Large Scale Training

argonne-lcf / ai-science-training-series

Sam Foreman

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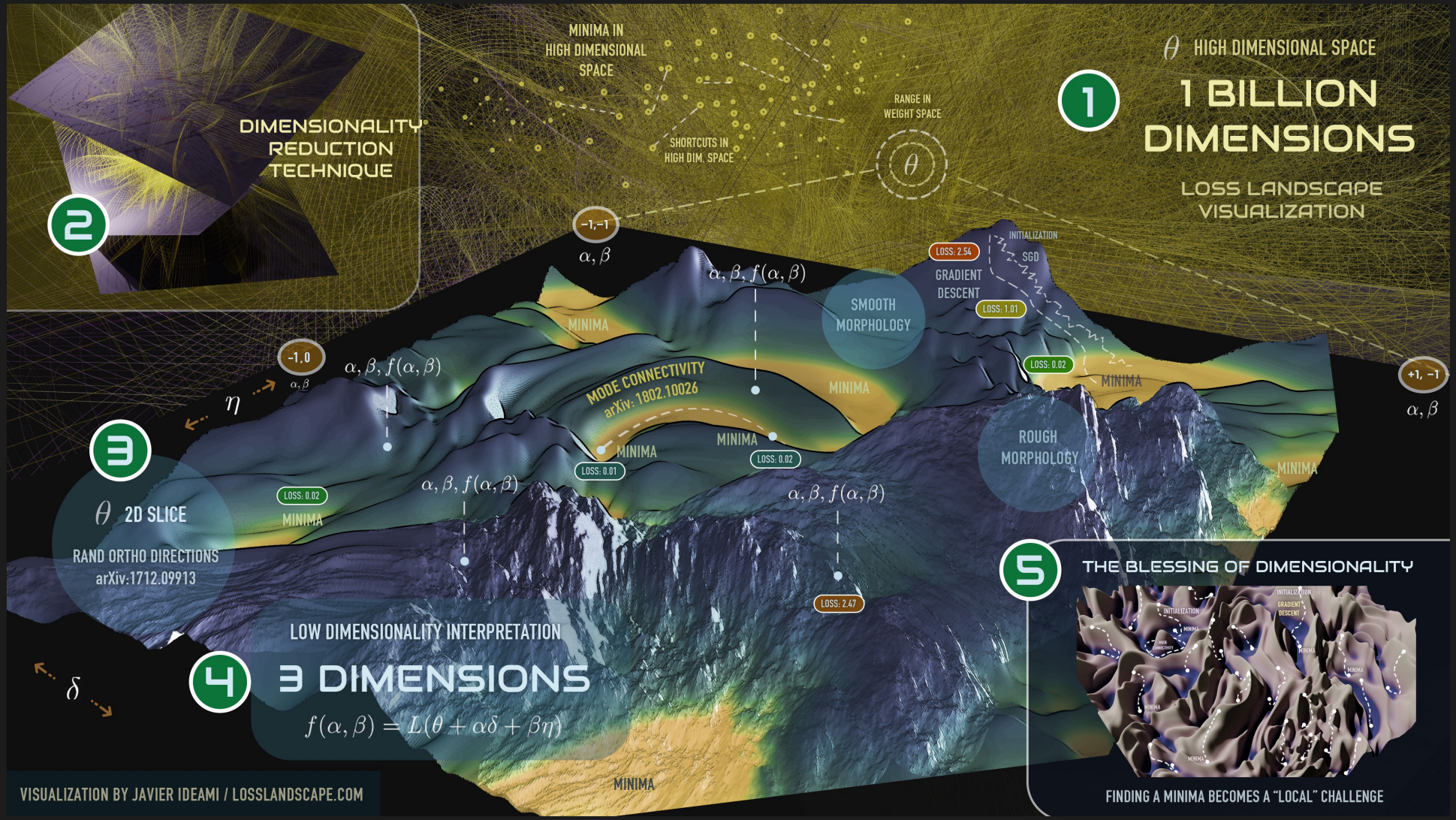
Why Distributed Training?

- Large batches may not fit in GPU memory
- Splitting data across workers → larger batch size
- Smooth loss landscape
- Improved gradient estimators
- Less iterations needed for same number of epochs
    - May need to train for more epochs if another change is not made
    - e.g. scaling learning rate
- See Large Batch Training of Convolutional Networks


MINIMA IN HIGH DIMENSIONAL SPACE
SHORTCUTS IN HIGH DIM. SPACE
RANGE IN WEIGHT SPACE
θ HIGH DIMENSIONAL SPACE
1
1 BILLION DIMENSIONS
LOSS LANDSCAPE VISUALIZATION
DIMENSIONALITY REDUCTION TECHNIQUE
2
−1,−1
α, β
α, β, f(α, β)
MINIMA
SMOOTH MORPHOLOGY
INITIALIZATION
SGD
GRADIENT DESCENT
LOSS: 2.54
LOSS: 1.01
LOSS: 0.02
MINIMA
+1, −1
α, β
-1, 0
α, β
α, β, f(α, β)
η
MODE CONNECTIVITY
arXiv: 1802.10026
MINIMA
LOSS: 0.01
MINIMA
LOSS: 0.02
ROUGH MORPHOLOGY
MINIMA
3
θ 2D SLICE
RAND ORTHO DIRECTIONS
arXiv:1712.09913
LOSS: 0.02
MINIMA
α, β, f(α, β)
α, β, f(α, β)
LOSS: 2.47
LOW DIMENSIONALITY INTERPRETATION
4
3 DIMENSIONS
$f(\alpha, \beta) = L(\theta + \alpha\delta + \beta\eta)$
δ
MINIMA
5
THE BLESSING OF DIMENSIONALITY
FINDING A MINIMA BECOMES A "LOCAL" CHALLENGE
VISUALIZATION BY JAVIER IDEAMI / LOSSLANDSCAPE.COM

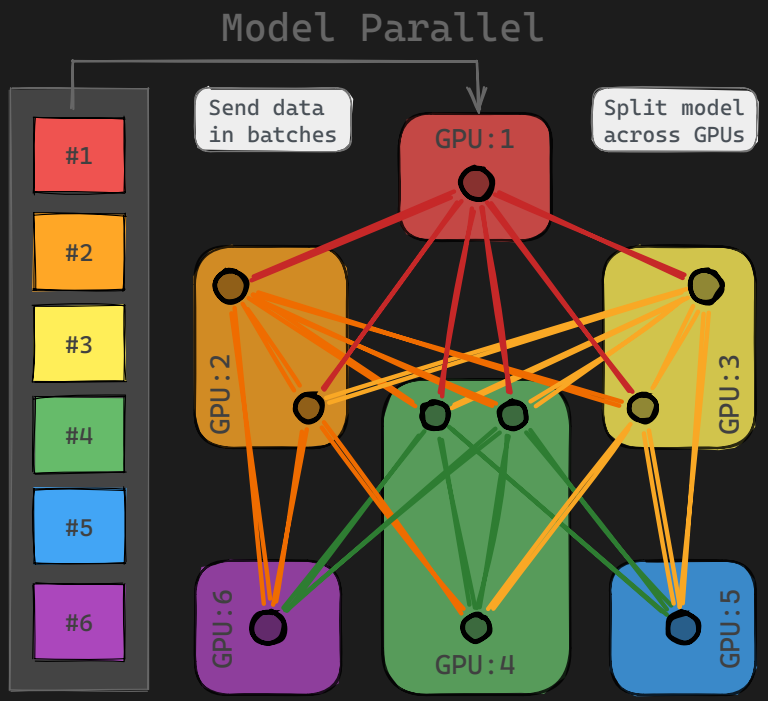
Recent Progress

Year	Author	Batch Size	Processor	DL Library	Time	Accuracy
2016	He et al. [1]	256	Tesla P100 x8	Caffe	29 Hrs	75.3%
	Goyal et al. [2]	8192	Tesla P100	Caffe 2	1 hour	76.3%
	Smith et al. [3]	8192 → 16,384	full TPU pod	TensorFlow	30 mins	76.1%
	Akiba et al. [4]	32,768	Tesla P100 x1024	Chainer	15 mins	74.9%
	Jia et al. [5]	65,536	Tesla P40 x2048	TensorFLow	6.6 mins	75.8%
	Ying et al. [6]	65,536	TPU v3 x1024	TensorFlow	1.8 mins	75.2%
	Mikami et al. [7]	55,296	Tesla V100 x3456	NNL	2.0 mins	75.29%
2019	**Yamazaki et al**	**81,920**	**Tesla V100 x 2048**	**MXNet**	**1.2 mins**	**75.08%**

Model Parallel Training

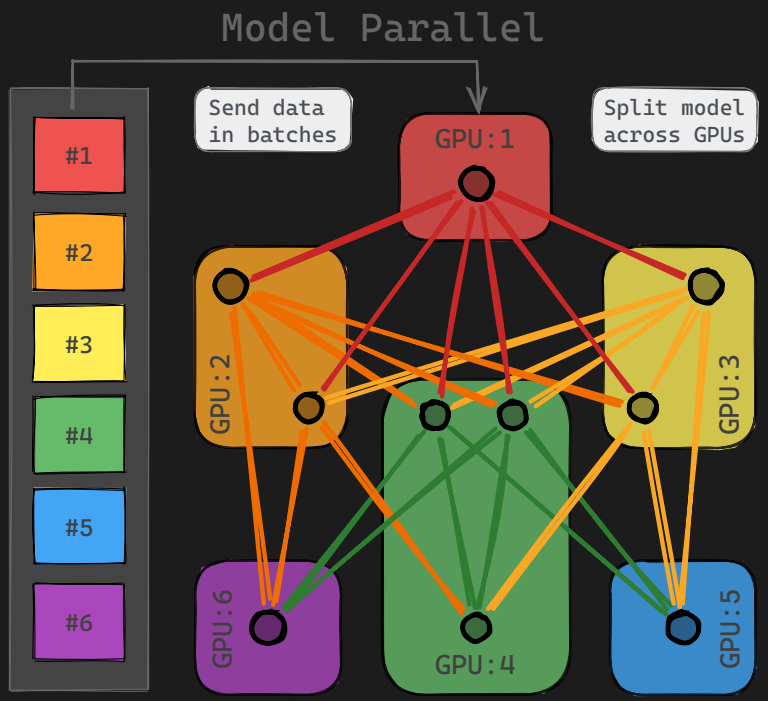
Model Parallel Training

- Split up network over multiple workers
  - Each receives disjoint subset
  - All communication associated with subsets are distributed
- Communication whenever dataflow between two subsets
- Typically **more complicated** to implement than data parallel training
- Suitable when the model is too large to fit onto a single device (CPU / GPU)



Model Parallel Training

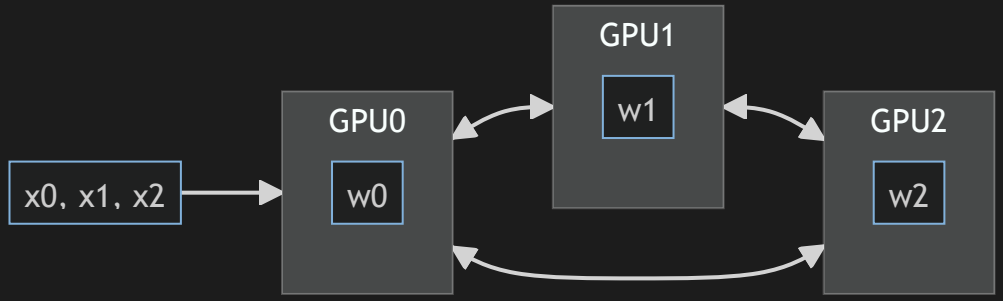
- Suitable when the model is too large to fit onto a single device
  - Partitioning the model into different subsets **is not an easy task**
  - Might introduce load imbalancing issues limiting scale efficiency
- 🤗 huggingface/transformers useful reference
  - Excellent series of posts in their documentation on Model Parallelism



Model Parallel Training: Example

$$y = w_0 * x_0 + w_1 * x_1 + w_2 * x_2$$

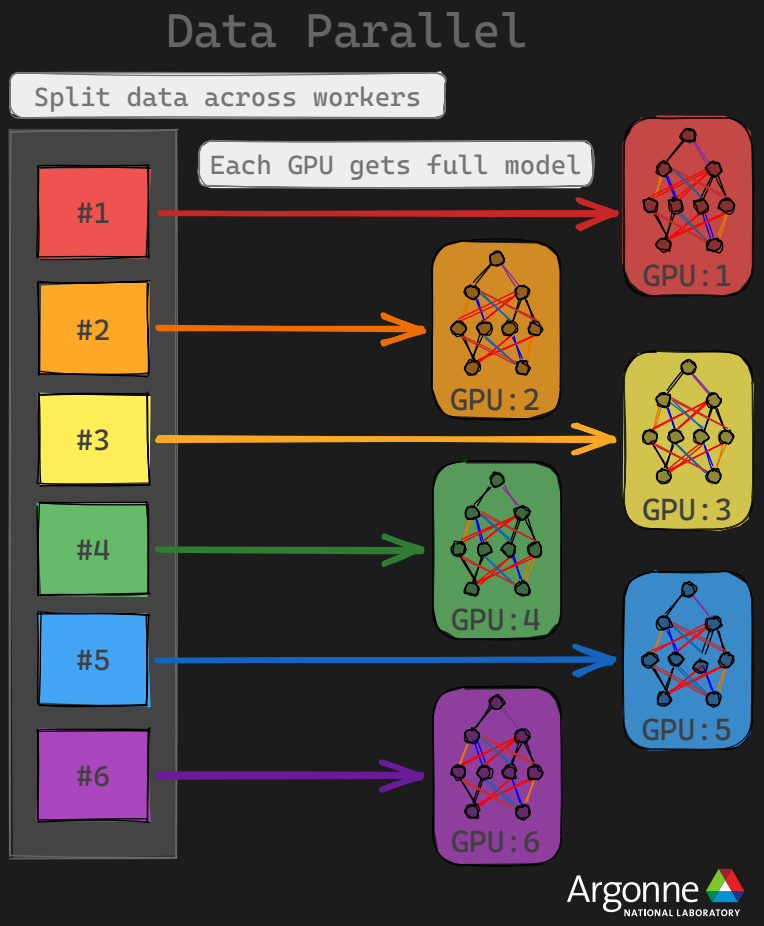
1. Compute $y_0 = w_0 * x_0$ and send to $\rightarrow$ GPU1
2. Compute $y_1 = y_0 + w_1 * x_1$ and send to $\rightarrow$ GPU2
3. Compute $y = y_1 * w_2 * x_2$ ✅



Data Parallel Training

Data Parallel Training

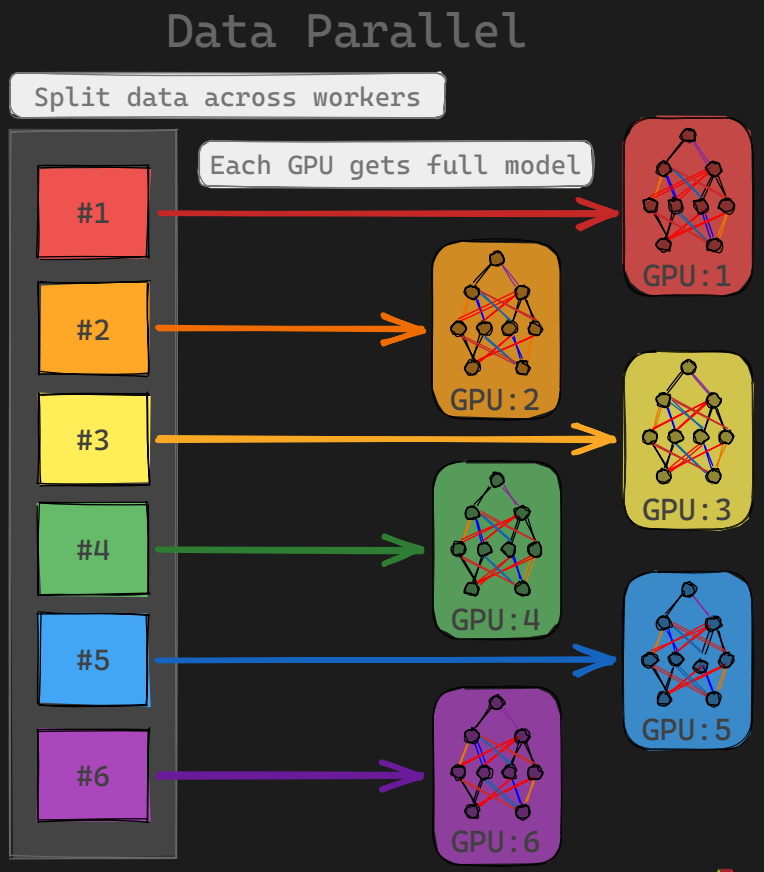
- Typically easier to implement
- Existing frameworks (Horovod, DeepSpeed, DDP, etc)
- Relatively simple to get up and running (minor modifications to code)[1]
- Recent presentation on data-parallel training available on YouTube

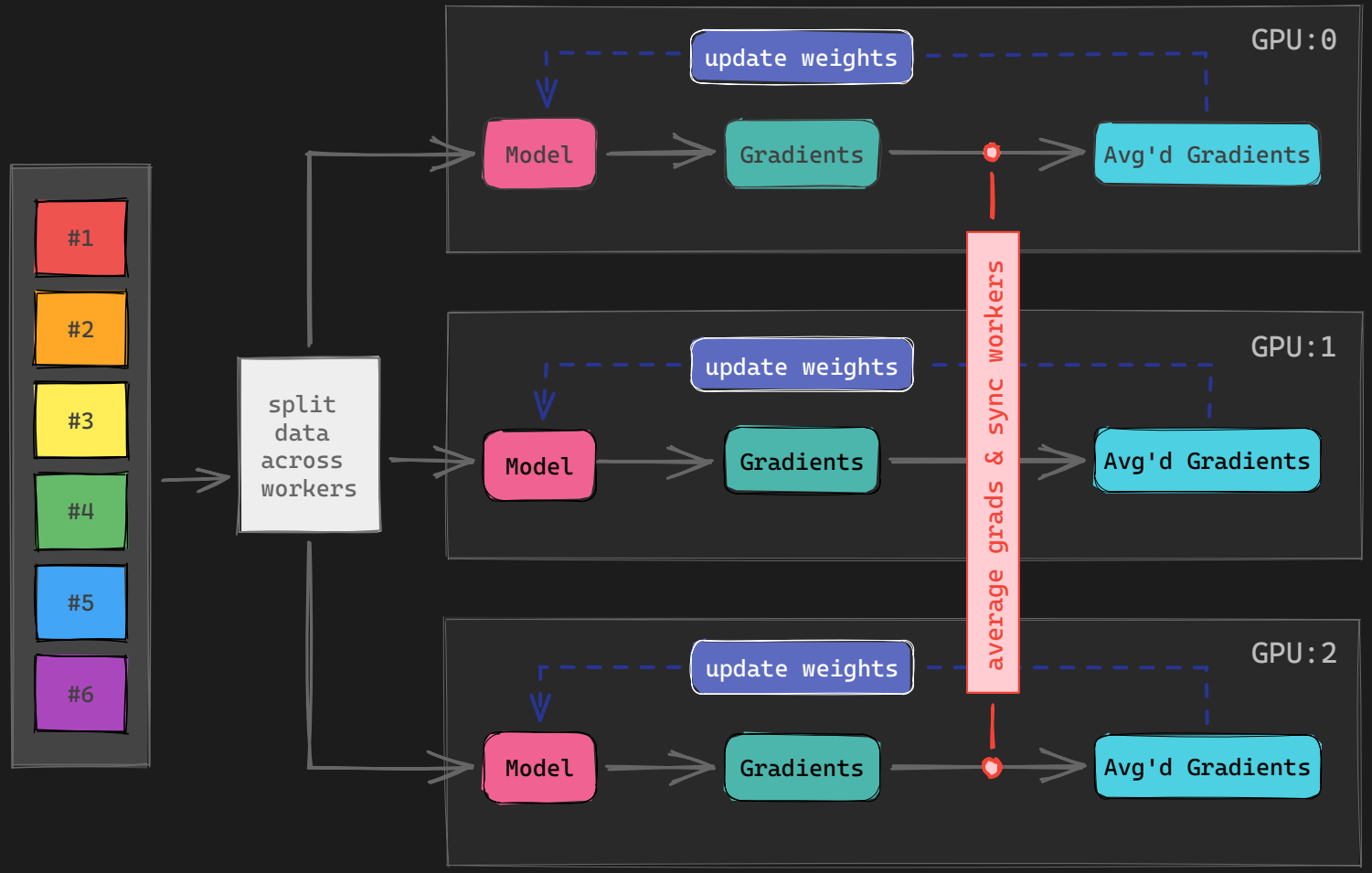


1. Concepts: Horovod

Data Parallel Training

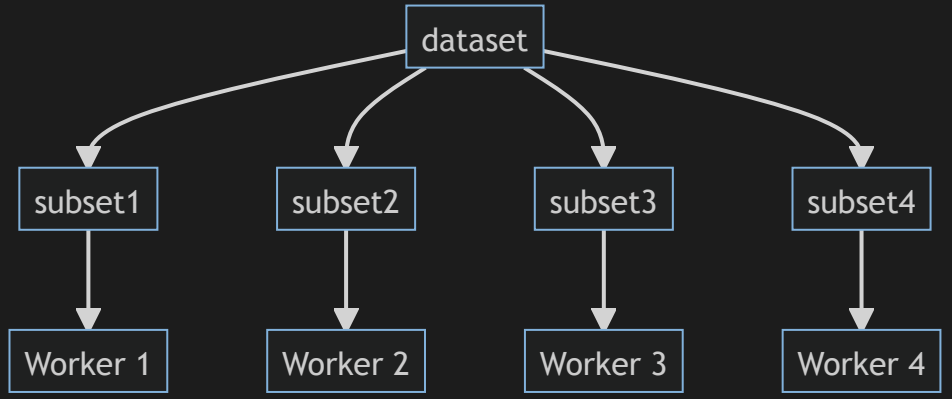
- Each worker has **copy of complete model**
- Global batch of data split into multiple mini-batches
  - Each worker computes the corresponding **loss and gradients from local data**
- Before updating parameters, loss and gradients averaged across workers





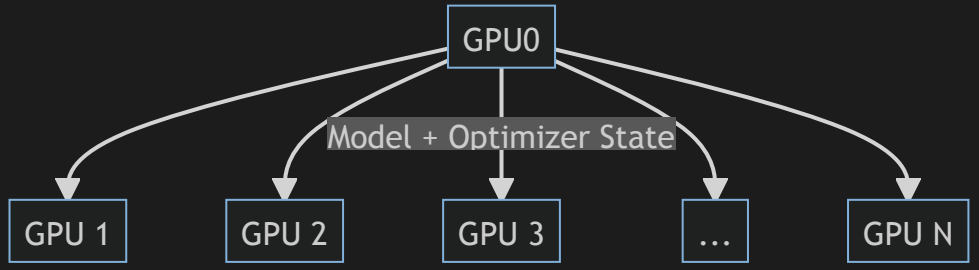
Data Parallel Training

- Each worker has identical copy of model
- **Global batch of data split across workers**
- Loss + Grads averaged across workers before updating parameters



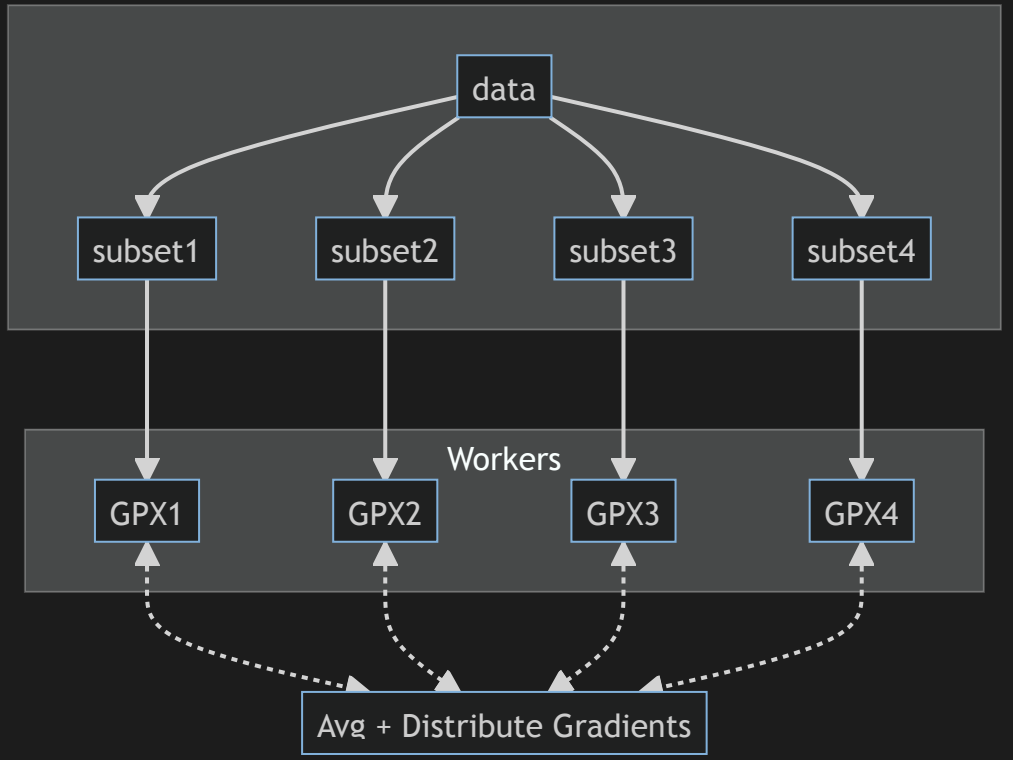
Broadcast Initial State

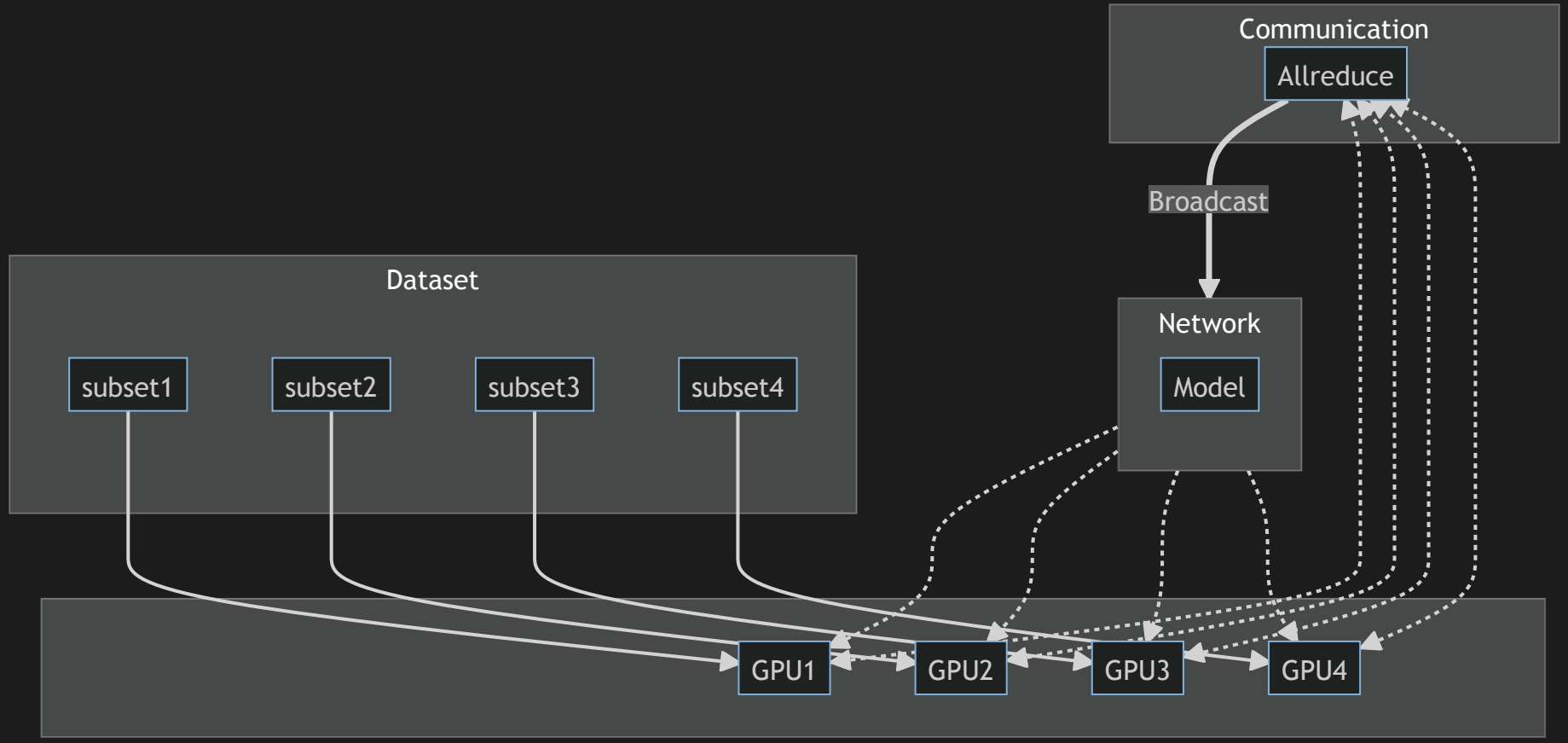
- At the start of training (or when loading from a checkpoint), we want all of our workers to be initialized consistently
  - **Broadcast** the model and optimizer states from `hvd.rank() == 0` worker



Data Parallel Training

- Disjoint subsets of a neural network are assigned to different devices
- Each worker receives:
  - **identical copy of model**
  - **unique subset of data**




Communication
Allreduce
Broadcast
Dataset
subset1
subset2
subset3
subset4
Network
Model
GPU1
GPU2
GPU3
GPU4

Best Practices

- Use parallel IO whenever possible
    - Feed each rank from different files
    - Use MPI IO to have each rank read its own batch from a file
    - Use several ranks to read data, MPI to scatter to remaining ranks
        - Most practical in big *at-scale* training

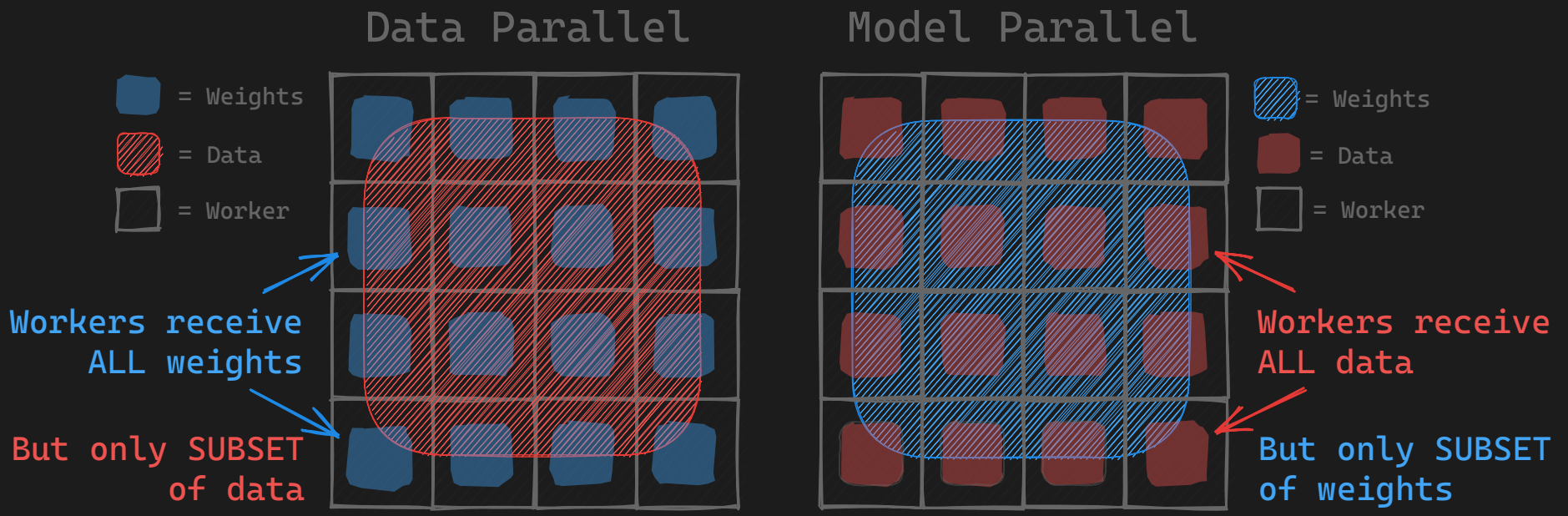
⚠ **Computation stalls during communication!**

Keeping the communication to computation ratio small is important for effective scaling

Best Practices

- Take advantage of data storage
  - Use striping on lustre
  - Use the right optimizations for Aurora, Polaris, etc.
- Preload data when possible
  - Offloading to a GPU frees CPU cycles for loading the next batch of data
    - **minimize IO latency this way**

Comparison


Data Parallel
= Weights
= Data
= Worker
Workers receive ALL weights
But only SUBSET of data
Model Parallel
= Weights
= Data
= Worker
Workers receive ALL data
But only SUBSET of weights

Horovod: Overview

1. Initialize Horovod[1]
2. Assign GPUs to each rank
3. Scale the initial learning rate by num. workers
4. Distribute gradients + broadcast state
    - Distribute gradients by wrapping `tf.GradientTape` with `hvd.DistributedGradientTape`
    - Ensure consistent initialization by broadcasting model weights and optimizer state from `rank == 0` to other workers
5. Ensure workers are always receiving unique data
6. Take global averages when calculating `loss`, `acc`, etc. using `hvd.allreduce(...)`
7. Save checkpoints *only* from `rank == 0` to prevent race conditions

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1. Horovod with Tensorflow

TensorFlow + Horovod

- Initialize Horovod:

```
import horovod.tensorflow as hvd
hvd.init()
```

- Set one GPU per process ID (`hvd.local_rank()`)

```
gpus = tf.config.experimental.list_physical_devices('GPU')
for gpu in gpus:
    tf.config.experimental.set_memory_growth(gpu, True)
if gpus:
    local_rank = hvd.local_rank()
    tf.config.experimental.set_visible_devices(gpus[local_rank], 'GPU')
```

Scale the Learning Rate

1. Scale by the number of workers to account for increased batch size

```
import horovod.tensorflow as hvd
optimizer = tf.optimizers.Adam(lr_init * hvd.size())
```

TensorFlow + Horovod

- Training step then looks like:

```
@tf.function
def train_step(data, model, loss_fn, optimizer, first_batch):
    batch, target = data
    with tf.GradientTape() as tape:
        output = model(batch, training=True)
        loss = loss_fn(target, output)
    tape = hvd.DistributedGradientTape(tape)
    grads = tape.gradient(loss, model.trainable_variables)
    optimizer.apply_gradients(zip(grads, model.trainable_variables))
    if first_batch:
        hvd.broadcast_variables(model.variables, root_rank=0)
        hvd.broadcast_variables(optimizer.variables, root_rank=0)
    return loss, output
```

Deal with Data

- At each training step, we want to ensure that **each worker receives unique data**
- This can be done in one of two ways:
    1. Manually partition data (ahead of time) and assign different sections to different workers
        1. Each worker can only see their local portion of the data
    2. From each worker, randomly select a mini-batch
        1. Each worker can see the full dataset

> ⚠ **Don't forget your seed!**
>
> When randomly selecting, it is important that each worker uses different seeds to ensure they receive unique data

Deal with Data

```
(images, labels), (xtest, ytest) = (
    tf.keras.datasets.mnist.load_data(path='mnist.npz')
)
dataset = tf.data.Dataset.from_tensor_slices(
    (tf.cast(images[..., None] / 255.0, tf.float32),
     tf.cast(labels, tf.int64))
)
test_dataset = tf.data.Dataset.from_tensor_slices(
    (tf.cast(xtest[..., None] / 255.0, tf.float32),
     tf.cast(ytest, tf.int64)))
)
dataset = dataset.repeat().shuffle(1000).batch(args.batch_size)
test_dataset = (
    test_dataset.shard(
        num_shards=hvd.size(),
        index=hvd.rank()
    ).repeat().batch(args.batch_size)
)
```

Average Across Workers

- Typically, we will want to take the global average of the loss across all our workers, for example:

```
global_loss = hvd.allreduce(loss, average=True)
global_acc = hvd.allreduce(acc, average=True)
```

Hands-On

1. Navigate to `ai-science-training-series`
2. `git pull`
3. Navigate into `07_largeScaleTraining/src/ai4sci`
4. To run (with a `batch_size=512`):

```
./main.sh batch_size=512 > main-bs-512.log 2>&1 &
```

5. View output:

```
tail -f "main-bs-512.log" $(tail -1 logs/latest)
```

Thank you!

- Organizers
- ALCF Data Science & Operations
- Feel free to reach out!

Acknowledgements

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