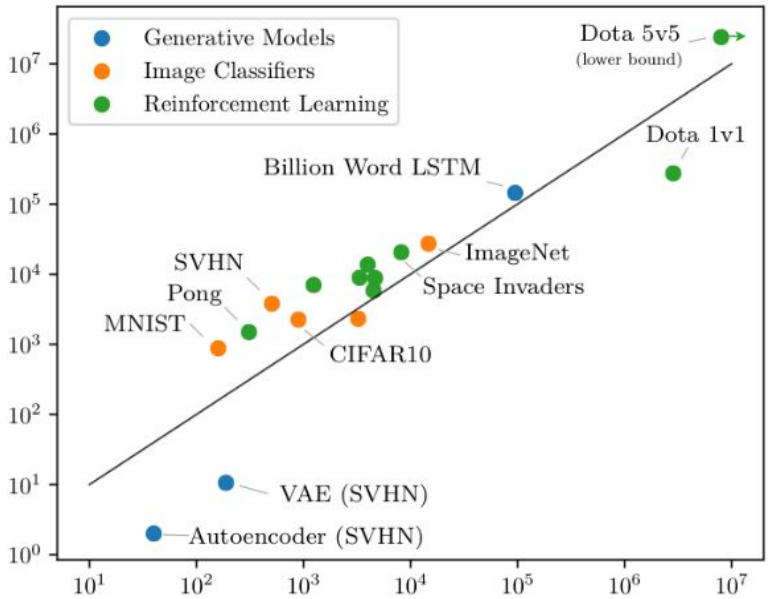
Limits of batch-size scaling

Recent empirical studies by OpenAI (arXiv:1812.06162) and Google Brain (arXiv:1811.03600) show that:

- A relationship between gradient noise scale and *critical* batch-size holds across many models, algorithms and datasets
- *gradient noise scale predicts maximum useful batch-size*
- More complex datasets/tasks have higher gradient noise, thus can benefit from training with larger batch-sizes

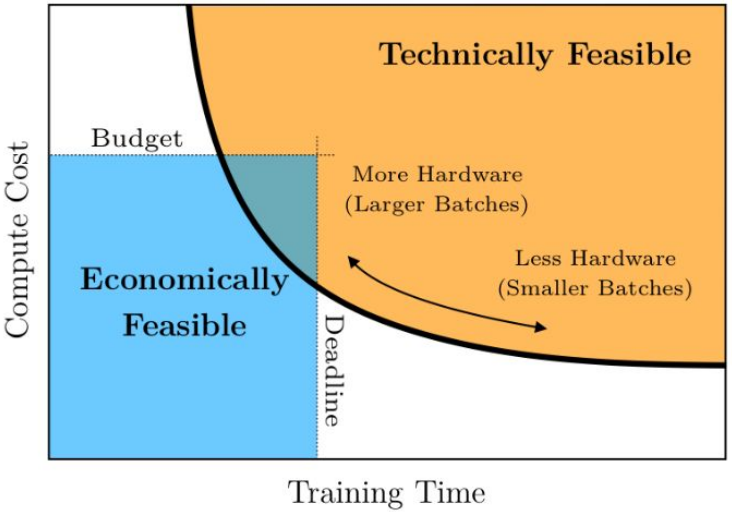
McCandlish, Kaplan and Amodei arXiv:1812.06162

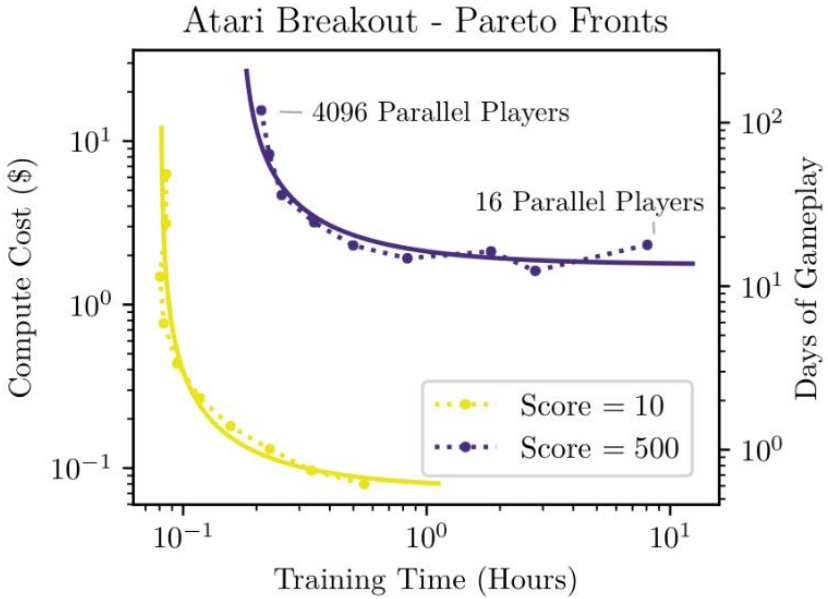
Gradient noise scale measures the variation of the gradients between different training examples



Critical batch size is the maximum batch size above which scaling efficiency decreases significantly

Computational cost vs. training time trade-off





"Increasing parallelism makes it possible to train more complex models in a reasonable amount of time… a Pareto frontier chart is [used] to visualize comparisons between algorithms and scales" -- blog.openai.com/science-of-ai

Figures from McCandlish, Kaplan and Amodei arXiv:1812.06162

Summary and outlook

- Distributed training is imperative for larger and more complex models/datasets
- Data parallelism distributes more data among more workers
- Large batch training is unstable and may impact generalization error if hyper-parameters are not *tuned* well
- Use learning-warm up and linear scaling to scale to modest scales < 10x. No guarantees that it will work for all models
- Batch-size scaling seems to be more robust across many models
- A simple statistic, gradient noise scale, can predict maximum useful batch-size

Let’s get practical

Distributed training hands-on session

We will use ResNet on CIFAR10 to demonstrate implementation and speedup.

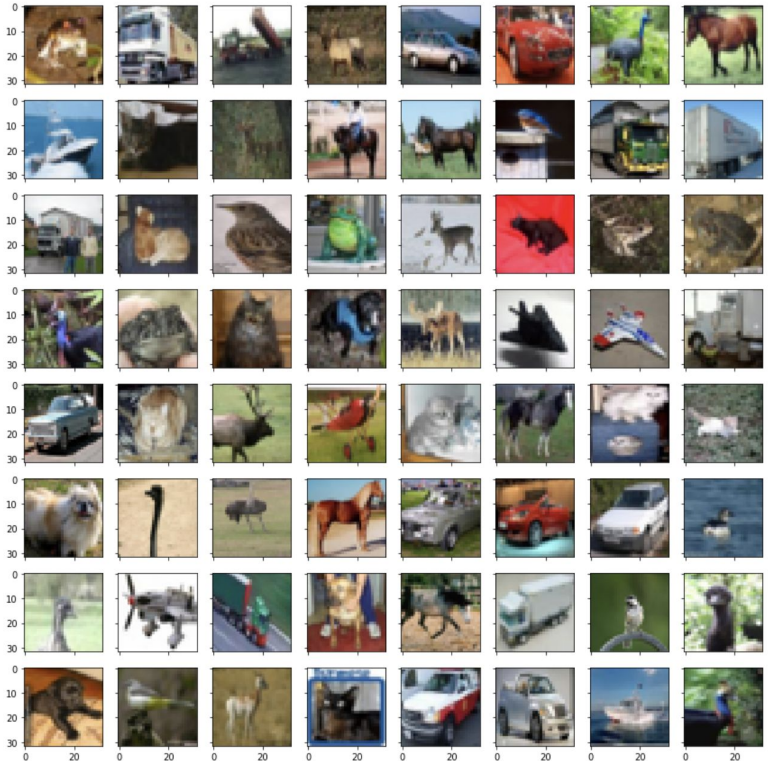
- Note that this small dataset doesn't necessarily *require* scale
- But it allows us to get some results in the allotted time frame

We will use Keras and Horovod/CPE ML for distributed training

- Easy to use/teach
- Fast (relies on optimized backend, MPI/RDMA)
- Only few code modifications necessary

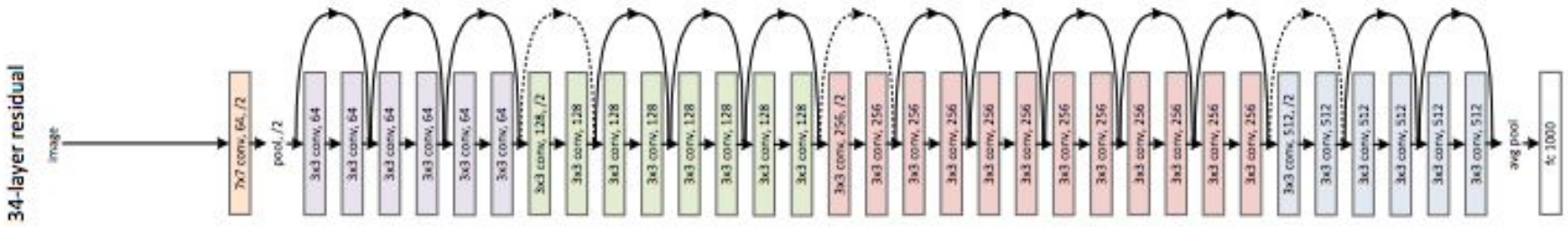
CIFAR-10

- prepared by University of Toronto
- slightly more complicated than MNIST, but less complex than Imagenet
- 60K, 32x32 color images
- 10 classes (plane, car, bird, car, deer, dog, frog, horse, ship, truck)
- 50K training, 10K test
- cifar-10 link
- intuitive, fast training/model development times, good for demonstrating the essentials of distributed training
- **good for tutorials**



ResNet Topology (34-layer-version)

- convolution layers arranged in blocks
- skip connections combine input and output of block (residual learning)
- FC layer for classification
- ResNet performs well on image classification tasks

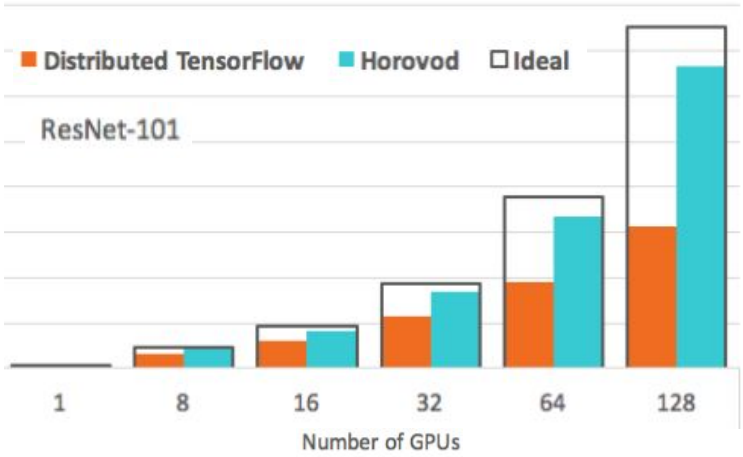


Horovod

Enables distributed synchronous data-parallel training with minimal changes to user code

Uses efficient all-reduces from MPI to collectively combine gradients across workers

Such approaches shown to scale better than parameter-server approaches (e.g. distributed TensorFlow with gRPC)



https://eng.uber.com/horovod/

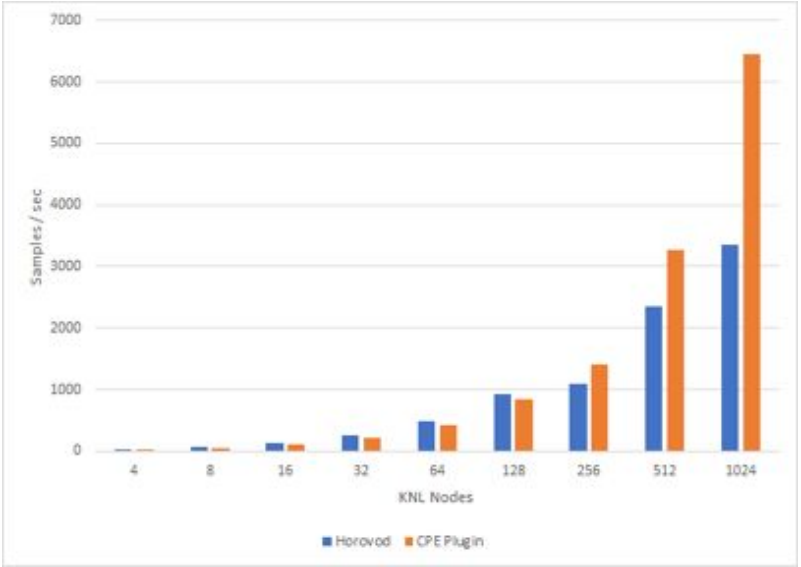
CPE ML (Cray Programming Environment ML Plugin)

Enables distributed synchronous data-parallel training with minimal changes to user code

Uses RDMA operations or reductions

Might perform better than Horovod on large networks and large scales

Advanced training features already implemented: pipelining, warmup, cooldown, etc.

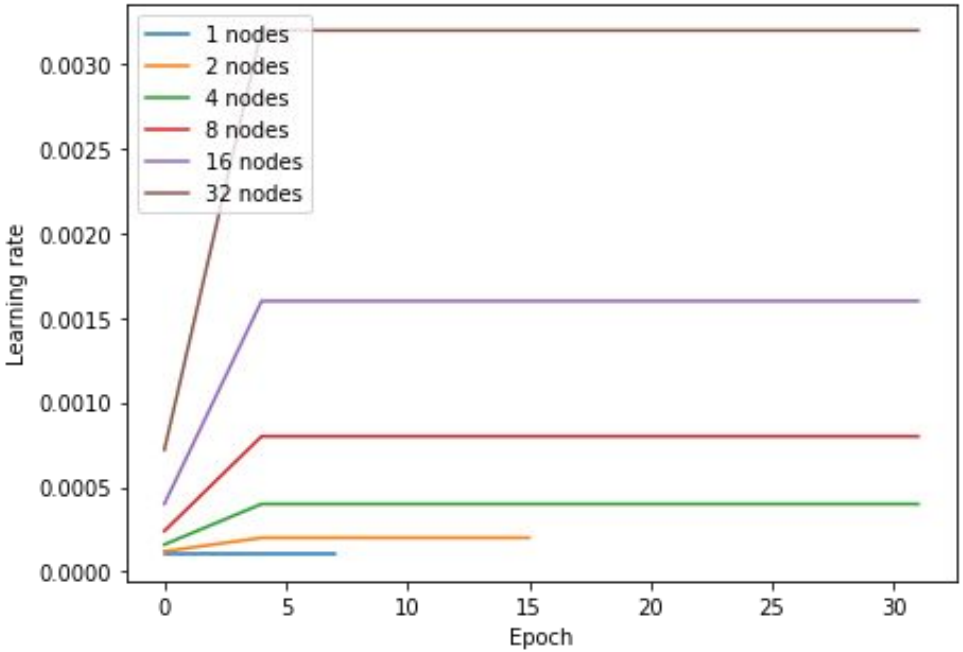


NERSC CosmoFlow

Scaling concepts demonstrated today

Today we will utilize:

- Synchronous data-parallel training (weak scaling) using Horovod/CPE ML
- Learning rate linear warmup
- Linear learning rate scaling, $\eta \rightarrow N * \eta$, followed by original decay schedule



Ingredients for multi-node training (Horovod)

Initialize Horovod and MPI:

```
hvd.init()
```

Wrap your optimizer in the Horovod distributed optimizer:

```
opt = keras.optimizers.SGD(lr=lr*hvd.size(), …)
opt = hvd.DistributedOptimizer(opt)
```

Linearly scaling the learning rate

Construct the variables broadcast callback:

```
callbacks =
[hvd.callbacks.BroadcastGlobalVariablesCallback(0), …]
```

Comparison Horovod vs. CPE ML - Initialization

```
# Import and MPI Initialization

 import keras
 from keras.datasets import mnist
 from keras.models import Sequential
 from keras.layers import Dense, Dropout, Flatten
 from keras.layers import Conv2D, MaxPooling2D
 from keras import backend as K

#  import Horovod library
 import horovod.keras as hvd

# initialize Horovod
 hvd.init()
```

Horovod

```
# Import and MPI Initialization

 import keras
 from keras.datasets import mnist
 from keras.models import Sequential
 from keras.layers import Dense, Dropout, Flatten
 from keras.layers import Conv2D, MaxPooling2D
 from keras import backend as K

 # Additional pkgs used to calculate buffer sizes, etc.
 import numpy as np
 import math
 import tensorflow as tf

# import Cray ML library and user defined
# Callbacks, Distributed Optimizer
 import ml_comm as mc

 from plugin_keras import InitPluginCallback,
 BroadcastVariablesCallback, DistributedOptimizer

 # initialize CPE
 mc.init_mpi()
```

CPE ML

Comparison Horovod vs. CPE ML - Model

```
# Optimizer and model compile

 base_lr = 1.0

# Adjust epochs based on parallel throughput
 epochs = int(epochs/hvd.size())

# Non-distributed compile
 optimizer = optimizer=keras.optimizers.Adadelta(base_lr)

# Horovod: Add Distributed Optimizer
 optimizer = keras.optimizers.Adadelta(lr=1.0*hvd.size())
 optimizer = hvd.DistributedOptimizer(optimizer)

 # Run the training loop
model.compile(loss=keras.losses.categorical_crossentropy,
              optimizer=optimizer,metrics=['accuracy'])
```

Horovod

```
# Optimizer and model compile

 base_lr = 1.0

# Adjust epochs based on parallel throughput
 epochs = int(epochs/mc.get_nranks())

# Non-distributed compile
 optimizer = optimizer=keras.optimizers.Adadelta(base_lr)

# Cray ML Plugin: Add Distributed Optimizer
 optimizer =
keras.optimizers.Adadelta(lr=1.0*mc.get_nranks())
 optimizer = DistributedOptimizer(optimizer)

 # Run the training loop
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```

CPE ML

CPE ML - DistributedOptimizer Implementation example

- implementation example for DistributedOptimizer
- extracting gradients and reducing them explicitly
- allows to inject/wrap other optimizations such as gradient manipulation (LARS/LARC)
- can be done in Horovod as well

```
class _DistributedOptimizer(keras.optimizers.Optimizer):
  """
  Leveraging approach used in horovod.keras.DistributedOptimizer.
  """
  def __init__(self, name, **kwargs):
      if name is None:
          name = "Distributed%s" % self.__class__.__base__.__name__
      self._name = name
      super(self.__class__, self).__init__(**kwargs)

  def get_gradients(self, loss, params):
      grads = super(self.__class__, self).get_gradients(loss, params)
      grads_mc = mc.gradients(grads, 0)
      return grads_mc

  def DistributedOptimizer(optimizer, name=None):
      """
      An optimizer that wraps another keras.optimizers.Optimizer
      """
      cls = type(optimizer.__class__.__name__, (optimizer.__class__,),
                 dict(_DistributedOptimizer.__dict__))
      return cls(name, **optimizer.get_config())
```

Ingredients for multi-node training (Horovod/CPE ML)

Train model as usual; it should now synchronize at every mini-batch step:

```
model.fit(..., callbacks=callbacks)
```

Launch your script with MPI

```
srun -n ${SLURM_NNODES} … -u python train.py …
```

(we'll use SLURM and srun instead of mpirun for generic MPI installations)

Running the multi-node training

Refer again to the documentation on the github repo:

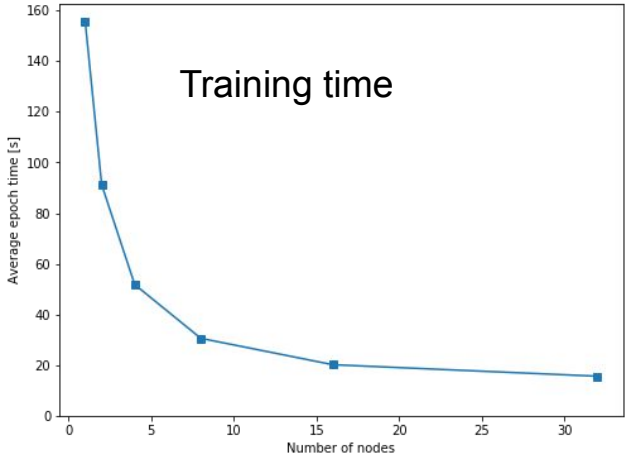
https://github.com/NERSC/cug19-da-tutorial

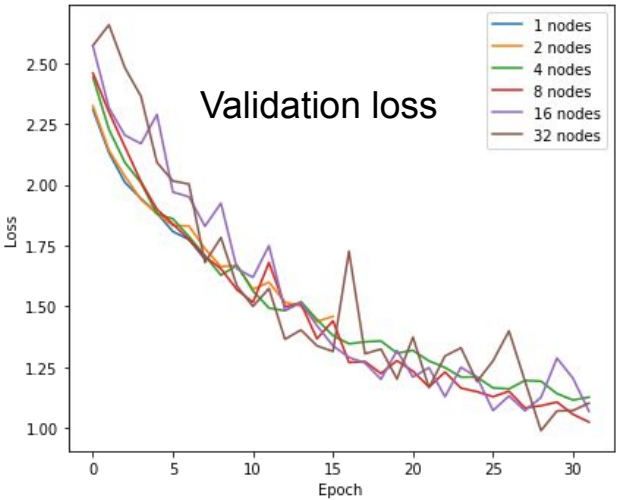
You can try these examples out on your own system

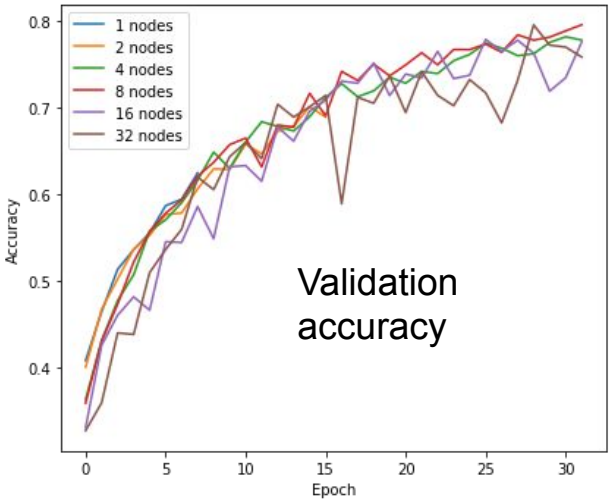
Feel free to try and tweak things and get better performance

- Change optimizer
- Change learning rate, number of warmup epochs, decay schedule
- Change learning rate scaling (e.g., lr*sqrt(N) instead of lr*N)

Scaling results for ResNet CIFAR10







Training time goes down

Training loss and accuracy are still converging at similar rates

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Thank You