

Hands-on Lecture: Deep learning Framework on Fugaku

--- CEA-RIKEN HPC School 2022 ---
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Slides: RIKEN-CEA-school2022-AI-kento.pdf

Please run this command to reserve an interactive node during the break:

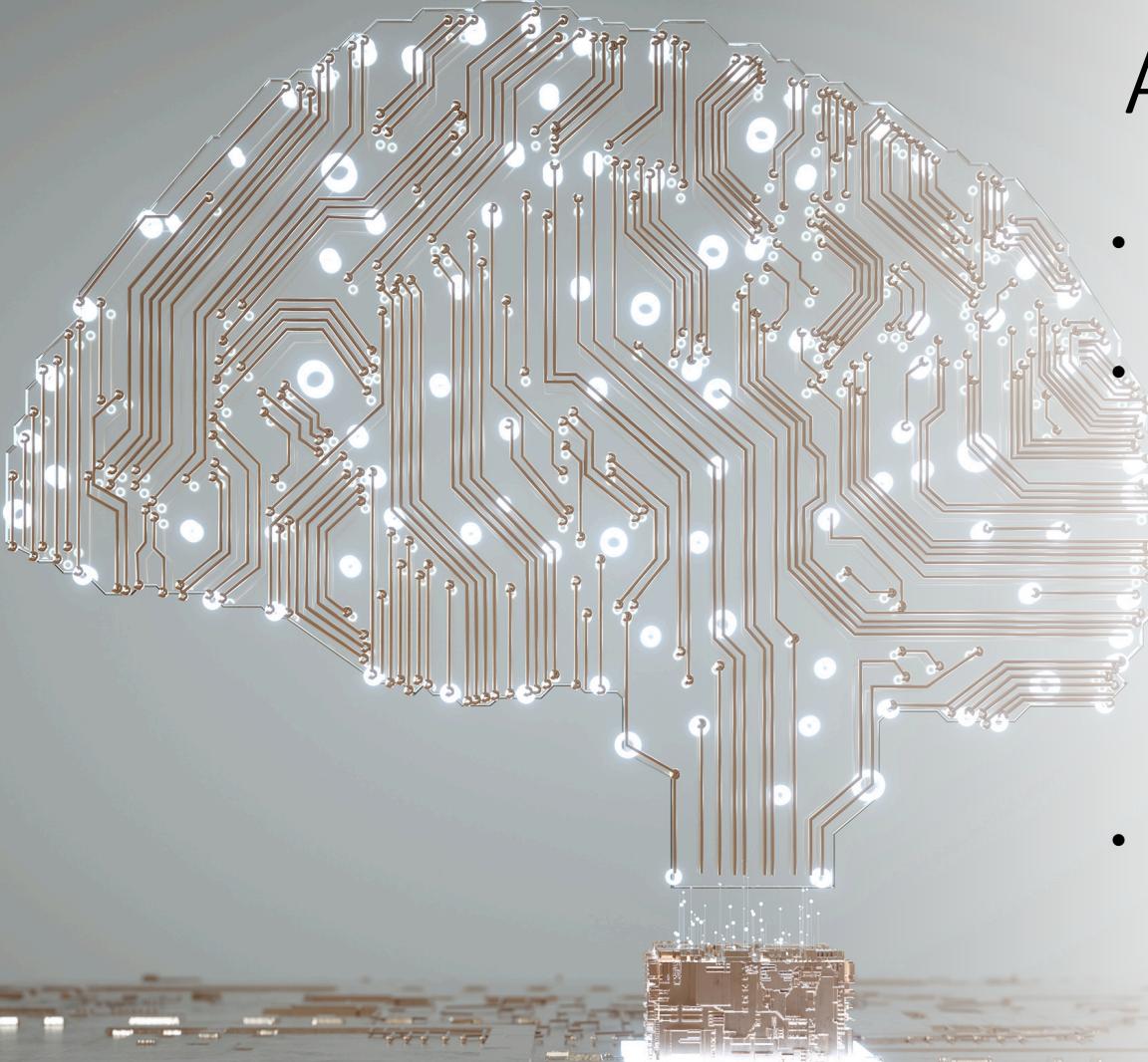
```
$ pbsub --interact -L "node=1" -L "rscgrp=int" -L "elapse=2:00:00" --sparam "wait-time=6000" --mpi "proc=8"  
-x "PJM_LLI0_GFSCACHE=/vol0004"
```

Self-introduction

- Kento Sato (佐藤賢斗)
- Team leader of High Performance Big Data Research team at RIKEN R-CCS



<https://www.hpbd.r-ccs.riken.jp>



Agenda

- In this lecture, you learn how to use one of AI frameworks (PyTorch) on Fugaku
- Especially you learn basics of how to
 - Use Tensor operations on PyTorch/Python
 - Load a dataset with dataloaders
 - Build a neural network
 - Train a neural netowrk
 - Save and load a trained neural network
 - Extend your code for distributed training
- You have hands-on exercise during this lecture, please login to Fugaku !

Preparation for hands-on

- Login to Fugaku

```
$ ssh <user name>@fugaku.r-ccs.riken.jp
```

- Download lecture materials

```
$ mkdir cea-riken-school-2022
$ cd cea-riken-school-2022
$ git clone https://github.com/kento/hpc_tools_examples.git
$ cd ./hpc_tools_examples/deep_learning/pytorch_fugaku/00_basics
```

- Reserve an interactive node

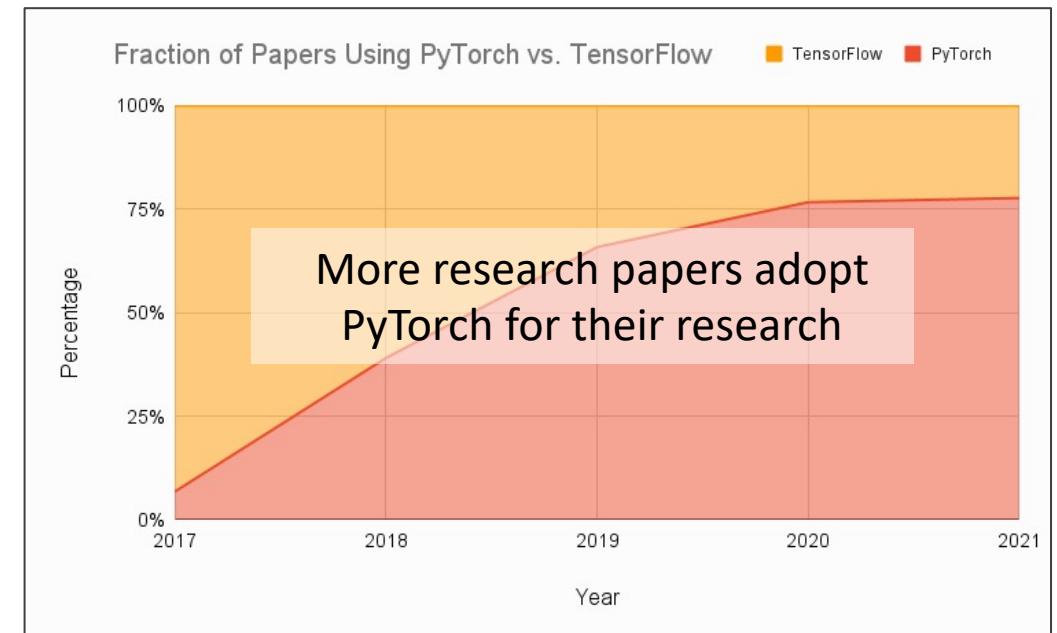
```
$ pbsub --interact -L "node=1" -L "rscgrp=int" -L "elapse=3:00:00" --sparam "wait-time=600" --mpi "proc=8"
-x "PJM_LLI0_GFSCACHE=/vol0004"
```

- Today, we use an interactive node, please reserve your interactive node !
- An interactive node is a compute node which you can keep using as if it is your own compute node without submiting a job to the batch scheduler

PyTorch vs. TensorFlow

- Today, we use PyTorch
- Both PyTorch and TensorFlow are very mature frameworks, and their core Deep Learning features overlap significantly
- PyTorch has become the *de facto* "research framework" after its explosive adoption by the research community

PyTorch



Source: <https://www.assemblyai.com/blog/pytorch-vs-tensorflow-in-2022/>

Set environment variables

- Set environment variables
 - By running a script “fugaku_setup.sh”

```
$ . ./.fugaku_setup.sh
```

- By setting one by one

```
$ export PYTORCH_PATH=/home/apps/oss/PyTorch-1.7.0
$ export LD_LIBRARY_PATH=${PYTORCH_PATH}/lib:${LD_LIBRARY_PATH}
$ export PATH=${PYTORCH_PATH}/bin:${PATH}
```



Tensors

- Tensors are a specialized data structure that are very similar to arrays and matrices
- In PyTorch, you use tensors to encode the inputs and outputs of a model, as well as the model's parameters
- Tensors are like NumPy's ndarrays (e.g., Matrix operations between arrays)
 - Except that tensors can run on GPUs or other hardware accelerators with the same interface

```
# Directly from data
import torch
data = [[1, 2], [3, 4]]
x_data = torch.tensor(data)
print (data)
print (x_data)
```

```
# From a NumPy array
import numpy as np
np_array = np.array(data)
x_np = torch.from_numpy(np_array)
print (data)
print (x_np)
```

```
print (x_np + x_np)
print (x_np * x_np)
```

Exercise

- Compute following tensor operations with Tensor data type

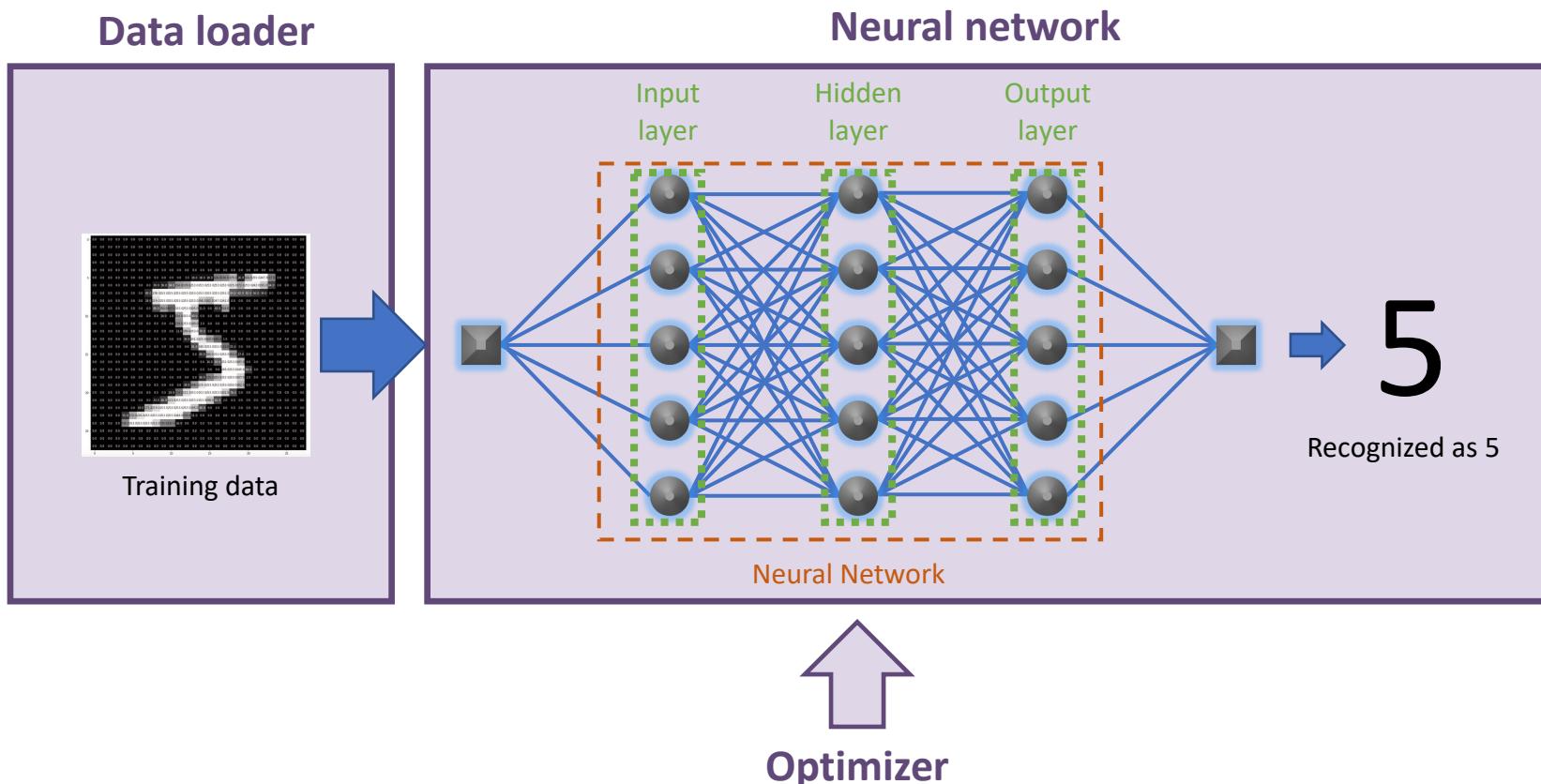
1.
$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 5 \end{pmatrix} + \begin{pmatrix} 5 & 4 & 3 \\ 4 & 3 & 2 \\ 3 & 2 & 1 \end{pmatrix} = ?$$

2.
$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 5 \end{pmatrix} * \begin{pmatrix} 5 & 4 & 3 \\ 4 & 3 & 2 \\ 3 & 2 & 1 \end{pmatrix} = ?$$

Answer: [00_basics/00_tensors_ex.py](#)

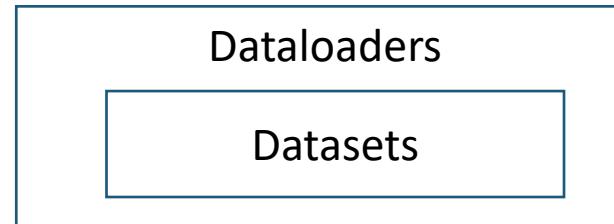
Basic concept of PyTorch

- Major three components
 - **Neural network**: Define a class and implement **neural networks** that you want to train
 - **Data loader**: Interface to **datasets** for training and test
 - **Optimizer**: Optimize parameters of a **neural network** trained with **datasets**



Datasets and Dataloaders

- Decoupling data processing code from model training code for better readability and modularity
- PyTorch provides two data primitives that allow you to use pre-loaded datasets as well as your own data
 - Dataset: `torch.utils.data.Dataset`
 - Stores the data and its corresponding labels
 - Provides a number of pre-loaded datasets (such as MNIST) for prototyping and benchmarking your model
 - Image Datasets: <https://pytorch.org/vision/stable/datasets.html>
 - Text Datasets: <https://pytorch.org/text/stable/datasets.html>
 - Audio Datasets: <https://pytorch.org/audio/stable/datasets.html>
 - Dataloader: `torch.utils.data.DataLoader`
 - Wrapper wraps an iterable around the Dataset to enable easy access to the samples.



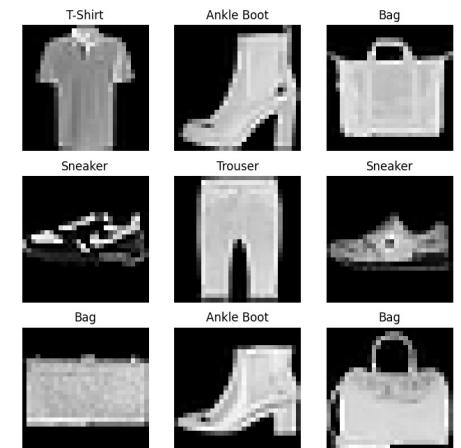
Loading a Dataset:

```
import torch
from torch.utils.data import Dataset
from torchvision import datasets
from torchvision.transforms import ToTensor

training_data = datasets.FashionMNIST(root="../data", train=True, download=True,
transform=ToTensor())

test_data = datasets.FashionMNIST(root="../data", train=False, download=True,
transform=ToTensor())
```

- **root (string)** – Root directory of dataset where you want to cache
- **train (*bool*, optional)** – If True, creates dataset from training.pt, otherwise from test.pt.
- **download (*bool*, optional)** – If true, downloads the dataset from the internet and puts it in root directory. If dataset is already downloaded, it is not downloaded again.
- **transform (*callable*, optional)** – A function/transform that takes in an PIL image and returns a transformed version. E.g., transforms.RandomCrop
 - Please specify ToTensor() → It transforms an image into tensor datatype



Fashion-MNIST

Exercise

- Modify 01_datasets.py to download MNIST instead of FashionMNIST by referring to PyTorch API documents
- MNIST is a dataset of handwritten digits that is commonly used for training various image processing systems
- PyTorch API documents
 - <https://pytorch.org/vision/stable/datasets.html>

The screenshot shows the PyTorch documentation website at https://pytorch.org/vision/stable/datasets.html. The top navigation bar includes links for Get Started, Ecosystem, Mobile, Blog, Tutorials, Docs (which is currently selected), Resources, and GitHub. The main content area is titled "PYTORCH DOCUMENTATION" and contains information about PyTorch being an optimized tensor library for deep learning. It includes sections on release status (Stable, Beta, Prototype), notes, language bindings, and a search bar.



Workflow for training NN

• Workflow

- **Step 1:** It retrieves multiple samples (“mini-batch” or “batch”) from a dataset
 - A minibatch refers to equally sized subsets of the dataset over which the gradient is calculated, and weights are updated
 - The number of samples in a mini-batch is called “batch size”
- **Step 2:** Run forward and backward operations, then updates parameters of a training neural network
- **Step 3:** Once all the samples are fed to the training neural network, it shuffles samples in a dataset and repeat from step 1

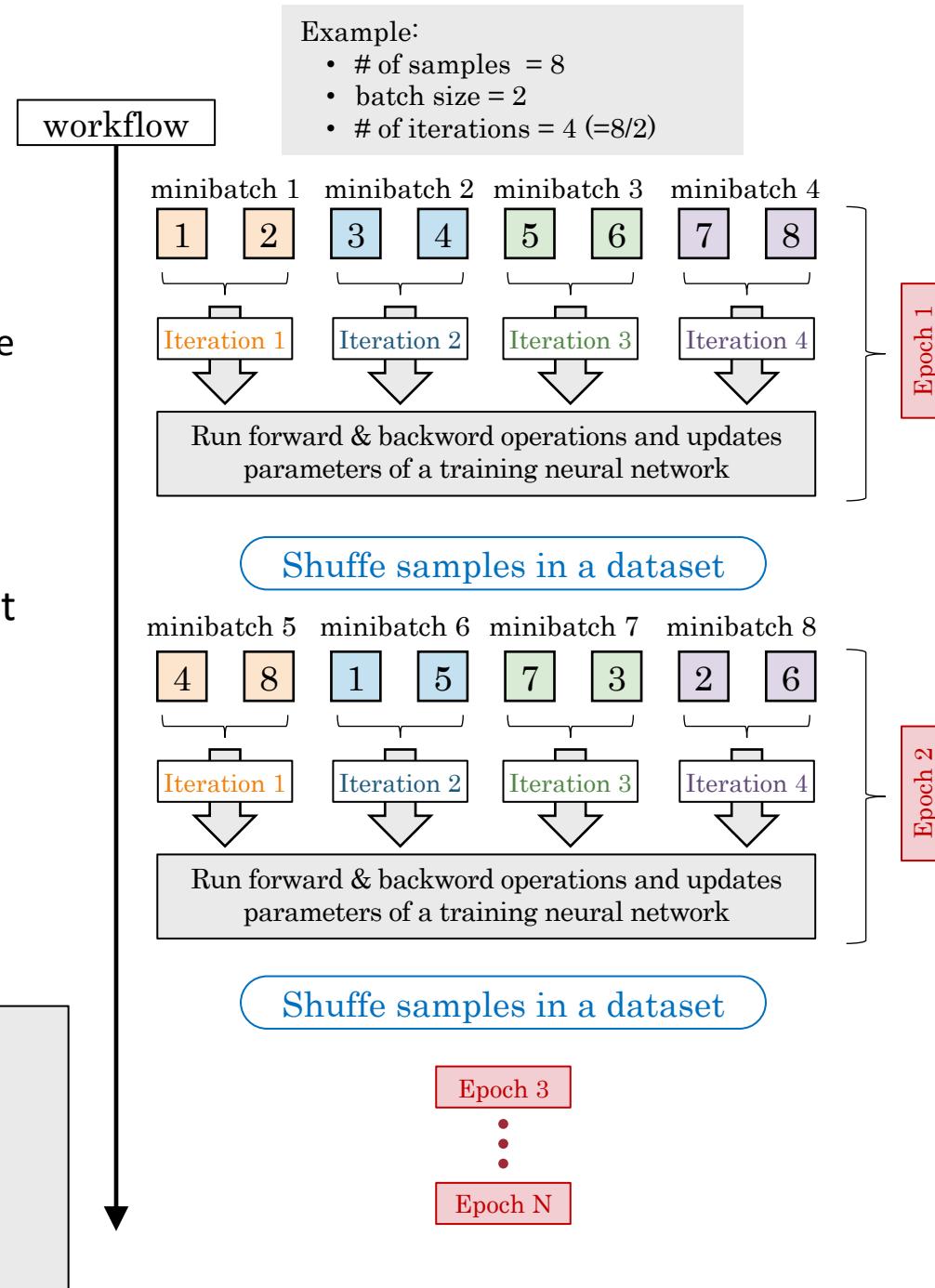
• Epoch

- One Epoch is when an ENTIRE dataset is passed forward and backward through the neural network only ONCE

• Iterations

- Iterations is the number of batches needed to complete one epoch

- Epoch 1
 - Iteration 1
 - ...
 - Iteration N
- Epoch 2
 - Iteration 1
 - ...
 - Iteration N
- Epoch 3
 - ...



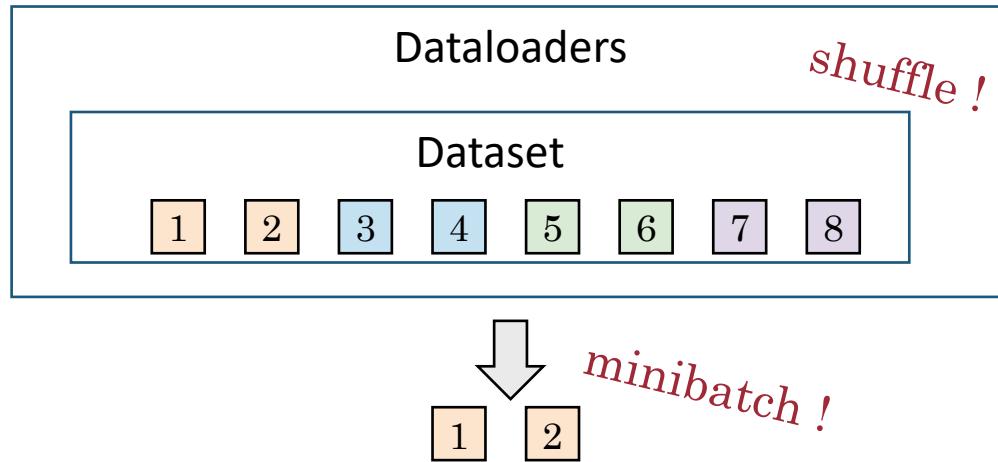
DataLoaders

- As explained in the previous slide, while training a model, we need to pass samples in a form of “mini-batches”, reshuffle the data at every epoch to reduce model overfitting
- The DataLoader abstracts this complexity for us in an easy API

Snippet (dataloaders)

```
from torch.utils.data import DataLoader

train_dataloader = DataLoader(dataset=training_data, batch_size=64, shuffle=True)
test_dataloader = DataLoader(dataset=test_data, batch_size=64, shuffle=True)
```



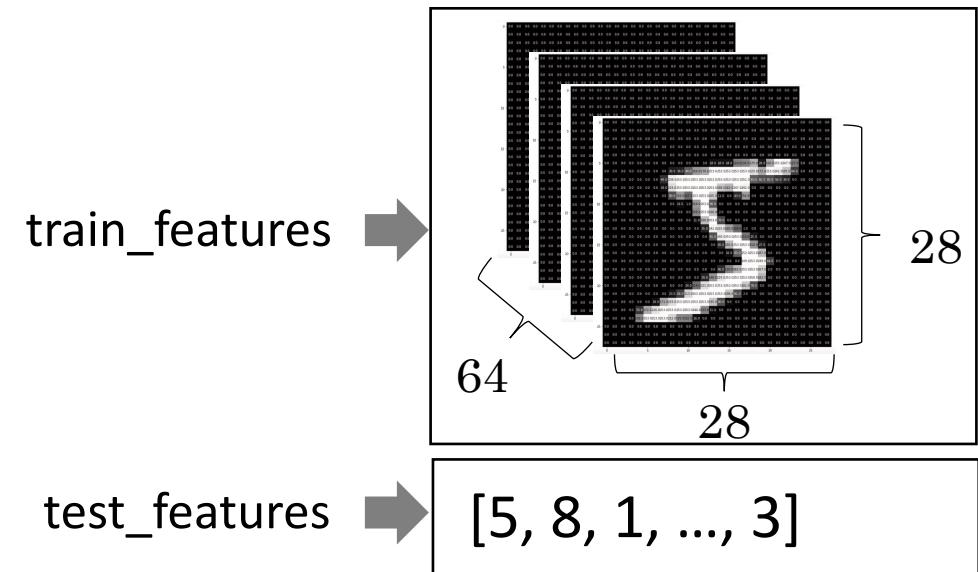
- **dataset** (*Dataset*) – dataset from which to load the data.
- **batch_size** (*int, optional*) – how many samples per batch to load (default: 1).
- **shuffle** (*bool, optional*) – set to True to have the data reshuffled at every epoch (default: False).

Preparing data for training with DataLoaders

- We have loaded that dataset into the DataLoader and can iterate through the dataset as needed
- Each iteration below returns a batch of "train_features" and "train_labels"
 - batch_size=64 features and labels respectively
- Because we specified shuffle=True, the data is shuffled after we iterate over all batches,

Snippet (dataloaders print)

```
# Display image and label
train_features, train_labels = next(iter(train_dataloader))
print(f"Feature batch shape: {train_features.size()}")
print(f"Labels batch shape: {train_labels.size()}")
img = train_features[0] # get the first image from mini-batch
label = train_labels[0] # get the first label
print(f"Label class: {label}")
```



```
Feature batch shape: torch.Size([64, 1, 28, 28])
Labels batch shape: torch.Size([64])
Label: 8
```

Exercise

- Get the first MNIST minibatch from dataloaders and print out shape of the minibatch and the labels by extending “01_datasets_ex.py”
- Hint: Adding the code snippets to 01_datasets_ex.py

00_basics/01_datasets_ex.py

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Snippet (dataloaders)

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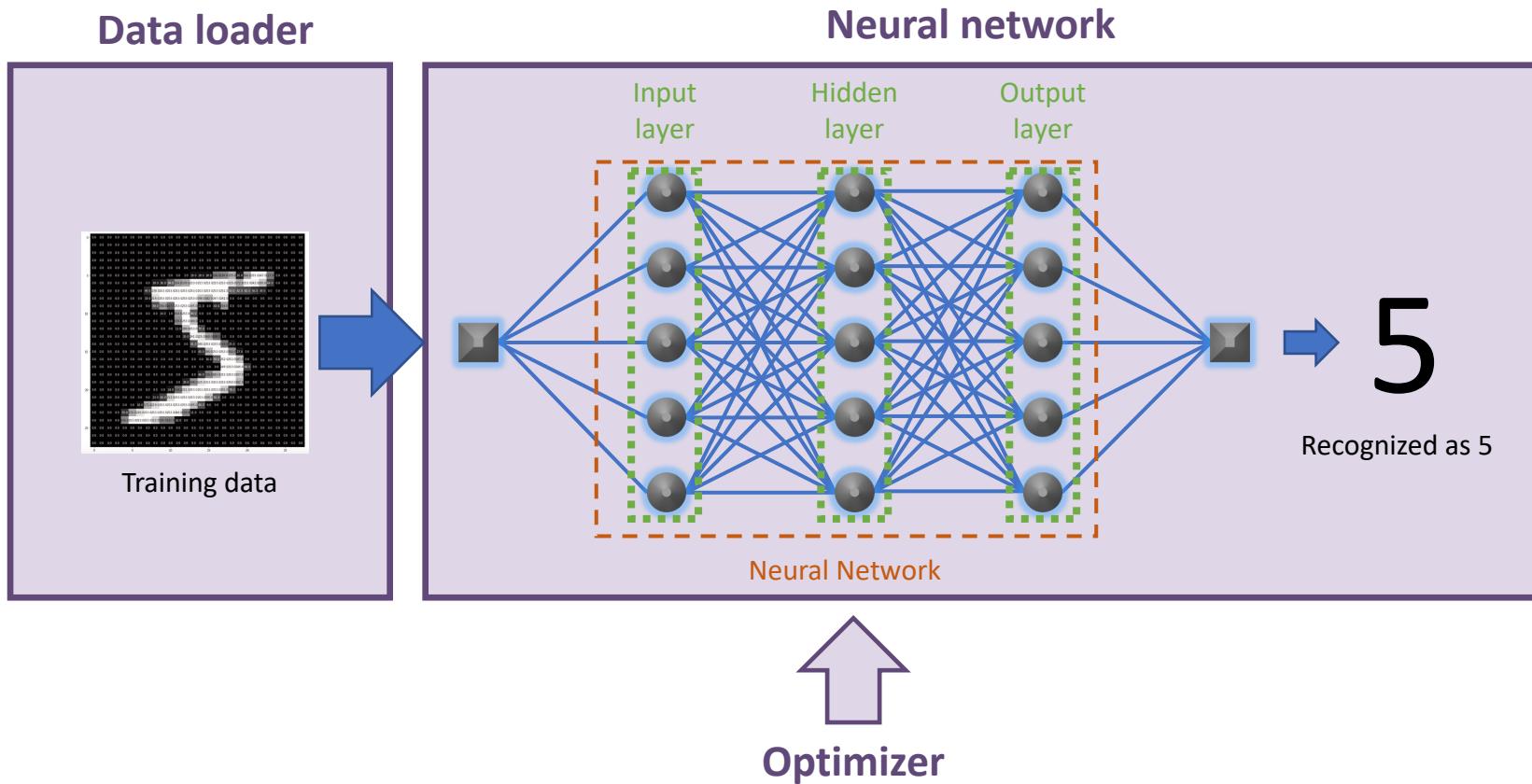
Snippet (dataloaders print)



Answer:

00_basics/02_dataloaders.py

Basic concept of PyTorch



Building a neural network

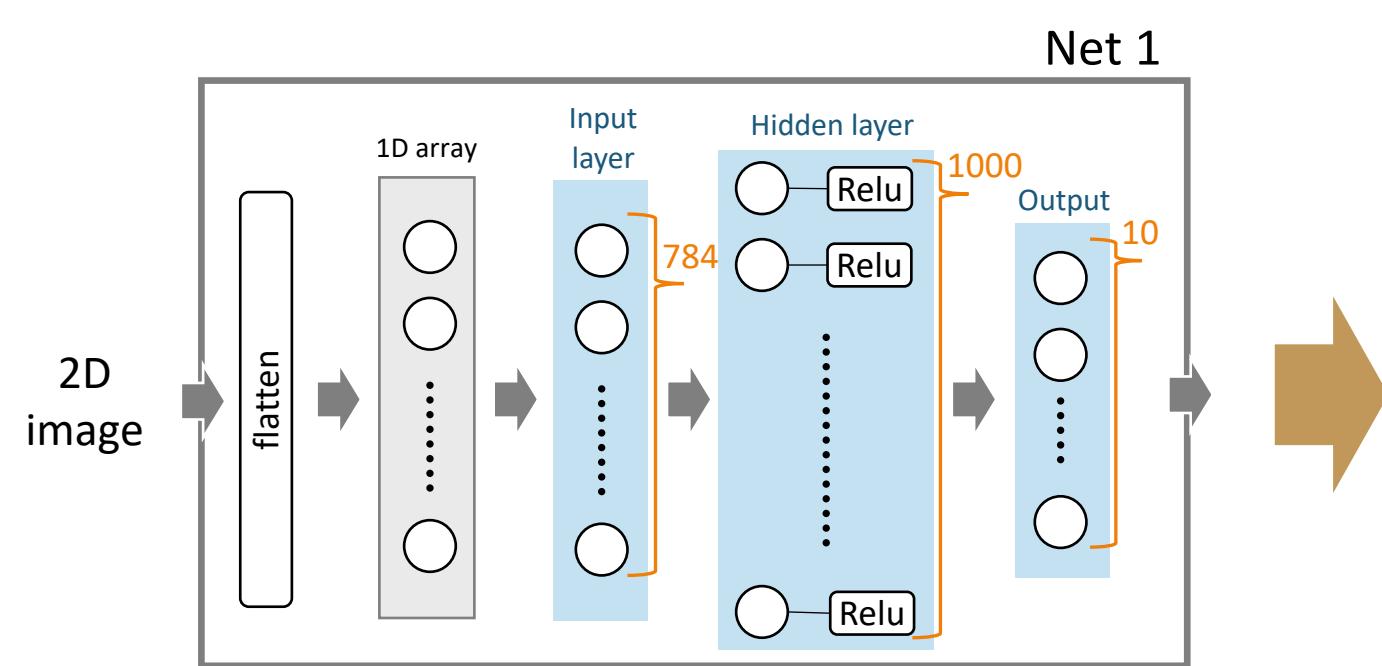
- Neural networks comprise of layers/modules that perform operations on data.
 - The torch.nn namespace provides all the building blocks that you need to build your own neural network
 - Every module in PyTorch subclasses the nn.Module
 - A neural network is a module itself that consists of other modules (such as layers)
 - This nested structure allows for building and managing complex architectures easily
-
- Necessary modules to import:

Snippet (import nn & functional)

```
from torch import nn  
from torch.nn import functional as F
```

Building a 3-layer neural network

- Now, we define our neural network (**Net1**) by subclassing nn.Module and initialize the neural network layers in **(1) __init__**
 - In `__init__`, we initialize layers
- Every nn.Module subclass implements the operations on input data in the **(2) forward method**
 - In `forward`, we codify how to connect the initialized layers



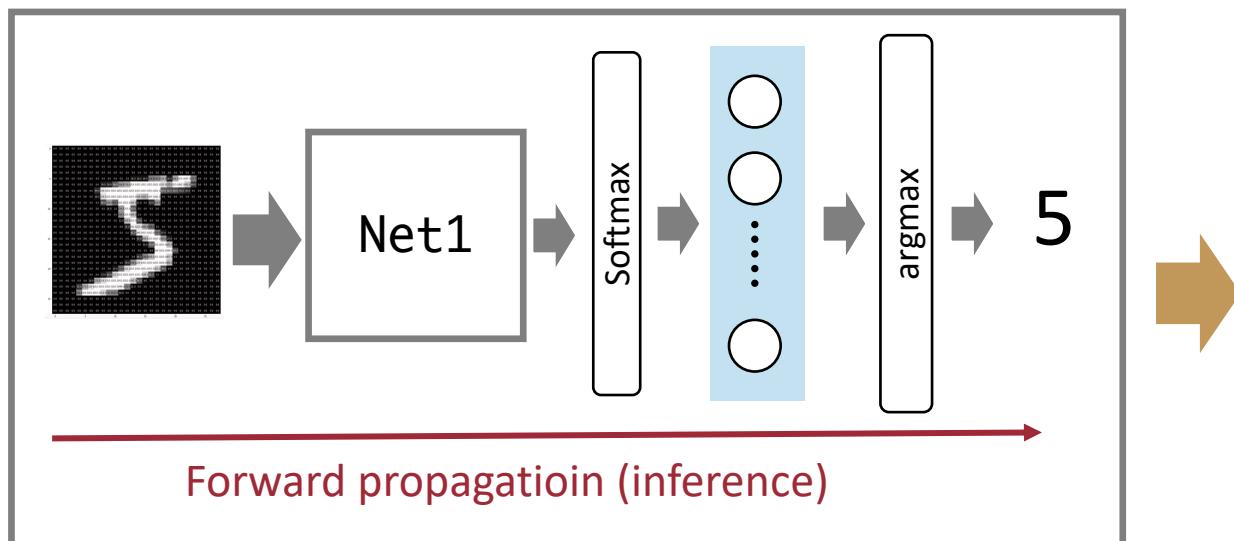
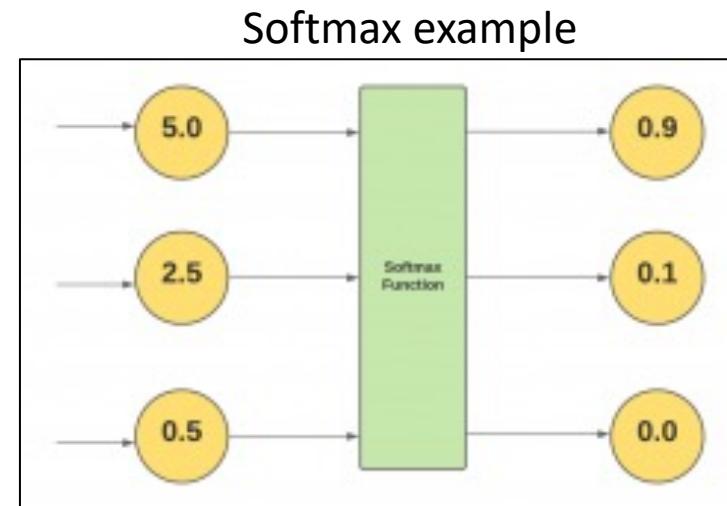
Snippet (Building Net1)

```
class Net1(nn.Module): 1. __init__ : init layers
    def __init__(self):
        super(Net1, self).__init__()
        self.flatten = nn.Flatten()
        self.fc1 = nn.Linear(28 * 28, 1000)
        self.fc2 = nn.Linear(1000, 10)

    def forward(self, x):
        x = self.flatten(x)
        x = self.fc1(x)
        x = F.relu(x)
        x = self.fc2(x)
        return x
2. forward: Connect layers
```

Running inference of Net 1

- To run inference with the built model, we pass the input data to the model
 - This is done by executing the model's forward
- Calling the model on the input returns a 10-dimensional tensor with raw predicted values for each class
- We get the prediction probabilities by passing it through an instance of the "nn.Softmax" module.
- To get the inference result, we get the index whose prediction probability is highest by calling "argmax"



Snippet (Running inference)

```
model = Net1()
print(model)
logits = model(img)
pred_probab = nn.Softmax(dim=1)(logits)
img_pred = pred_probab.argmax(1)
print(f"Predicted class: {img_pred}")
```

$$\text{Softmax}(x_i) = \frac{\exp(x_i)}{\sum_j \exp(x_j)}$$

Exercise

- Build Net1 and run inference of the untrained Net1 on the first image of MNIST by extending “02_dataloaders.py”
- Hint: Adding the code snippets to 02_dataloaders.py

00_basics/02_dataloaders.py

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Snippet (import nn & functional)

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Snippet (Building Net1)

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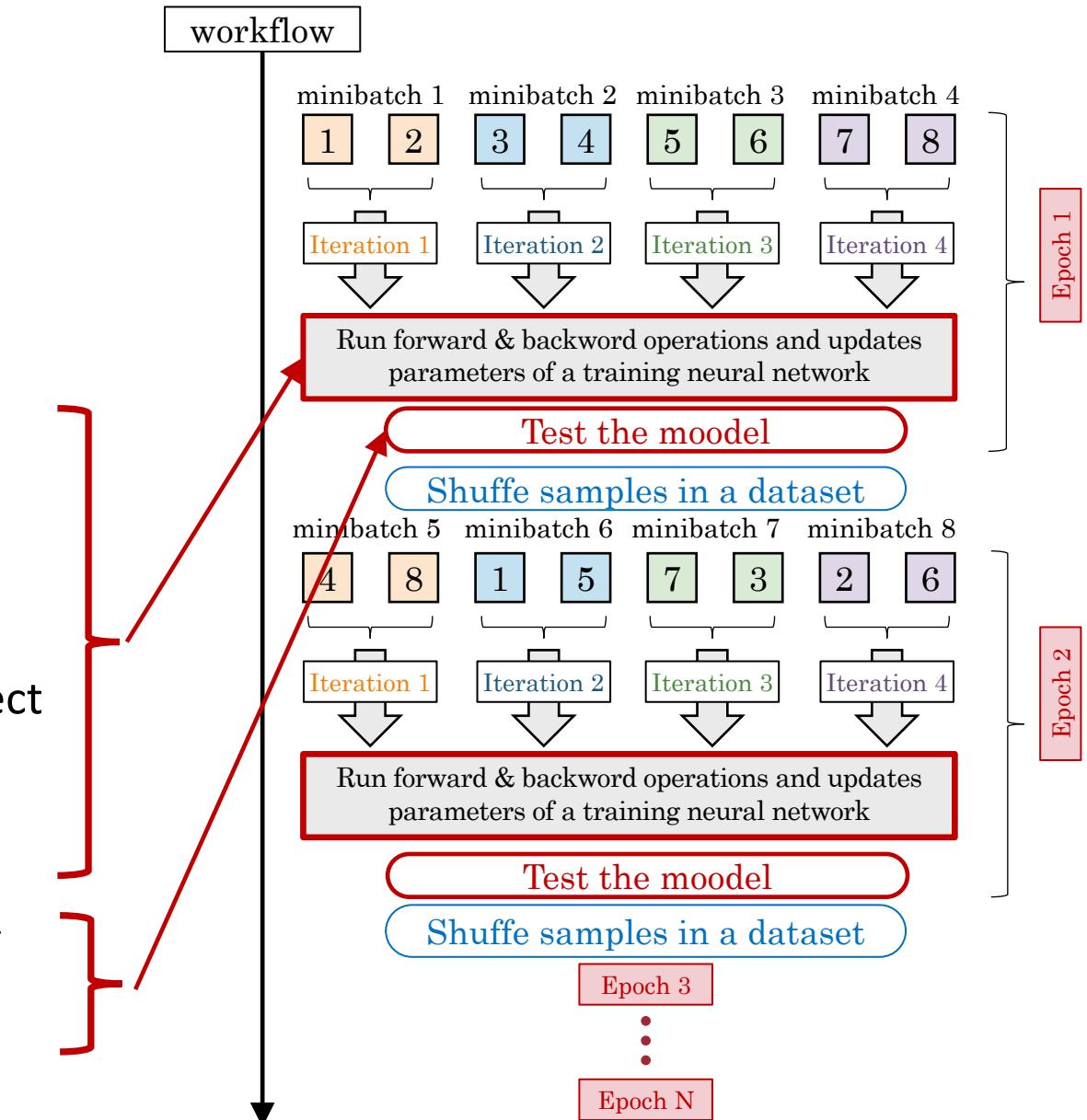
Snippet (Running inference)

Answer:

00_basics/03_build_NN.py

Training: Optimizing Model Parameters

- Now, we have a model and data
- It's time to train and test our model by optimizing its parameters on our data
- Training a model is an iterative process
 - In each iteration with “training data”, the model
 - **makes** a guess about the output (forward)
 - **calculates** the error in its guess (*loss*)
 - **collects** the derivatives of the error with respect to its parameters
 - **optimizes** these parameters using gradient descent
 - After each epoch, test the model accuracy with “test data”

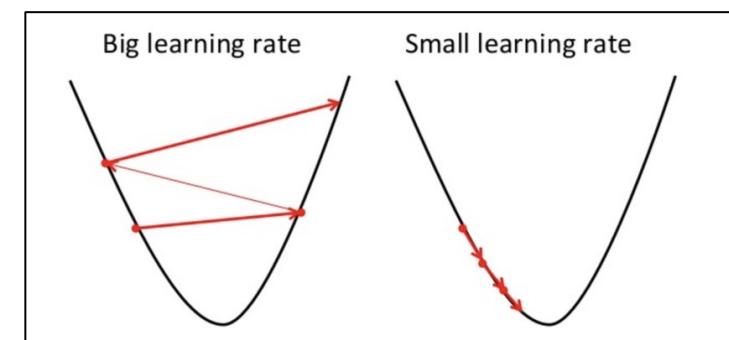


Hyperparameters

- Hyperparameters are adjustable parameters that let you control the model optimization process
- Different hyperparameter values can impact model training and convergence rates
 - c.f) Hyperparameter tuning
https://pytorch.org/tutorials/beginner/hyperparameter_tuning_tutorial.html
- We define the following hyperparameters for training:
 - **Number of Epochs:** the number times to iterate over the dataset
 - **Batch Size:** the number of data samples propagated through the network before the parameters are updated
 - Specify how many samples (e.g., image frames) to be trained at one time
 - **Learning Rate:** how much to update model parameters at each batch
 - Smaller values yield slow learning speed, while large values may result in unpredictable behavior during training

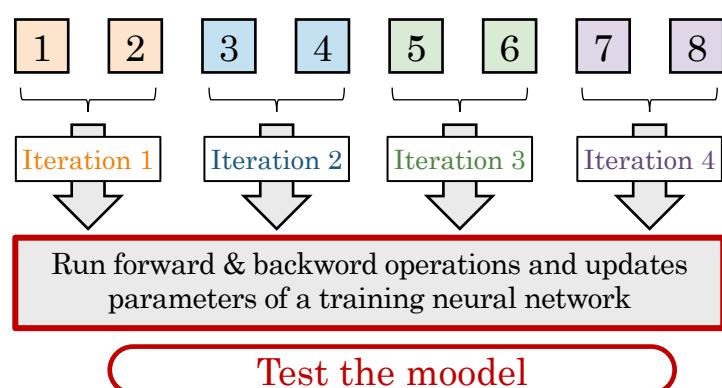
Snippet (Hyperparameters)

```
learning_rate = 1e-3  
batch_size = 64  
epochs = 1
```



Optimization Loop (i.e., *Epoch loop*) : Training + Testing

- Once we set our hyperparameters, we can then train and optimize our model with an optimization loop
- Each iteration of the optimization loop is called an **epoch**.
- Each epoch consists of two main parts
 - The Train Loop:** iterate over the training dataset and try to converge to optimal parameters.
 - The Test Loop:** iterate over the test dataset to check if model accuracy is improving without overfitting to training data



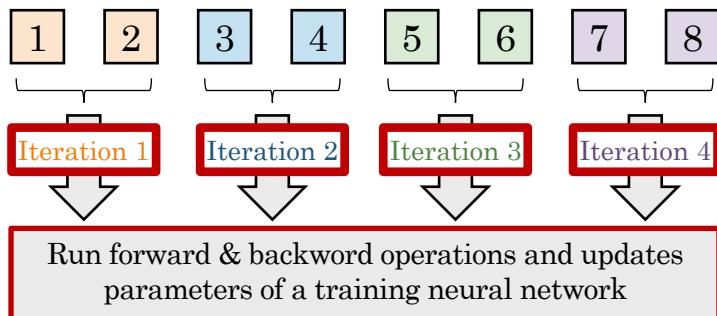
Snippet (Optimization loop)

```
for t in range(epochs):
    print(f"Epoch {t+1}\n-----")
    train_loop(train_dataloader, model, loss_fn, optimizer)
    test_loop(test_dataloader, model, loss_fn)
```

Train loop (i.e., Iterations)

- Inside the training loop, optimization happens in six steps
 - (1) Get a **minibatch** from dataloader in each loop
 - (2) Call **model(X)** to Compute forward propagation
 - (3) Call a **loss function** to compute loss
 - (4) Call **optimizer.zero_grad()** to reset the gradients of model parameters
 - Gradients by default add up; to prevent double-counting, we explicitly zero them at each iteration
 - (5) Backpropagate the prediction loss with a call to **loss.backward()**
 - PyTorch deposits the gradients of the loss w.r.t. each parameter
 - (6) Once we have our gradients, we call **optimizer.step()** to adjust the parameters by the gradients collected in the backward pass

Snippet (Training loop)



```
def train_loop(dataloader, model, loss_fn, optimizer):  
    for batch, (X, y) in enumerate(dataloader): # (1)  
        # Compute prediction and loss  
        pred = model(X) # (2)  
        loss = loss_fn(pred, y) # (3)  
        #Backpropagation  
        optimizer.zero_grad() # (4)  
        loss.backward() # (5)  
        optimizer.step() # (6)
```

Train loop (i.e., *Iterations*) with progress print

- Periodic prints will help you to know the progress of training

Snippet (Training loop with progress print)

```
def train_loop(dataloader, model, loss_fn, optimizer):
    size = len(dataloader.dataset)
    for batch, (X, y) in enumerate(dataloader):
        # Compute prediction and loss
        pred = model(X) # forward propagation
        loss = loss_fn(pred, y) # compute loss
        #Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        if batch % 100 == 0:
            loss, current = loss.item(), batch * len(X)
            print(f"loss: {loss:>7f}\n [{current:>5d}/{size:>5d}]")
```

Loss Function

- When presented with some training data, our untrained network (Net1) is likely not to give the correct answer
- Loss function measures the degree of dissimilarity of obtained result to the target value, and it is the loss function that we want to minimize during training
- To calculate the loss we make a prediction using the inputs of our given data sample and compare it against the true data label value
- Common loss functions include:
 - nn.MSELoss (Mean Square Error) for regression tasks
 - nn.NLLLoss (Negative Log Likelihood) for classification
 - nn.CrossEntropyLoss combines nn.LogSoftmax and nn.NLLLoss
- We pass our model's output logits to **nn.CrossEntropyLoss**, which will normalize the logits and compute the prediction error

Snippet (Loss function)

```
loss_fn = nn.CrossEntropyLoss()
```

Cross Entropy Loss

$$H(p, q) = - \sum_i p(x) \log q(x)$$

Optimizer

- Optimization is the process of adjusting model parameters to reduce model error in each training step (i.e., minimizing a result of the loss function)
- **Optimization algorithms** define how this process is performed
- All optimization logic is encapsulated in the optimizer object
- Here, we use the SGD (Stochastic Gradient Descent) optimizer
 - Additionally, there are many different optimizers available in PyTorch such as ADAM and RMSProp, that work better for different kinds of models and data.
- We initialize the optimizer by registering the model's parameters that need to be trained, and passing in the learning rate hyperparameter.

Snippet (Optimizer)

```
optimizer = torch.optim.SGD(model.parameters(), lr=learning_rate)
```

Test loop

- **The Test Loop:** iterate over the test dataset to check if model accuracy is improving without overfitting to training data
- When testing, disabling gradient calculation is useful for inference by calling “`torch.no_grad()`”, when you are sure that you will not run backpropagation
- It will reduce memory consumption for computations that would otherwise have `requires_grad=True`.

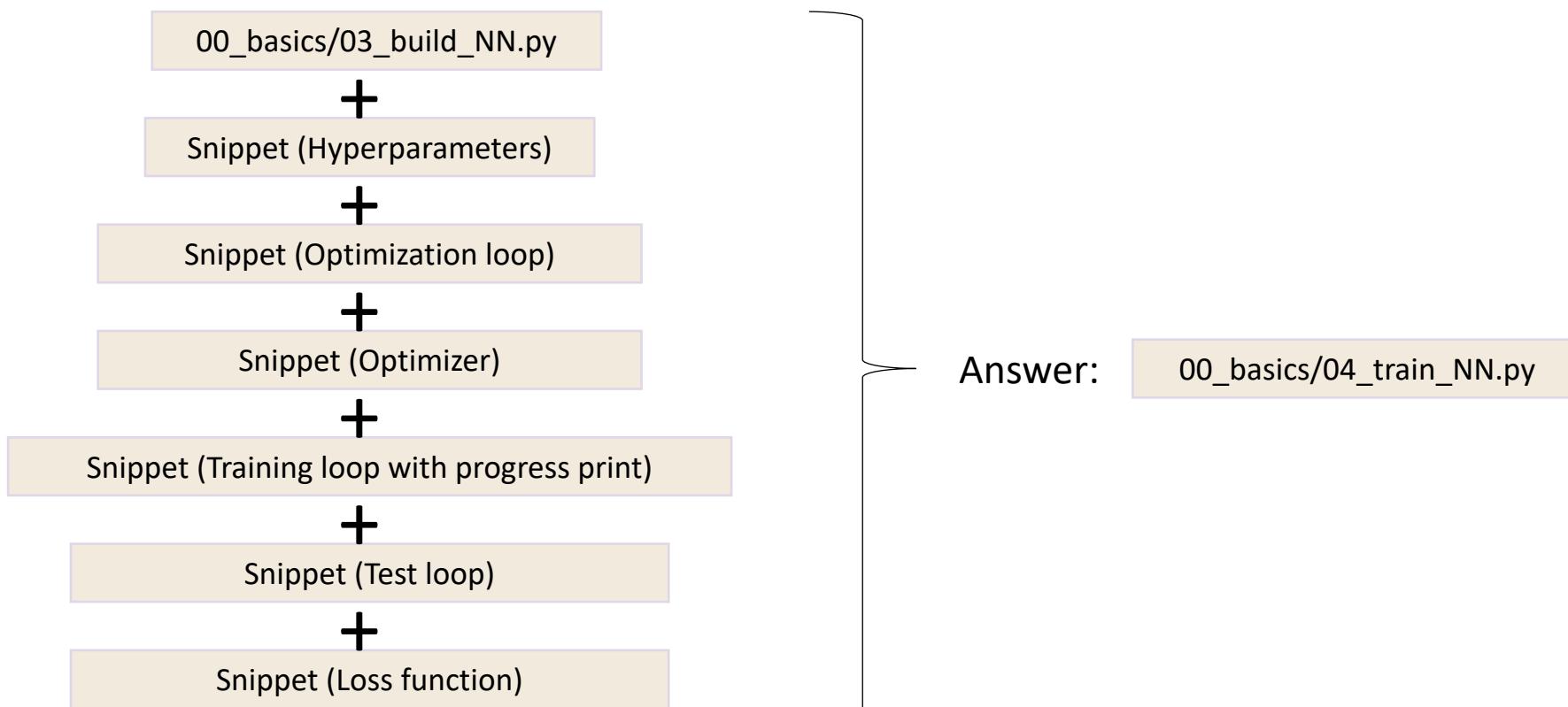
Snippet (Test loop)

```
def test_loop(dataloader, model, loss_fn):  
    size = len(dataloader.dataset)  
    num_batches = len(dataloader)  
    test_loss, correct = 0, 0  
    with torch.no_grad():  
        for X, y in dataloader:  
            pred = model(X)  
            test_loss += loss_fn(pred, y).item()  
            correct += (pred.argmax(1) == y).type(torch.float).sum().item()  
    test_loss /= num_batches  
    correct /= size  
    print(f"Test Error: \n Accuracy: {(100*correct):>0.1f}%, Avg loss: {test_loss:>8f} \n")
```

```
# item() returns a value of tensor when one  
element  
>>> x = torch.tensor([1.0])  
>>> x.item()  
1.0
```

Exercise

- Write a code to train Net1 with MNIST by extending 03_build_NN.py
- Hint: Add all the code snippets for training



Save and Load the model

- Once you finished training the model, you need to persist its model state with saving, loading and running model prediction
 - Save:** PyTorch models store the learned parameters in an internal state dictionary, called "state_dict". These can be persisted via the `torch.save` method:
 - Load:** To load model weights, you need to create an instance of the same model first, and then load the parameters using `load_state_dict()` method.

Snippet (save model)

```
# Saving model  
torch.save(model.state_dict(), "Net1_weights.pth")  
print("Saving Done!")
```

Snippet (load model)

```
# Load Model  
model.load_state_dict(torch.load('Net1_weights.pth'))  
model.eval()  
print("Loading model Done !")
```

Exercise: Save the model

- Save the trained model by extending “04_train_NN.py”
- Hint: Add the code snippet to 04_train_NN.py

00_basics/04_train_NN.py

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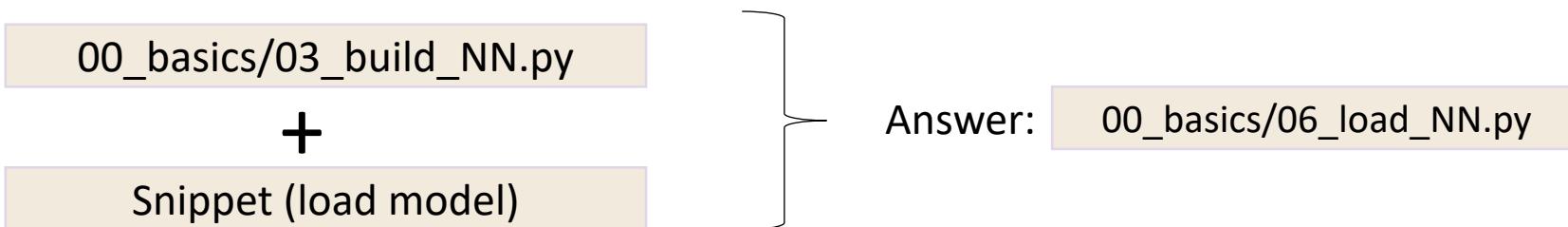
Snippet (save model)

Answer:

00_basics/05_save_NN.py

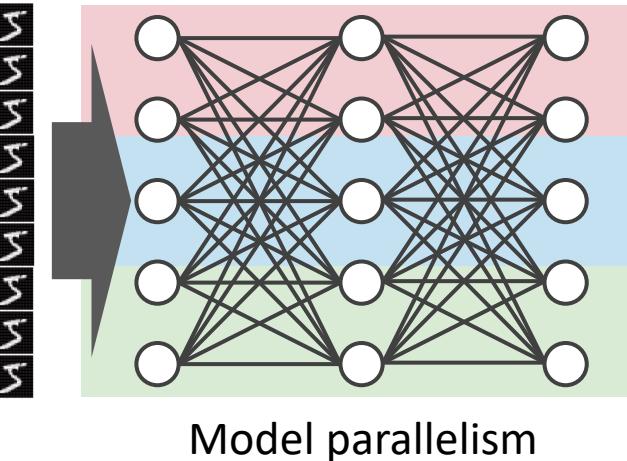
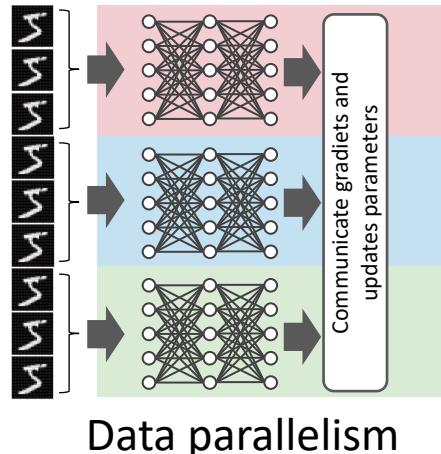
Exercise: Load the model

- Load the trained model by extending “03_build_NN.py”
 - Please recall 03_build_NN.py creates Net1 but does not train so it gave many wrong answers
 - By loading trained model before inference 03_build_NN.py will give more correct answers
- Hint: Add the code snippet to 03_train_NN.py



Distributed training

- Overview
 - Distributed training distribute training workloads across multiple PEs (e.g., cores/CPUs/GPUs) to accelerate process by training samples in parallel
- Data parallelism v.s. Model parallelism
 - Data parallelism
 - Data parallelism **devides training data** and distribute across multiple PEs
 - Each PEs trains a copy of the model on a different batch of training data and communicate its results (i.e., gradients) after computation to keep the model parameters synchronized across all PEs
 - Model parallelism
 - Model parallelism **devides the model** itself into parts
 - The parts are trained simultaneously across different PEs by using the same dataset across different PEs

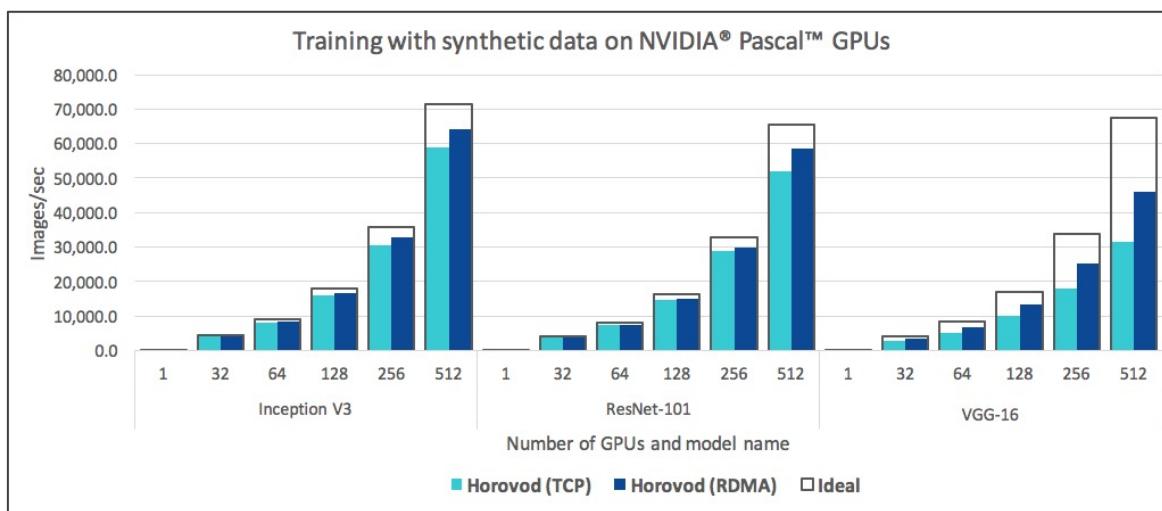


→ Data parallelism is more common so we focus on data parallelism



Horovod

- High coverage across different DL frameworks
 - Horovod is an MPI-based distributed deep learning training framework for TensorFlow, Keras, PyTorch, and Apache MXNet
- Easy-to-use
 - The goal of Horovod is to make distributed deep learning fast and easy to use
 - Once a training script has been written for scale with Horovod, it can run on a single-CPU/GPU, multiple-CPUs/GPUs, or even multiple hosts without any further code changes
- Performance
 - Horovod achieves 90% scaling efficiency for both Inception V3 and ResNet-101, and 68% scaling efficiency for VGG-16



128 servers with 4 Pascal GPUs each connected by RoCE-capable 25 Gbit/s network:

Modification to a single-PE script with 5 Steps

- 1. import Horovod module

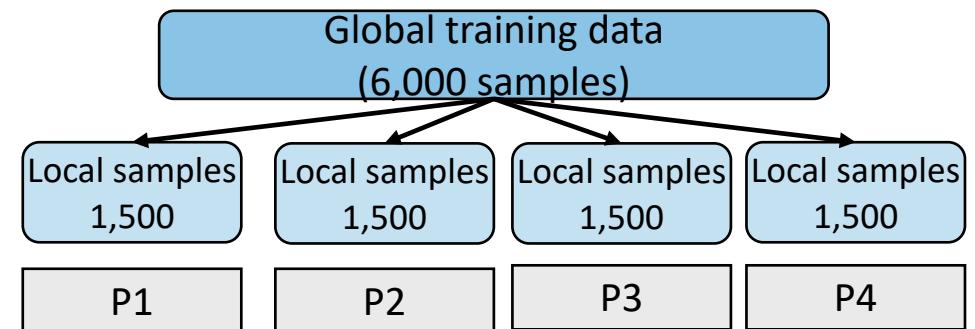
Snippet (import horovod)

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

- 2. Add Initialization
 - Call **hvd.init()**

- 3. Modify the Dataloader part

- Partition dataset among workers by adding **DistributedSampler**
- **Dataset → DistributedSampler → DataLoader**
- shuffle is handled by DistributedSampler so remove “shuffle=True” in DataLoader



```
train_dataloader = DataLoader(dataset=training_data, batch_size=batch_size, shuffle=True)  
test_dataloader = DataLoader(dataset=test_data, batch_size=batch_size, shuffle=True)
```



Snippet (Distributed Sampler)

```
train_sampler = torch.utils.data.distributed.DistributedSampler(training_data, num_replicas=hvd.size(), rank=hvd.rank())  
test_sampler = torch.utils.data.distributed.DistributedSampler(test_data, num_replicas=hvd.size(), rank=hvd.rank())  
  
train_dataloader = DataLoader(dataset=training_data, batch_size=batch_size, sampler=train_sampler)  
test_dataloader = DataLoader(dataset=test_data, batch_size=batch_size, sampler=test_sampler)
```

Modification to a single-PE script with 5 Steps

- 4. Modify Optimizer part
 - Wrap the optimizer in **hvd.DistributedOptimizer**
 - **Optimizer → DistributedOptimizer**
- 5. Add Broadcast for synchronizing the initial variable states from rank 0 to all other ranks
 - Call **hvd.broadcast_parameter**

Snippet (DistributedOptitmizer and Broadcast)

```
optimizer = hvd.DistributedOptimizer(optimizer, named_parameters=model.named_parameters())  
hvd.broadcast_parameters(model.state_dict(), root_rank=0)
```

Other modifications (1/2)

- Learning rate and batch size [1]

- In general, if you increase batch size too high, it decrease its accuracy
- Roughly speaking, it is known that we can keep up accuracy by increasing both learning rate and batch size as long as the number of training samples is high enough
- We increase learning rate depending on the number of processes

```
optimizer = torch.optim.SGD(model.parameters(), lr=learning_rate)
```



```
optimizer = torch.optim.SGD(model.parameters(), lr=learning_rate * hvd.size())
```

Global batch size = 64

local batch size
= 64

P1

Global batch size = 256

local batch size
= 64

P1

P2

P3

P4

[1] Samuel L. Smith, Pieter-Jan Kindermans, Chris Ying, Quoc V. Le. *Don't Decay the Learning Rate, Increase the Batch Size*. 2017. ICLR 2018
<https://arxiv.org/abs/1711.00489>

Other modifications (2/2)

- Get # of local training testing samples

```
def train_loop(dataloader, model, loss_fn):  
    size = len(dataloader.dataset)
```



```
def train_loop(dataloader, model, loss_fn):  
    size = len(dataloader.sampler)
```

```
def test_loop(dataloader, model, loss_fn):  
    size = len(dataloader.dataset)
```



```
def test_loop(dataloader, model, loss_fn):  
    size = len(dataloader.sampler)
```

- Printing by only rank 0 and flush
 - mpirun buffers the stdout and dump it later
 - “flush=True” enables immediate print out on stdout

```
print("...")
```



```
if hvd.rank() == 0: print("...", flush=True)
```

Running distributed training and CPU binding

- Reserving an interactive node

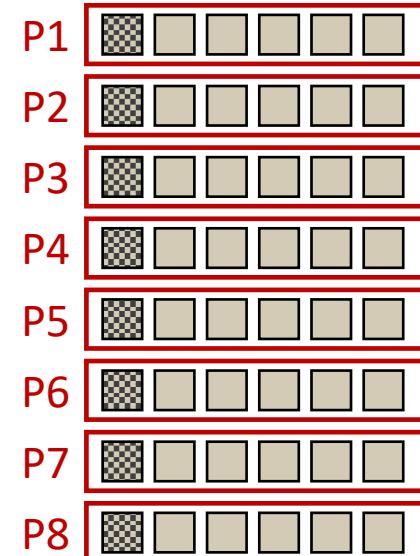
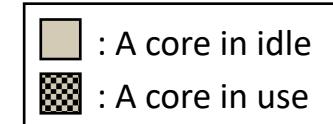
```
$ pbsub --interact -L "node=1" -L "rscgrp=int" -L "elapse=3:00:00" --sparam "wait-time=600" --mpi "proc=8"  
-x "PJM_LLI0_GFSCACHE=/vol0004"
```

- Since Horovode is based on MPI, we use mpirun for launching processes

```
$ mpirun -n 8 ./07_dist_train_NN.py
```

- Process topology on A64FFX

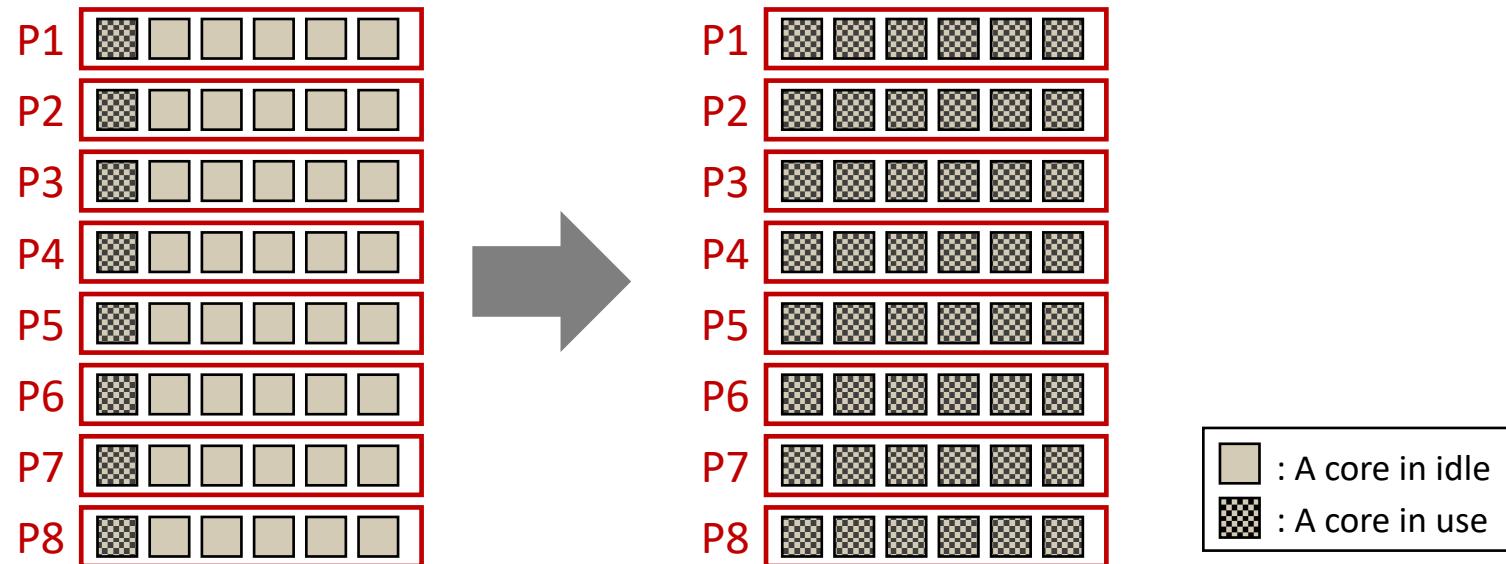
- Fugaku/A64FX has 48 computation cores
- --mpi “procs=8” lets to use 8 processes at maximum
 - Also, 8 processes are binned to each isolated set of 6 cores



Tuning for Fugaku: MPI+OpenMP

- To make use of idle cores, we need to enable multi-threading
 - However, use of all the cores can rather degrate the performance due to contentionn with other threads (e.g., communication)

```
torch.set_num_threads(3)
```
- Another way is to use flat MPI with 48 processes, but in my experience MPI+OpenMP runs faster on Fugaku in PyTorch+Horovod



Exercise: Distributed training with data parallelism

- Write a code for distributed training with data parallelism by extending “05_save_NN_cleaned.py”
 - We have been accumulating unnecessary code used in earlier exercises, I removed these unnecessary code in “05_tran_NN_cleaned.py”
- Hint: Add and Modify the code based on the snippets

00_basics/05_save_NN_cleaned.py

+

Snippet (import horovod)

+

Modify based on Snippet (Distributed Sampler)

+

Snippet (DistributedOptimizer and Broadcast)

+

1. Other modifications

2. Tuning for Fugaku: MPI+OpenMP

Answer:

00_basics/07_dist_train_NN.py

Hint: Template code

```
import ...
import horovod.torch as hvd

# Initialize Horovod
hvd.init()

# Define dataset...
training_dataset = ...

# Partition dataset among workers using DistributedSampler
train_sampler = torch.utils.data.distributed.DistributedSampler(training_data, num_replicas=hvd.size(), rank=hvd.rank())
test_sampler = ...
train_loader = torch.utils.data.DataLoader(training_data, batch_size=..., sampler=train_sampler)
test_loader = ...

# Build model...
model = ...

# Add Horovod Distributed Optimizer
optimizer = torch.optim.SGD(model.parameters(), lr=learning_rate * hvd.size())
optimizer = hvd.DistributedOptimizer(optimizer, named_parameters=model.named_parameters())

# Broadcast parameters from rank 0 to all other processes.
hvd.broadcast_parameters(model.state_dict(), root_rank=0)

# Start training
for t in range(epochs):
    ...
```

Exercise: Performance measurement

- Measure training times with 1, 2, 4, 8 processes

References

- PyTorch
 - <https://pytorch.org/tutorials/index.html>
- HOROVOD
 - <https://horovod.readthedocs.io/en/stable/pytorch.html>
- Machine Learning Testing: A Step to Perfection
 - <https://serokell.io/blog/machine-learning-testing>

