



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

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- 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

• Typically, you usually wrap the model build function with another function, and add in arguments for the hyperparameters



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)

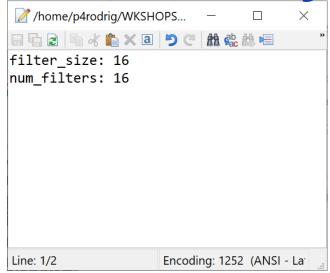
- Consider how long each a model runs for 1 configuration of hyperparameters for 1 dataset
- Organize jobs into reasonable chunks of work
- For large models consider model-checkpoints
- Tensorboard is available but needs to be secure (ask for details)



Organizing Configurations – one way

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

Create text file with "Parameter: Value" pairs



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

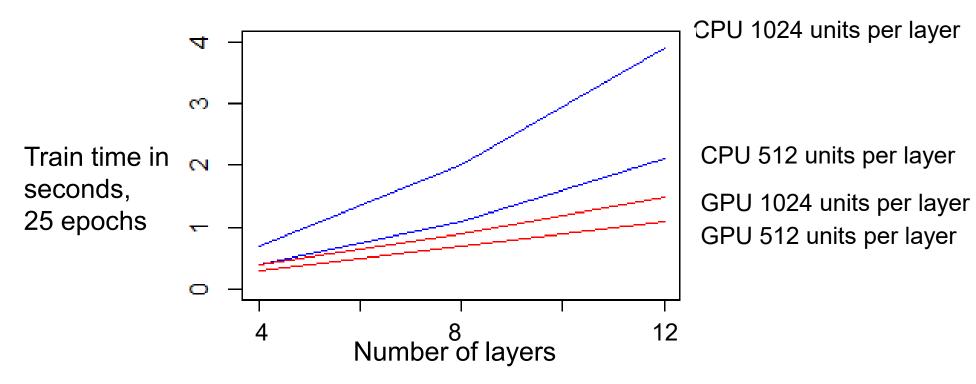
filter_size=mv_yaml.get("filter_size")
num_filters=my_yaml.get("num_filters")
print('arguments, filter_size:',filter_size,' num_filters',num_filters)
```

note on using GPU

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

Code snippet to check for GPU devices

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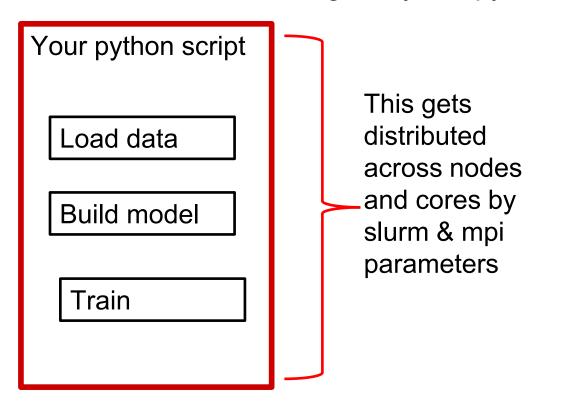
- Main functions:
- 1. mpirun command (also torchrun exists but I haven't tested it much)
- 2. Pytorch data loader will parallelize sampling
- 3. Pytorch DDP (**Distributed Data Parallel**) will wrap a model
- 4. DDP wil use the Pytorch 'init_backend' function

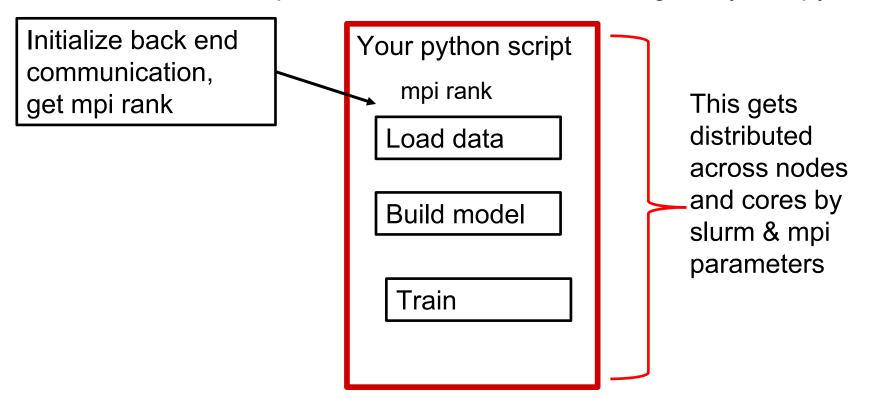
For example, single node, single device execution

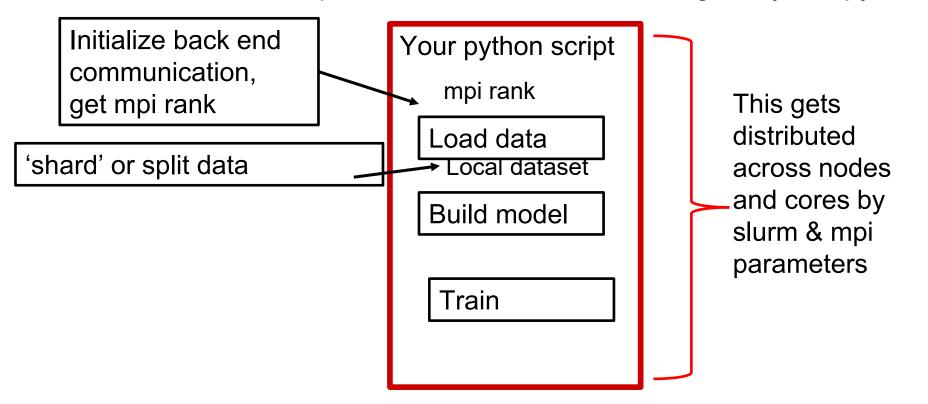
In slurm batch script:

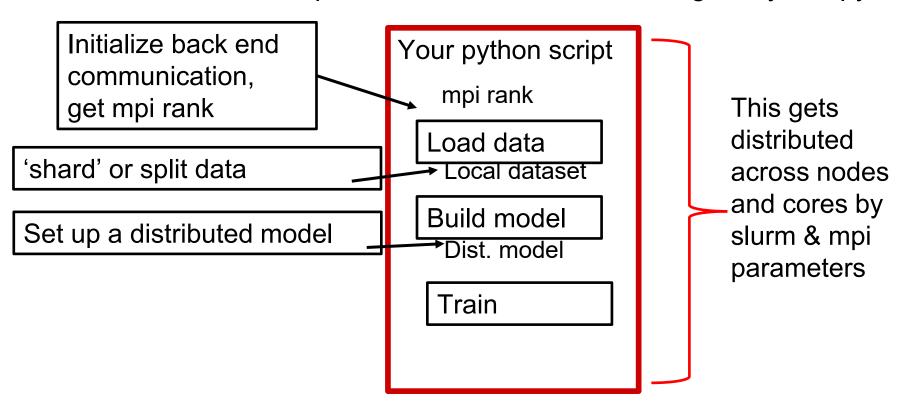
singularity → python

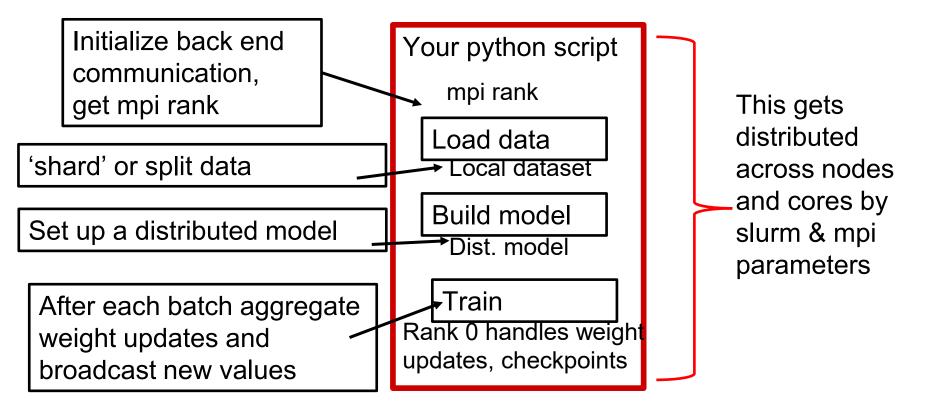
Your python script
Load data
Build model
Train











mpi launches one instance per processor

mpi launches one instance per processor

In slurm batch script:

mpirun –n **number of tasks** singularity \rightarrow python

device =GPU:0

device =GPU:1

device =GPU:N

Your python script

mpi rank

Load data

Local dataset

Build model

Dist. Model

Train

Rank 0 handles updates

Your python script

mpi rank

Load data

Local dataset

Build model

Dist. model

Train

Your python script

mpi rank

Load data

Local dataset

Build model

Dist. model

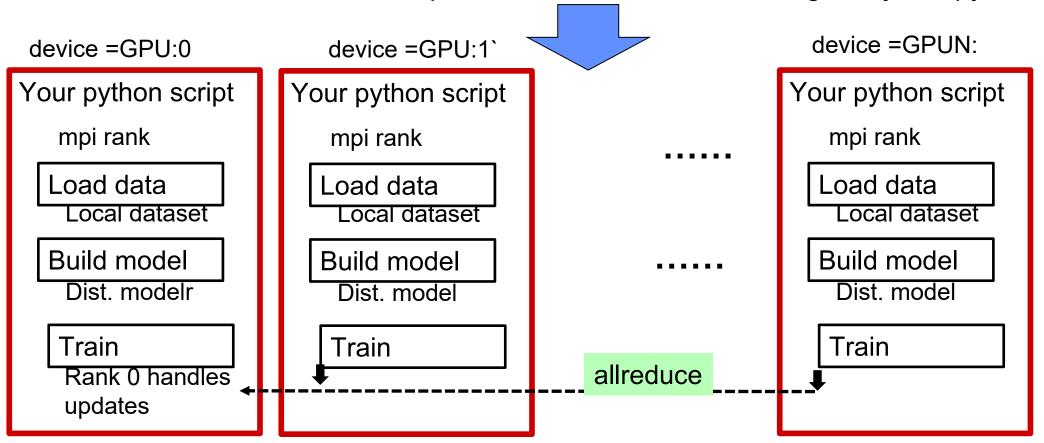
Train



For each batch: DDP will aggregate & share weights updates

In slurm batch script:

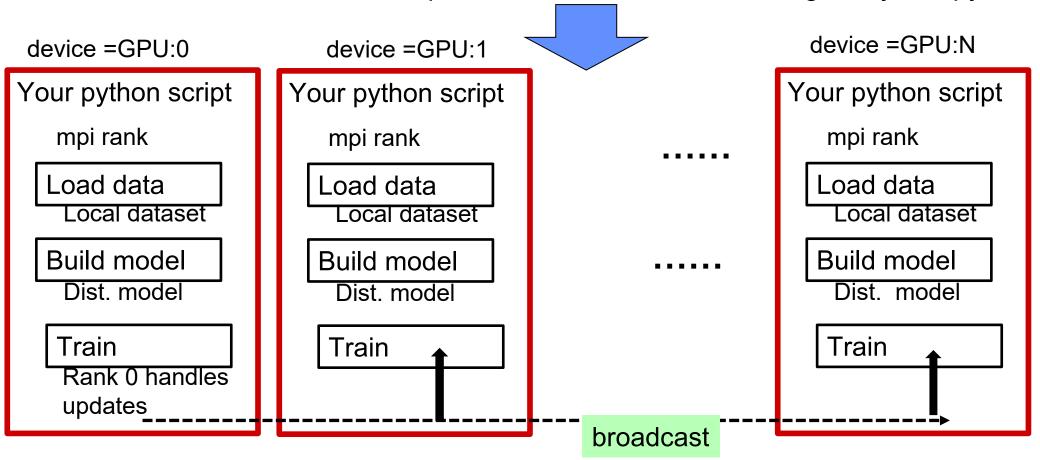
mpirun –n **number of tasks** singularity → python



For each batch: DDP will aggregate & share weights updates

In slurm batch script:

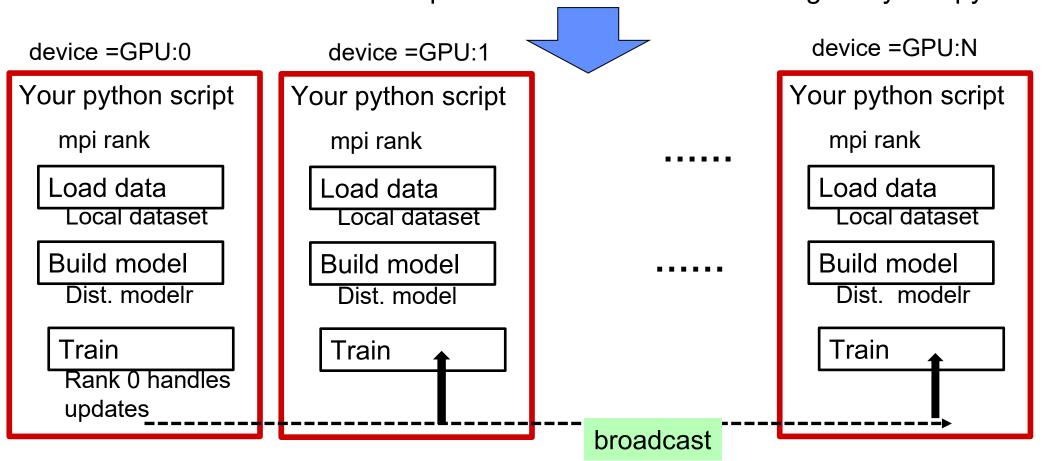
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For each batch: DDP will aggregate & share weights updates

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'])

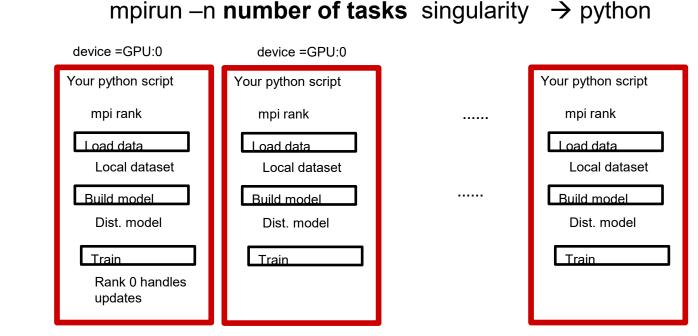
local_rank = int(os.environ['OMPI_COMM_WORLD_LOCAL_RANK'])

device = torch.cuda.set_device(local_rank)

torch.distributed.init_process_group('nccl',rank=rank,world_size=world_size)
```

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)



SLURM batch script highlights

#!/usr/bin/env bash #SBATCH --job-name=pyt-cpu Set up job #SBATCH --account=gue998 resources **#SBATCH** --partition=compute #SBATCH --nodes=2 #try 1 or 2 #SBATCH --ntasks-per-node=8 #try 8 or 16 or 32 etc... #set up ip addresses for communication Set up 'master' declare -xr MASTER_ADDR=\$(mpirun --allow-run-as-root -n 1 hostname -i declare -xr MASTER_PORT=\${MASTER_PORT:-15566}; ip address #use -n num-of-nodes * num-per-node mpirun - 16 - npernode 8 singularity exec -- bind /expanse, /scratch **Use mpirun** /cm/shared/apps/containers/singularity/pytorch/pytorch-latest.sif pyth command stdout_mnist_multinode_cpu.txt

2*8=16

Your task:

- run sbatch command for the slurm script
- \$ sbatch run-pyt-main-cpu2.sb
- ssh into node to see execution

```
$ squeue -u $USER
```

\$ ssh exp-##-##

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

(this will show your nodes)

(this will connect to a node)

(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]$ 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

