



Introduction to Deep Learning – Some Practical Guidelines

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Outline

- **Part II - Practical Guidelines for Running a Project:**

Choosing Hyperparameters – a bit of exploration and exploitation

Job workflow - make it efficient and easy to organize

CPUs vs GPUs

Parallelizing Models and Multinode/Multidevice Execution

Exercise/Demo, Multinode MNIST

Choosing Hyperparameters

- Hyperparameters are found by searching, not by the network algorithm
- Generally, hyperparameters related to:
 - architecture (layers, units, activation, filters, ...)
 - algorithm (learning rate, optimizer, epochs, ...)
 - efficient learning (batch size, normalization, initialization, ...)
- Some options are determined by task:
 - loss function, CNN vs MLP, ...
- Use what works, from related work or the latest recommendations,

Hyperparameters Search

- Can take a long time, hard to find global optimal
- Start with small data, short runs to get sense of range of good parameter values
- Easy but possibly time-consuming method:
grid search over uniformly spaced values
- Do “exploration” then “exploitation”, ie search wide then search deep
Keras Tuner functions can help with the wide search
Raytune is similar tool for Pytorch

Hyperparameter Search Tool

- Several search strategies, such as:

Hyperband is like a tournament of hyperparameter configurations

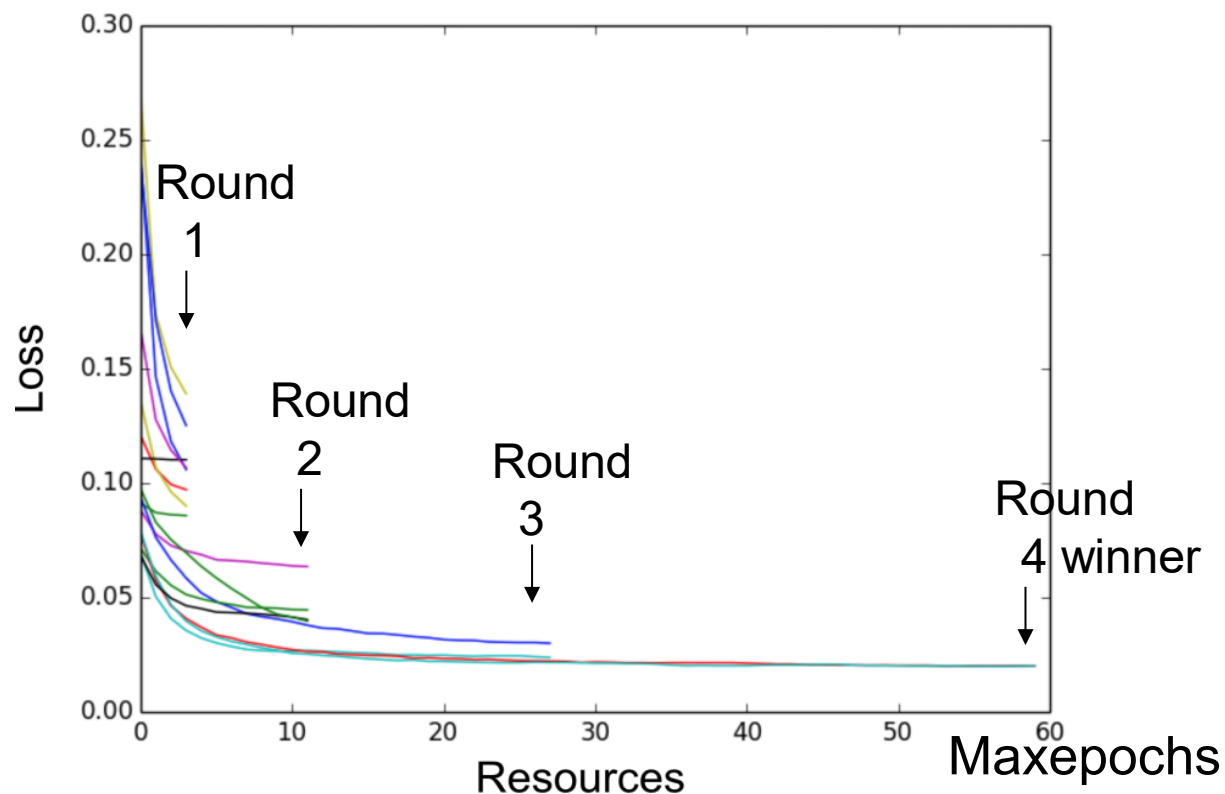
RandomSearch will search randomly through the space of configurations

Bayesian optimization is like a function approximation to pick out next configuration

- Typically, you usually wrap the model build function with arguments for hyperparameters

Hyperband Bracket

Each round runs several network configurations for small number of epochs
Several rounds with increasing epochs make up a bracket
Several brackets are run to end up with several possible overall winners.



Note, you could run a small grid search around hyperband winners to confirm performance

Keras Tuner code snippet

Set up function to
make the model

```
def build_model(numfilters,activation_choice): #<<-----add code: if you want to change the list and change code to match the list
    mymodel = keras.models.Sequential()
    mymodel.add(keras.layers.Convolution2D(numfilters,
                                            (3, 3),
                                            strides=1
```

Keras Tuner code snippet –

Set up function to
make the model

Set up
hyperparameter
choices

```
def build_model(numfilters, activation_choice): #<<-----add code: if you want to
# list and change code to your needs
mymodel = keras.models.Sequential()
mymodel.add(keras.layers.Convolution2D(numfilters,
(3, 3),
strides=1
```


Keras Tuner code snippet – put build-model inside a ‘wrapper’ function

Set up function to make the model

Set up hyperparameter choices

```
def build_model_hp(hp):  
    hp_numfilters = hp.Int('hpnumfilters', min_value=8, max_value=32, step=4)  
    #your variable name          ^^^ the parameter name in the hp object  
  
    return build_model(hp_numfilters, hp_Activation) #<<---- dont forget to pass the new  
  
def build_model(numfilters, activation_choice): #<<-----add code: if you  
    # list and change code to  
    mymodel = keras.models.Sequential()  
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```

Define ‘tuner’ object:
uses the wrapper
and model fit to
search configurations

```
tuner = kt.Hyperband(build_model_hp,  
                     objective = 'val_accuracy',  
                     max_epochs = num_max_epochs,  
                     factor = 3,  
                     hyperband_iterations=10,
```

Workflow and Organizing Jobs

Job Level: What makes sense to include in each job?

Model Level: run & test model for each parameter configuration

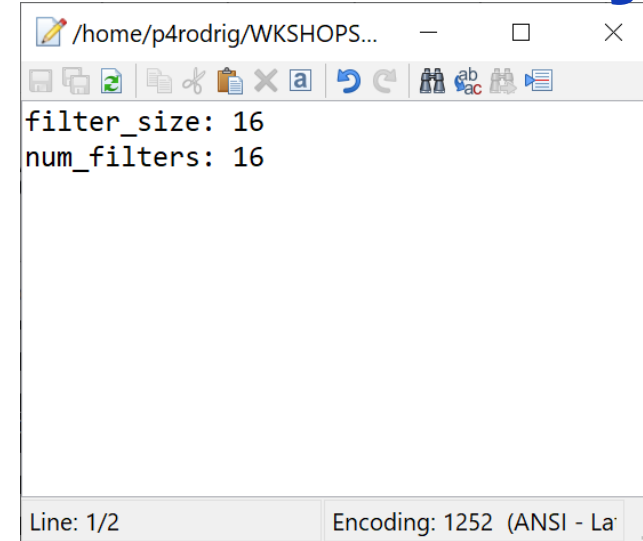
Data Level: loop through cross validation datasets (if applicable)

- **Consider how long each a model runs for 1 configuration of hyperparameters for 1 dataset**
- **Organize jobs into reasonable chunks of work**
- **For large models consider model-checkpoints**
- **Tensorboard is available but needs to be secure (ask for details)**

Organizing Configurations – one way

Code snippet:
using 'YAML' file to
set up
hyperparameter
configuration

Create text file with
"Parameter: Value"
pairs



A screenshot of a text editor window with the title bar "/home/p4rodrig/WKSHOPS...". The window contains a YAML file with two lines: "filter_size: 16" and "num_filters: 16". The status bar at the bottom indicates "Line: 1/2" and "Encoding: 1252 (ANSI - La)".

Read file as
python dictionary

```
import yaml

with open("./modelrun_args.yaml", "r") as f:
    my_yaml=yaml.safe_load(f) #this returns a python dictionary

filter_size=my_yaml.get("filter_size")
num_filters=my_yaml.get("num_filters")
print('arguments, filter_size:',filter_size,' num filters',num_filters)
```

note on using GPU

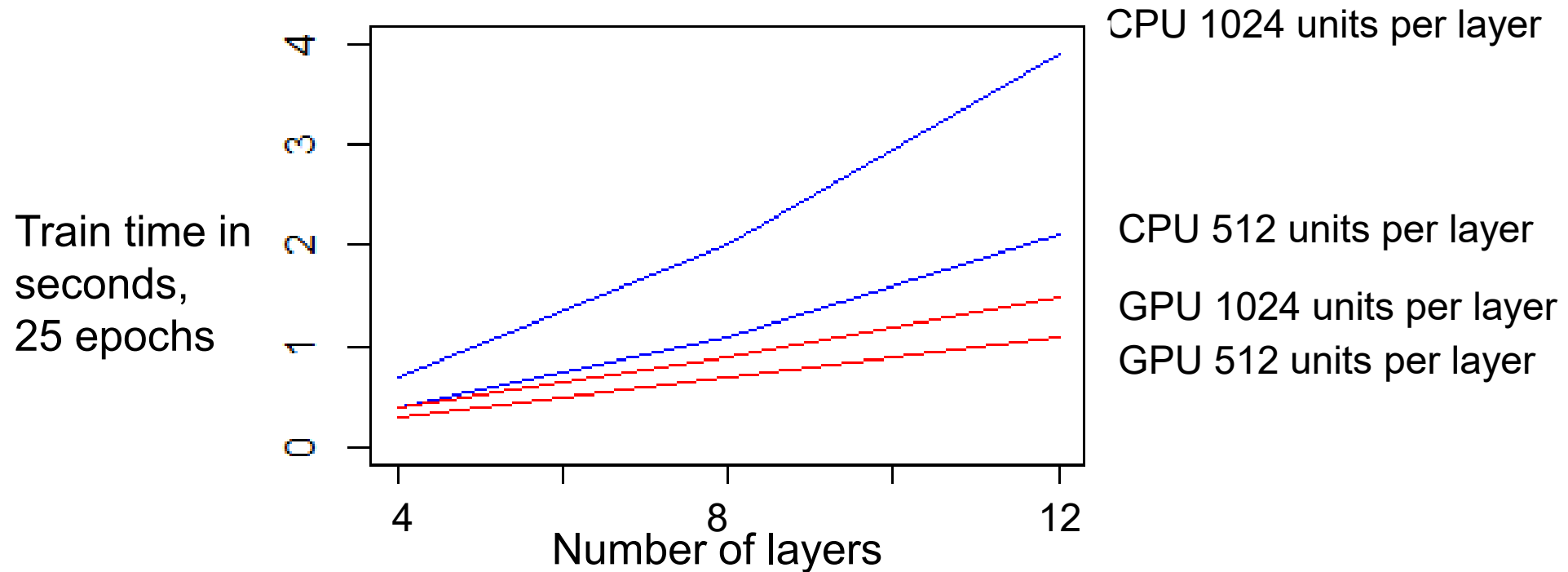
- GPU node has multiple GPU devices
- By default tensorflow will run on 0th gpu device if GPU is available, otherwise it will use all CPU cores

Code snippet to
check for GPU
devices

```
/home/p4rodrig/WKSHOPS/EXP-05192022/Intro_mnist_cnn2_forbatch.py - p4rodrig@login.exppanse.sdsc.edu - Editor - V
physical_devices = tf.config.list_physical_devices('GPU')
n_gpus = len(physical_devices)
print("Info,config,Num GPUs:", n_gpus)
if tf.test.gpu_device_name():
    print('Info, test,Default GPU Device:{}'.format(tf.test.gpu_device_name()))
```

GPU shared (V100) vs CPU (128 cores)

For MLP with Dense Layers, 80000x200 data matrix



GPUs faster, but you might have to wait more in job queue; also some memory limits compared to CPU, may need to use smaller batch size

Scaling in Deep Learning

- **Two Goals**

1 Speed Up Learning - parallelizing data and/or model

**2 Optimize Memory - as models scale up they take up too much memory
e.g. V100s have 32Gb limit and 8B float32 parameters would fill that**

Parallelism strategies

- **Data Parallelism:** partition data and copy the model across devices, (this is probably easiest thing to do, least programming)
- **Pipeline Parallelism:** split up the model so that layers are on different devices, ie inter-layer partitions (you organize layers)
- **Tensor Parallelism:** intra-layer partitions (model has to support it)

Parallel DL models with multiple nodes/devices

- **Data Parallel:**
 1. Launch your script on each device on each node
 2. Split up data
 3. Each device trains a copy of the model with a part of the data
 4. Aggregate parameter updates across devices/nodes

Parallel DL models with multiple nodes/devices

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- **Main functions:**

1. *mpirun* command (also *torchrun* exists but I haven't tested it much)
2. *Pytorch data loader will parallelize sampling*
3. *Pytorch DDP (Distributed Data Parallel) will wrap a model*
4. *DDP will use the Pytorch 'init_backend' function*

For example, single node, single device execution

In slurm batch script:
singularity → python

Your python script

Load data

Build model

Train

Multinode, mpi launches instances

In slurm batch script:

`mpirun -n number of tasks singularity → python`

Your python script

Load data

Build model

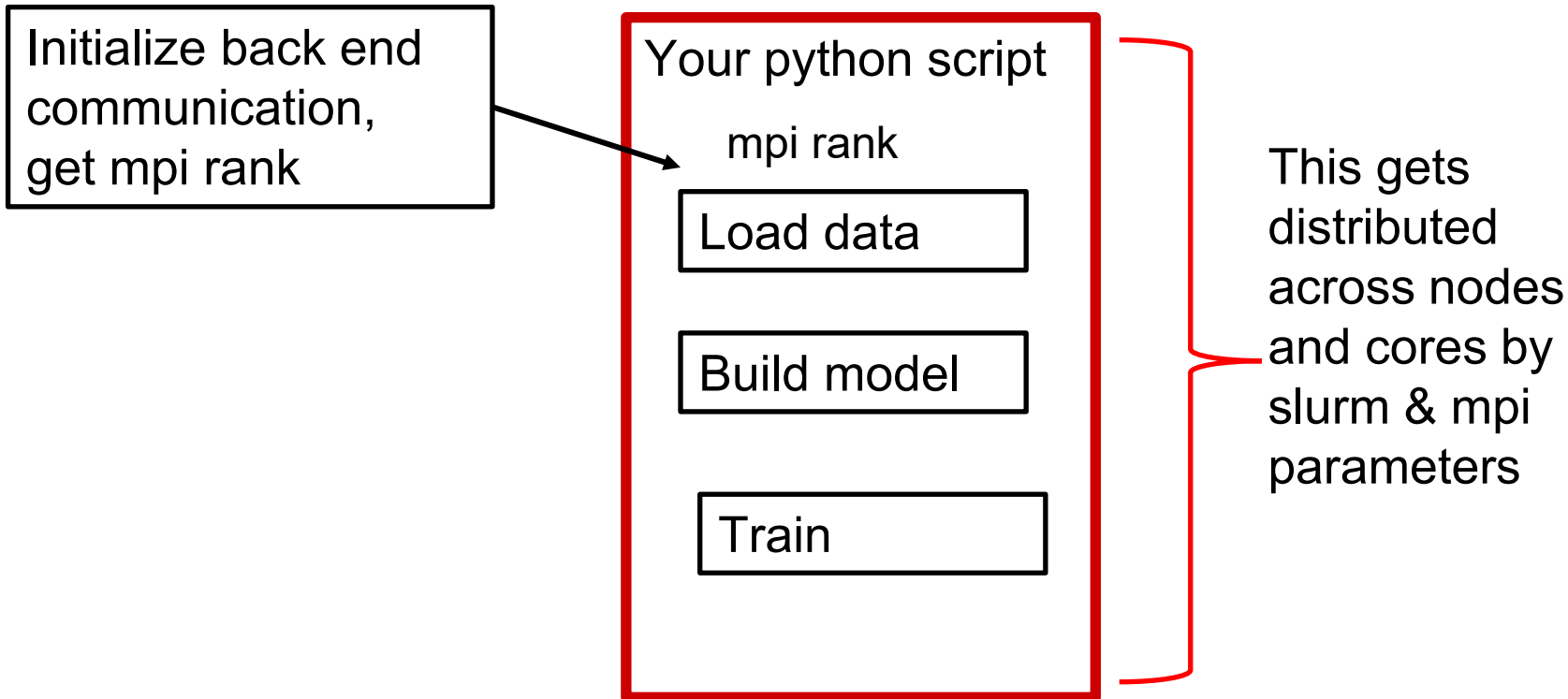
Train

This gets distributed across nodes and cores by slurm & mpi parameters

Multinode, mpi launches instances

In slurm batch script:

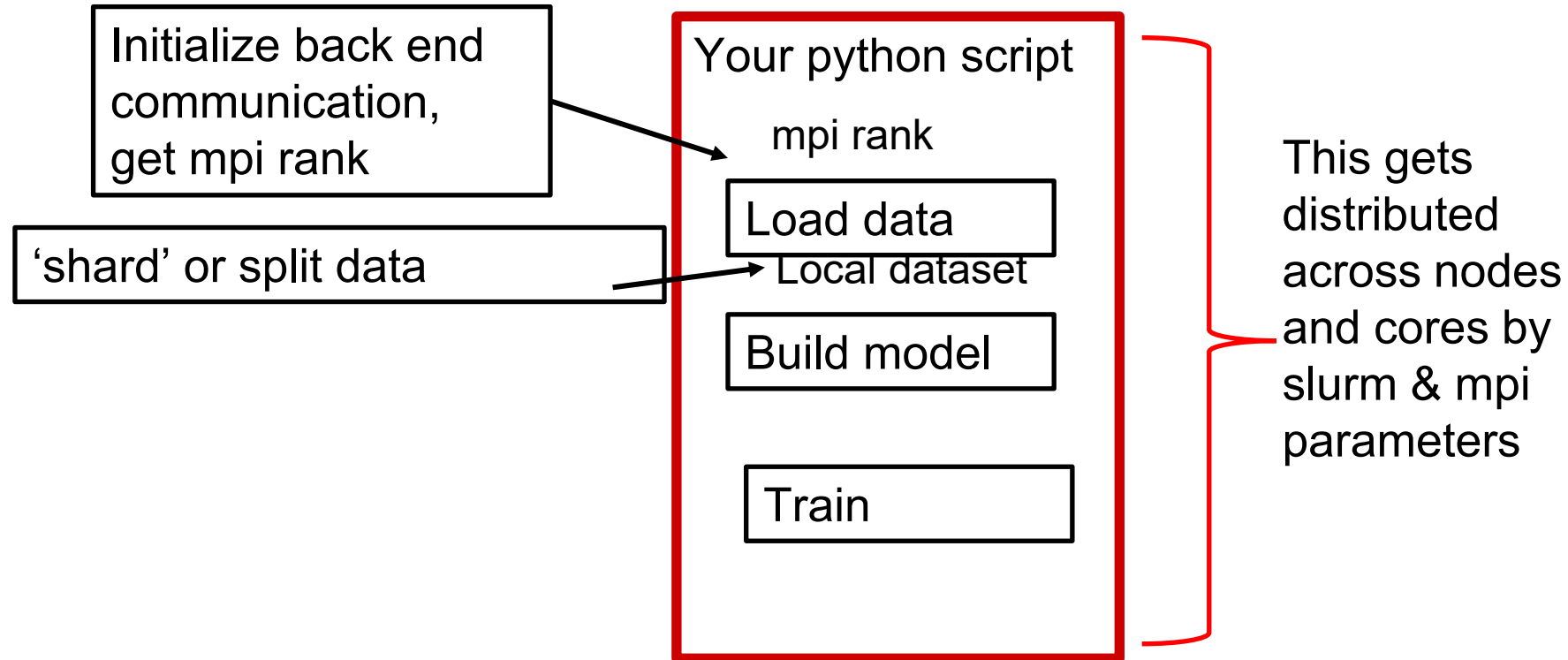
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Multinode, mpi launches instances

In slurm batch script:

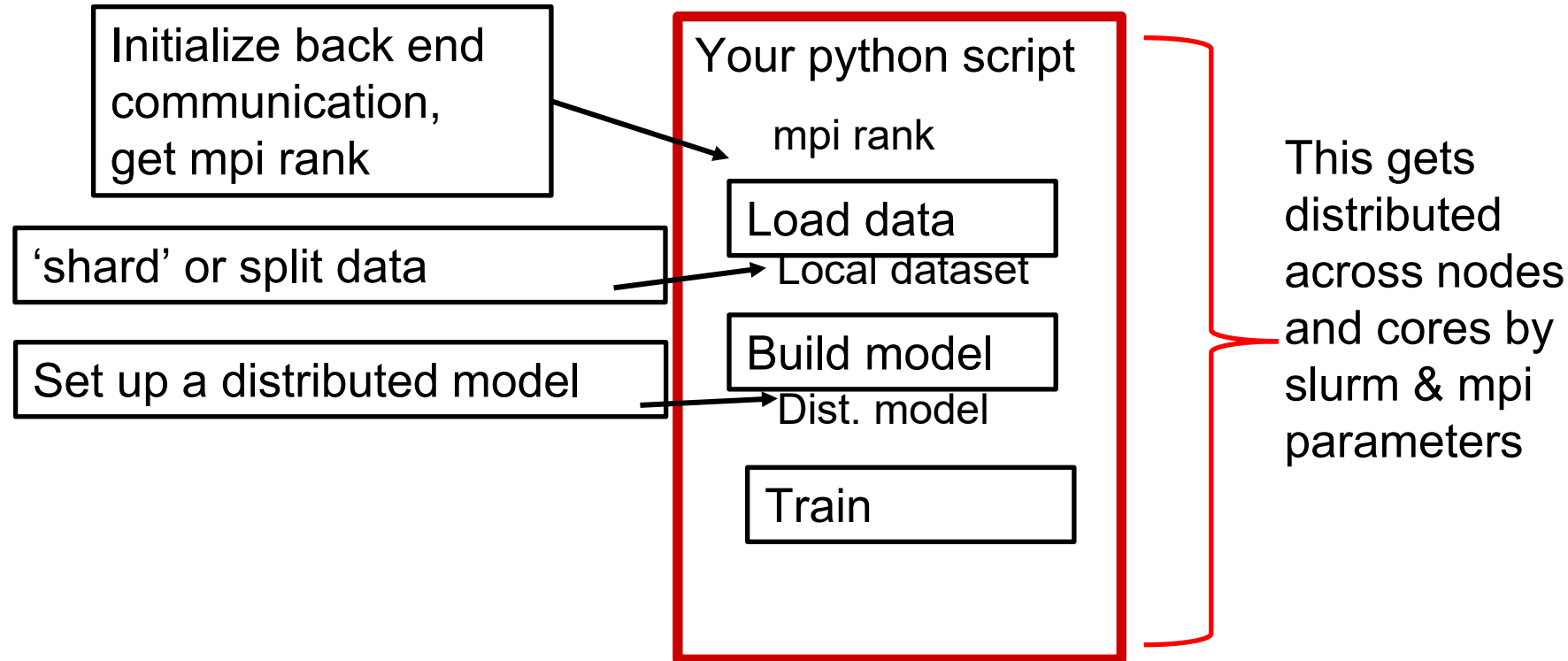
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Multinode, mpi launches instances

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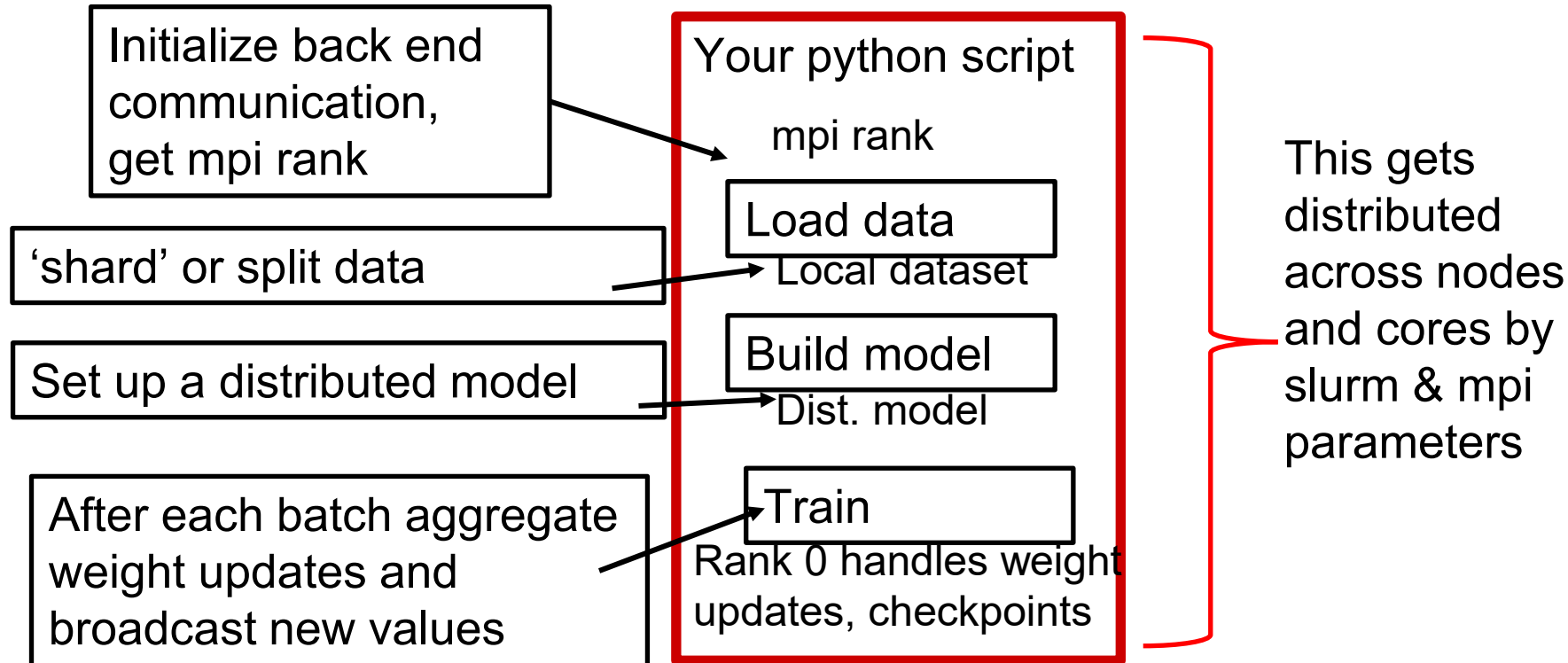
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Multinode, mpi launches instances

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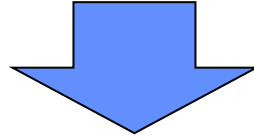
`mpirun -n number of tasks singularity → python`



mpi launches one instance per processor

In slurm batch script:

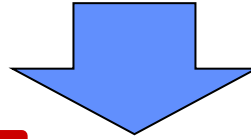
```
mpirun -n number of tasks singularity → python
```



mpi launches one instance per processor

In slurm batch script:

`mpirun -n number of tasks singularity → python`



device =GPU:0

Your python script

mpi rank

Load data

Local dataset

Build model

Dist. Model

Train

Rank 0 handles
updates

device =GPU:1

Your python script

mpi rank

Load data

Local dataset

Build model

Dist. model

Train

.....

.....

device =GPU:N

Your python script

mpi rank

Load data

Local dataset

Build model

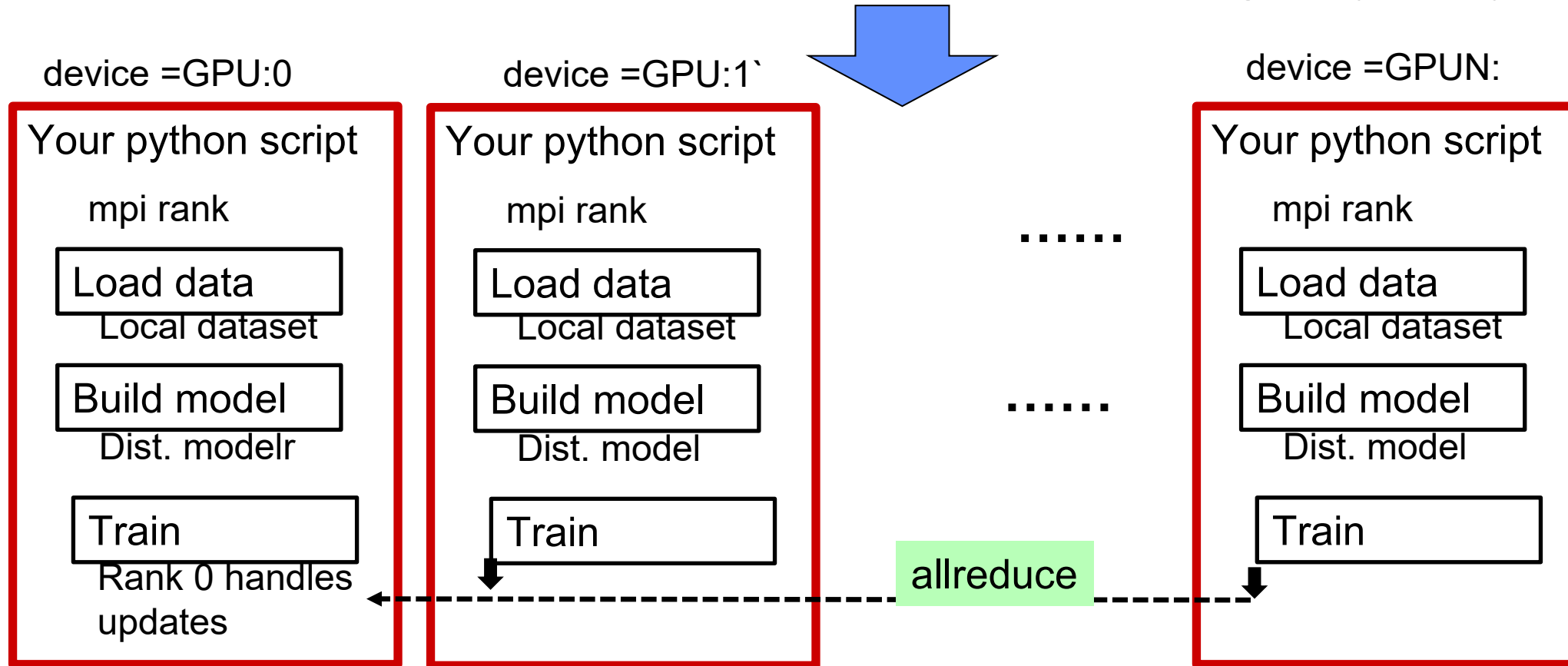
Dist. model

Train

For each batch: DDP will aggregate & share weights updates

In slurm batch script:

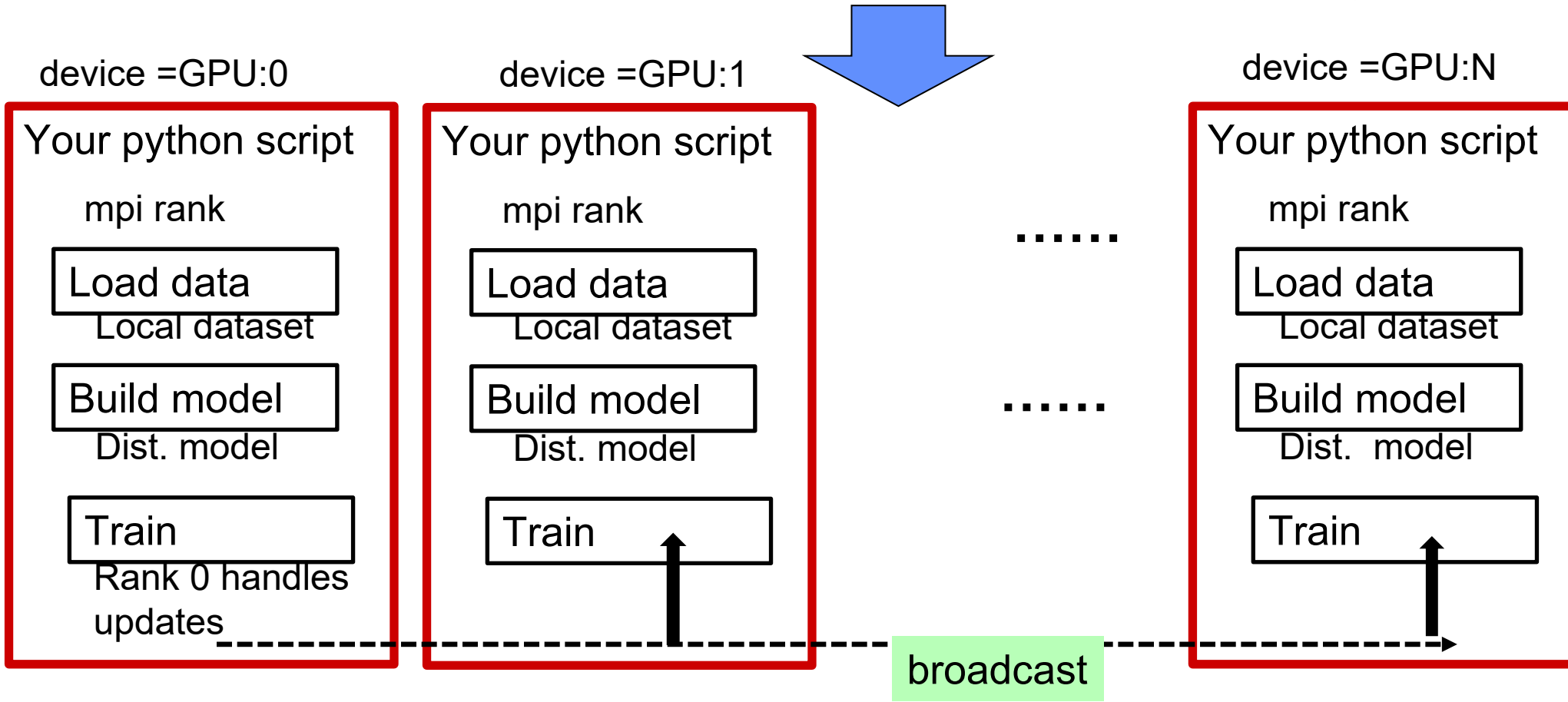
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For each batch: DDP will aggregate & share weights updates

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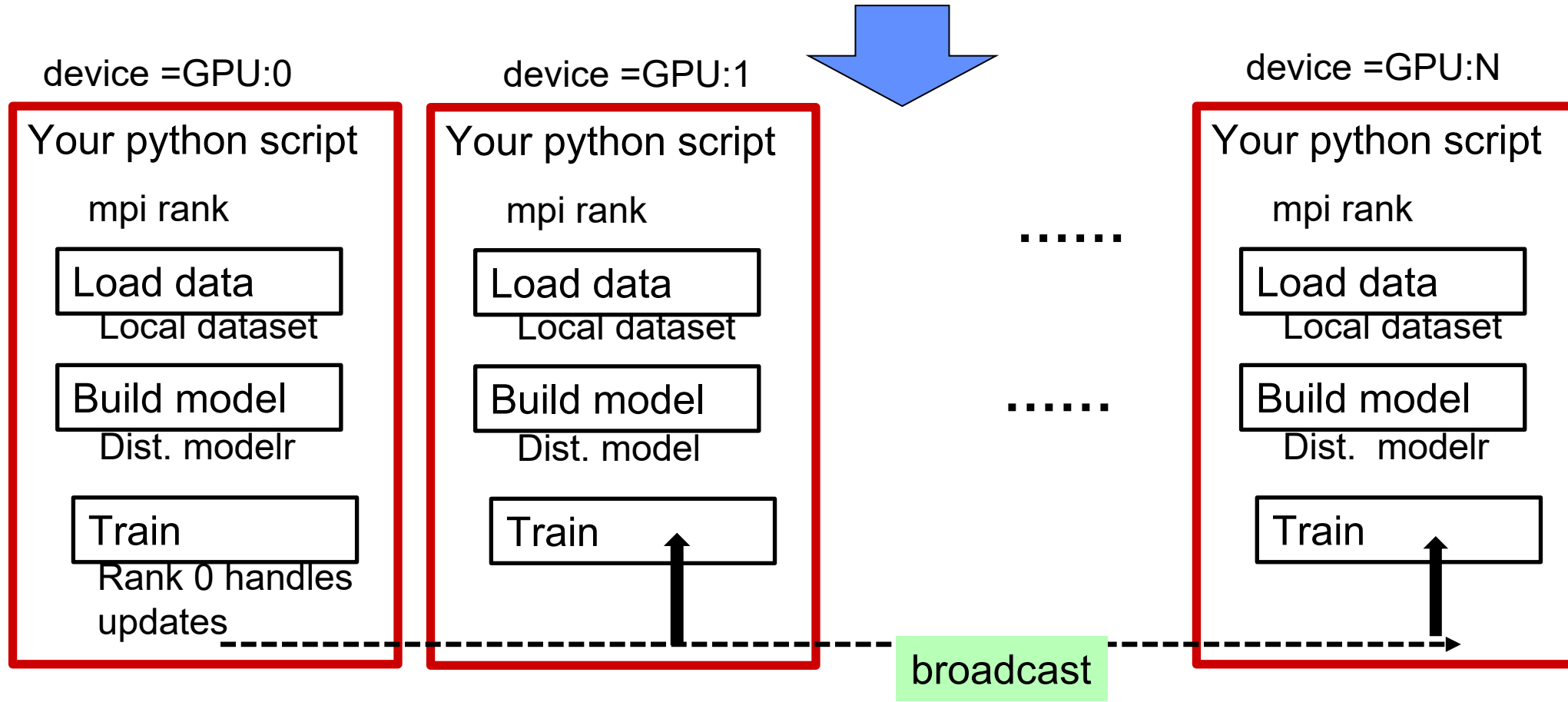
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For each batch: DDP will aggregate & share weights updates

In slurm batch script:

`mpirun -n number of tasks singularity → python`



Bigger batch size helps, but it uses more memory

Code snippets – Pytorch functions

Initialize back end communication, get mpi rank

```
world_size = int(os.environ['OMPI_COMM_WORLD_SIZE'])
rank       = int(os.environ['OMPI_COMM_WORLD_RANK'])
local_rank = int(os.environ['OMPI_COMM_WORLD_LOCAL_RANK'])
device = torch.cuda.set_device(local_rank)
torch.distributed.init_process_group('nccl', rank=rank, world_size=world_size)
```

'shard' or split data

```
train_sampler = torch.utils.data.distributed.DistributedSampler(dataset1)
train_loader = torch.utils.data.DataLoader(dataset1,
                                             batch_size=batch_size,
                                             sampler=train_sampler, ...)
```

Set up a distributed model

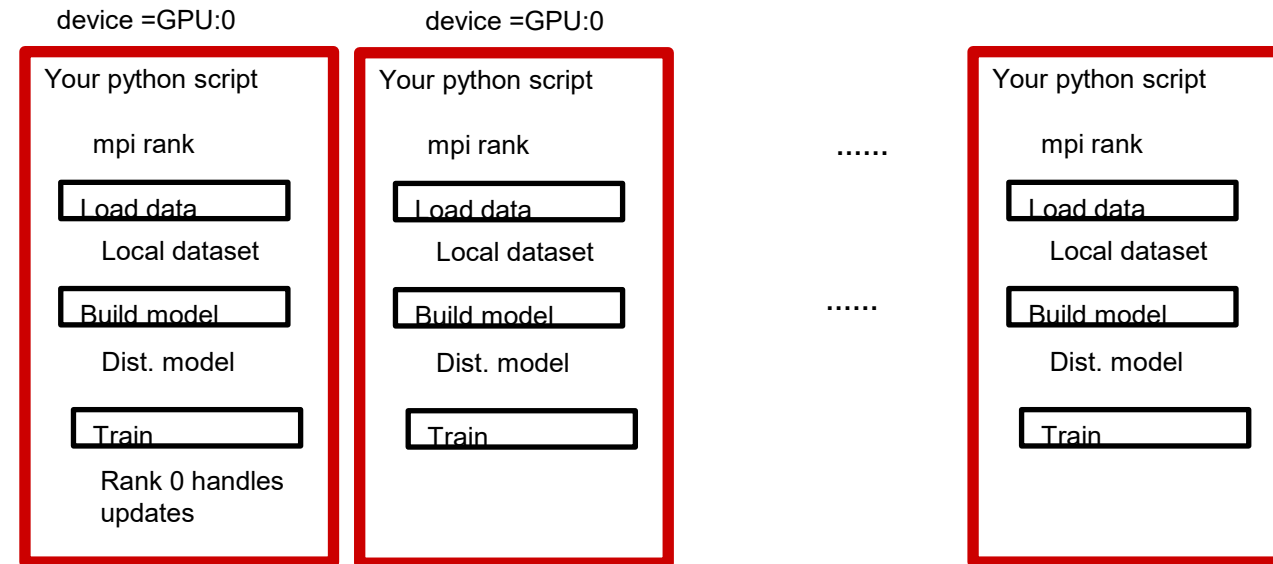
```
model = Net().to(device)
model = torch.nn.parallel.DistributedDataParallel() #with default args
```

After each batch aggregate weight updates and broadcast new values

Exercise, multinode MNIST execution

- **Goal: Get familiar with Pytorch coding for multinode execution on Expanse**
- **Goal: Get familiar with slurm batch script multinode parameters**
- **Let's login to a terminal window (see next page for tasks to try)**

```
mpirun -n number of tasks singularity → python
```



SLURM batch script highlights

- **Set up job resources**



```
#!/usr/bin/env bash
#SBATCH --job-name=pyt-cpu
#SBATCH --account=gue998
#SBATCH --partition=compute
#SBATCH --nodes=2 #try 1 or 2
#SBATCH --ntasks-per-node=8 #try 8 or 16 or 32 etc..
....
```

- **Set up 'master' ip address**



```
#set up ip addresses for communication
declare -xr MASTER_ADDR=$(mpirun --allow-run-as-root -n 1 hostname -i)
declare -xr MASTER_PORT=${MASTER_PORT:-15566};
```

- **Use mpirun command**
2*8=16



```
#use -n num-of-nodes * num-per-node
mpirun -n 16 -npnnode 8 singularity exec --bind /expance,/scratch
/cm/shared/apps/containers/singularity/pytorch/pytorch-latest.sif pyth
stdout_mnist_multinode_cpu.txt
```


Your task:

- run sbatch command for the slurm script
\$ sbatch run-pyt-main-cpu2.sb

- ssh into node to see execution

\$ squeue -u \$USER

(this will show your nodes)

\$ ssh exp-##-##

(this will connect to a node)

[exp-##-##] \$ top -u \$USER

(this will show what's running)

- review stdout output file

\$ grep 'training time' stdout_mnist_...txt

- homework: find trade offs in speed up vs communication

```
[etrain107@login02 MultiNode_v2]$ squeue -u etrain107
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
40567303	compute	pyt-cpu	etrain10	R	0:13	2	exp-5-[34-35]

```
etrain107@exp-5-34-~$ top - 22:44:29 up 21 days, 5:35, 1 user, load average: 419.73, 116.12, 55.52
```

Tasks: 1811 total, 9 running, 1801 sleeping, 0 stopped, 1 zombie

%Cpu(s): 99.6 us, 0.1 sy, 0.0 ni, 0.0 id, 0.0 wa, 0.3 hi, 0.0 si, 0.0 st

Mem: 257485.8 total, 239778.3 free, 11741.2 used, 5966.2 buff/cache

Swap: 0.0 total, 0.0 free, 0.0 used, 243939.4 avail Mem

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
1923907	etrain1+	20	0	13.4g	671832	216164	R	1597	0.3	10:03.77	python3
1923910	etrain1+	20	0	13.3g	631752	216164	R	1597	0.2	9:47.36	python3
1923911	etrain1+	20	0	13.4g	671496	216340	R	1597	0.3	10:01.92	python3
1923908	etrain1+	20	0	13.3g	634908	216164	R	1597	0.2	9:24.16	python3
1923912	etrain1+	20	0	13.4g	683004	218276	R	1597	0.3	10:24.23	python3
1923909	etrain1+	20	0	13.4g	734788	216164	R	1596	0.3	9:59.80	python3
1923913	etrain1+	20	0	13.4g	688748	216164	R	1596	0.3	9:51.26	python3
1923914	etrain1+	20	0	13.4g	707712	216164	R	1595	0.3	10:12.39	python3
1929064	etrain1+	20	0	60420	6336	3528	R	1.0	0.0	0:00.13	top
1923604	etrain1+	20	0	89740	9844	8236	S	0.0	0.0	0:00.06	systemd
1923609	etrain1+	20	0	158092	10728	0	S	0.0	0.0	0:00.00	(sd-pa
1923654	etrain1+	20	0	12984	3360	2832	S	0.0	0.0	0:00.01	bash
1923734	etrain1+	20	0	221900	12800	6316	S	0.0	0.0	0:00.09	mpirun
1923738	etrain1+	20	0	253768	7484	3716	S	0.0	0.0	0:00.00	srn
1923740	etrain1+	20	0	44548	888	0	S	0.0	0.0	0:00.00	srn

```
etrain107@login02 MultiNode_v2]$ grep 'training time' stdout_8.txt
```

NFO rank: 1 training time: 27.54175

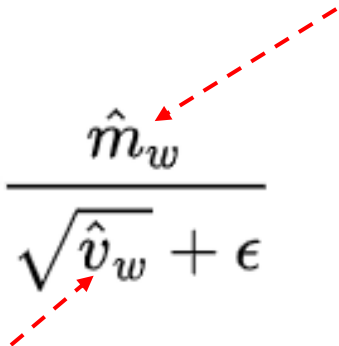
NFO rank: 14 training time: 27.54182

NFO rank: 2 training time: 27.54186

- **pause**

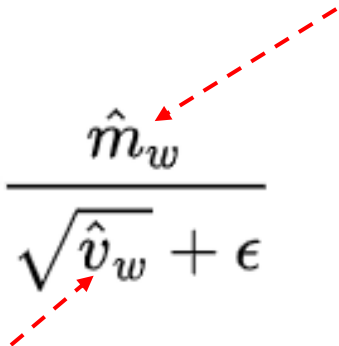
Deepspeed Memory Optimization

- Optimizers like Adam use a lot of memory **b/c** it tracks momentum and variances of gradients for *each* weight parameter update:

$$w^{(t+1)} \leftarrow w^{(t)} - \eta \frac{\hat{m}_w}{\sqrt{\hat{v}_w} + \epsilon}$$


Deepspeed Memory Optimization

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$$w^{(t+1)} \leftarrow w^{(t)} - \eta \frac{\hat{m}_w}{\sqrt{\hat{v}_w} + \epsilon}$$


- “Zero Redundancy” (ZeRO) optimizes memory storage by partitioning these terms to different devices and then gathering them only when needed

ZeRO: Memory Optimizations Toward Training Trillion Parameter Models 2020, Rajbhandari et al, Microsoft

Deepspeed: 3 stages of incrementally more partitioning

1. Optimizer state partitioning (ZeRO stage 1)
2. Gradient partitioning (ZeRO stage 2)
3. Parameter (weights) partitioning (ZeRO stage 3)

Deepspeed: 3 stages of incrementally more partitioning

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3. Parameter (weights) partitioning (ZeRO stage 3)

All options go in a json file and passed as argument

--deepspeed_config
ds_config.json

```
1-20:mnist_trialpipe$ more ds_config.json

"train_batch_size":16,
"bf16": { "enabled": true },
"fp16": { "enabled": false},
"gradient_clipping": 1.0,
"zero_optimization": { "stage": 0 },
"zero_allow_untested_optimizer": true
```

Deepspeed code snippets

Deepspeed initialization creates a “**model_engine**” to wrap the model

```
model_engine, opt, _, _ = deepspeed.initialize(model=model,  
model_parameters=model_params, args=args)
```

Deepspeed code snippets

Deepspeed initialization creates a “**model_engine**” to wrap the model

```
model_engine, opt, _, _ = deepspeed.initialize(model=model,  
model_parameters=model_params, args=args)
```

The training loop now uses **model_engine** for forward,backward processing

```
output = model_engine(data)  
loss = loss_function(output, target)  
model_engine.backward()  
model_engine.step()  
htcore.mark_step()
```

Launch program instances with mpirun, or deepspeed launcher

- End