
Machine Learning PyTorch Tutorial

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Outline

- Prerequisites
- What is PyTorch?
- PyTorch v.s. TensorFlow
- Overview of the DNN Training Procedure
- Tensor
- How to Calculate Gradient?
- Dataset & Dataloader
- torch.nn
- torch.optim
- Neural Network Training/Evaluation
- Saving/Loading a Neural Network
- More About PyTorch

Prerequisites

- We assume you are already familiar with...
 - **Python3**
 - if-else, loop, function, file IO, class, ...
 - refs: [link1](#), [link2](#), [link3](#)
 - **NumPy**
 - array & array operations
 - ref: [link](#)





What is PyTorch?

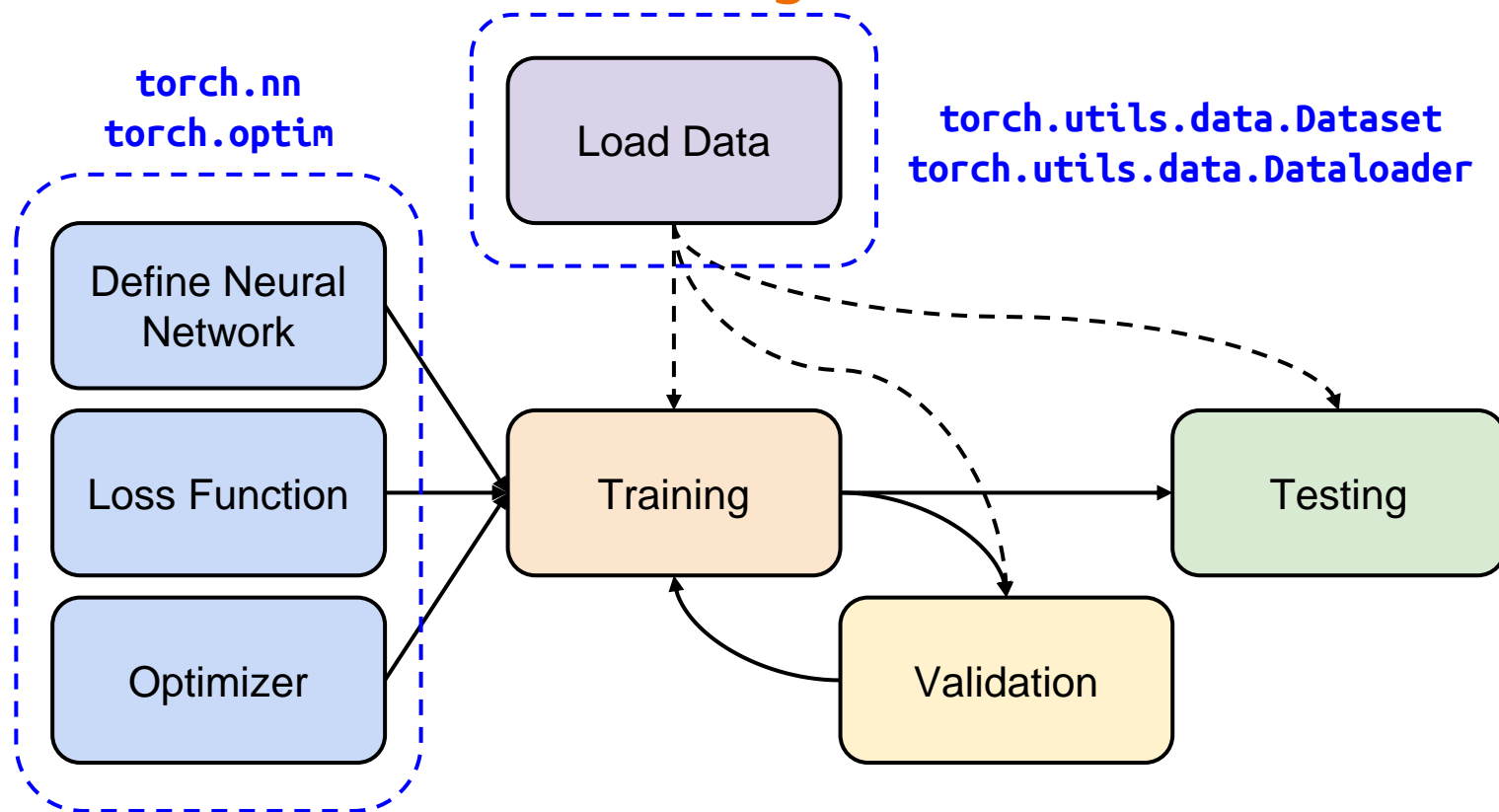
- An open source **machine learning framework**.
- A Python package that provides two high-level features:
 - **Tensor** computation (like NumPy) with strong **GPU acceleration**
 - Deep neural networks built on a **tape-based autograd** system



PyTorch v.s. TensorFlow

	PyTorch 	TensorFlow 
Developer	Facebook AI	Google Brain
Interface	Python & C++	Python, C++, JavaScript, Swift
Debug	Easier	Difficult (easier in 2.0)
Application	Research	Production

Overview of the DNN Training Procedure

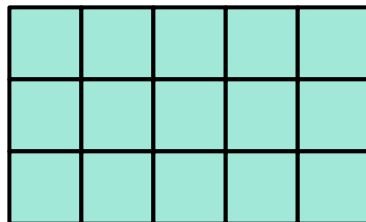


Tensor

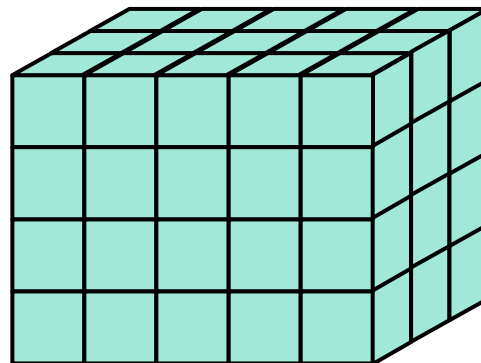
- High-dimensional matrix (array)



1-D tensor



2-D tensor



3-D tensor

Tensor -- Data Type

Data type	dtype	tensor
32-bit floating point	<code>torch.float</code>	<code>torch.FloatTensor</code>
64-bit integer (signed)	<code>torch.long</code>	<code>torch.LongTensor</code>

ref: <https://pytorch.org/docs/stable/tensors.html>

Tensor -- Shape of Tensors

- Shape

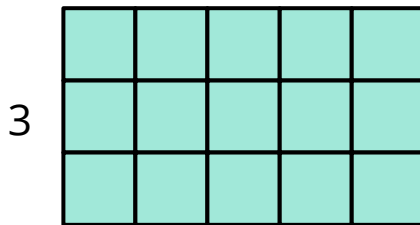


5

(5,)



dim 0



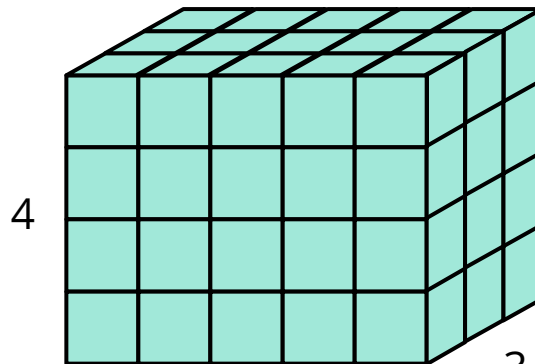
3

5

(3, 5)



dim 0 dim 1



4

5

3

(4, 5, 3)



dim 0 dim 1 dim 2

Note: **dim** in PyTorch == **axis** in NumPy

Tensor -- Constructor

- From list / NumPy array

```
x = torch.tensor([[1, -1], [-1, 1]])
```

```
x = torch.from_numpy(np.array([[1, -1], [-1, 1]]))
```

```
tensor([[1., -1.],  
        [-1., 1.]])
```

- Zero tensor

```
x = torch.zeros([2, 2])
```

```
tensor([[0., 0.],  
        [0., 0.]])
```

- Unit tensor

```
x = torch.ones([1, 2, 5])
```

```
tensor([[[[1., 1., 1., 1., 1.],  
          [1., 1., 1., 1., 1.]]]])
```



shape

Tensor -- Operators

- **Squeeze**: remove the specified dimension with length = 1

```
>>> x = torch.zeros([1, 2, 3])
```

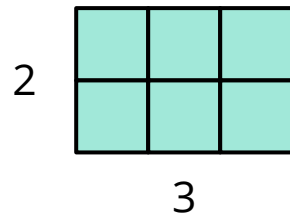
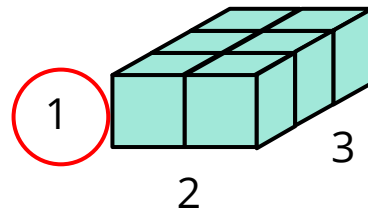
```
>>> x.shape
```

```
torch.Size([1, 2, 3])
```

```
>>> x = x.squeeze(0)  
                (dim = 0)
```

```
>>> x.shape
```

```
torch.Size([2, 3])
```



Tensor -- Operators

- **Unsqueeze**: expand a new dimension

```
>>> x = torch.zeros([2, 3])
```

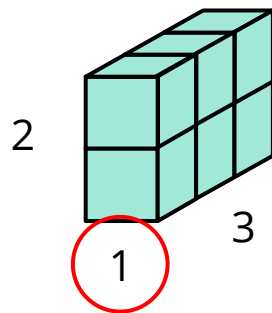
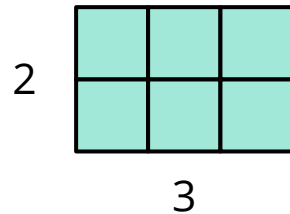
```
>>> x.shape
```

```
torch.Size([2, 3])
```

```
>>> x = x.unsqueeze(1) (dim = 1)
```

```
>>> x.shape
```

```
torch.Size([2, 1, 3])
```



Tensor -- Operators

- **Transpose:** transpose two specified dimensions

```
>>> x = torch.zeros([2, 3])
```

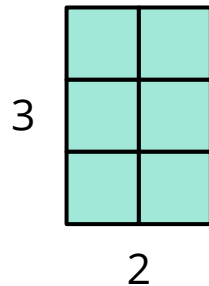
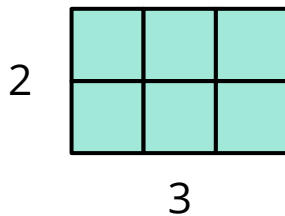
```
>>> x.shape
```

```
torch.Size([2, 3])
```

```
>>> x = x.transpose(0, 1)
```

```
>>> x.shape
```

```
torch.Size([3, 2])
```



Tensor -- Operators

- **Cat:** concatenate multiple tensors

```
>>> x = torch.zeros([2, 1, 3])
```

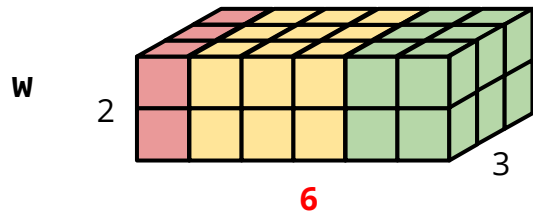
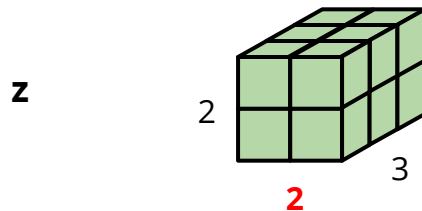
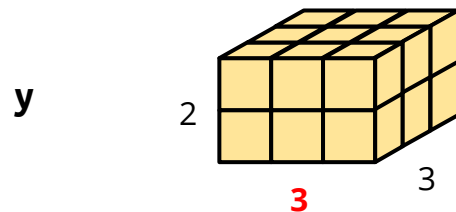
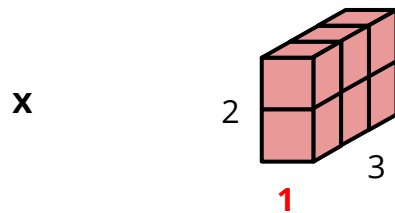
```
>>> y = torch.zeros([2, 3, 3])
```

```
>>> z = torch.zeros([2, 2, 3])
```

```
>>> w = torch.cat([x, y, z], dim=1)
```

```
>>> w.shape
```

```
torch.Size([2, 6, 3])
```



Tensor -- Operators

- Addition

$$z = x + y$$

- Subtraction

$$z = x - y$$

- Power

$$y = x.\text{pow}(2)$$

Tensor -- Operators

- Summation

```
y = x.sum()
```

- Mean

```
y = x.mean()
```

more operators: <https://pytorch.org/docs/stable/tensors.html>

Tensor -- PyTorch v.s. NumPy

- Attributes

PyTorch	NumPy
<code>x.shape</code>	<code>x.shape</code>
<code>x.dtype</code>	<code>x.dtype</code>

Tensor -- PyTorch v.s. NumPy

- Shape manipulation

PyTorch	NumPy
<code>x.reshape / x.view</code>	<code>x.reshape</code>
<code>x.squeeze()</code>	<code>x.squeeze()</code>
<code>x.unsqueeze(1)</code>	<code>np.expand_dims(x, 1)</code>

Tensor -- Device

- Default: tensors & modules will be computed with **CPU**

- CPU

```
x = x.to('cpu')
```

- GPU

```
x = x.to('cuda')
```

Tensor -- Device (GPU)



- Check if your computer has NVIDIA GPU

```
torch.cuda.is_available()
```

- Multiple GPUs: specify 'cuda:0', 'cuda:1', 'cuda:2', ...
- Why GPU?
 - Parallel computing
 - <https://towardsdatascience.com/what-is-a-gpu-and-do-you-need-one-in-deep-learning-718b9597aa0d>

How to Calculate Gradient?

1 `>>> x = torch.tensor([[1., 0.], [-1., 1.]], requires_grad=True)`

2 `>>> z = x.pow(2).sum()`

3 `>>> z.backward()`

4 `>>> x.grad`
`tensor([[2., 0.],`
 `[-2., 2.]])`

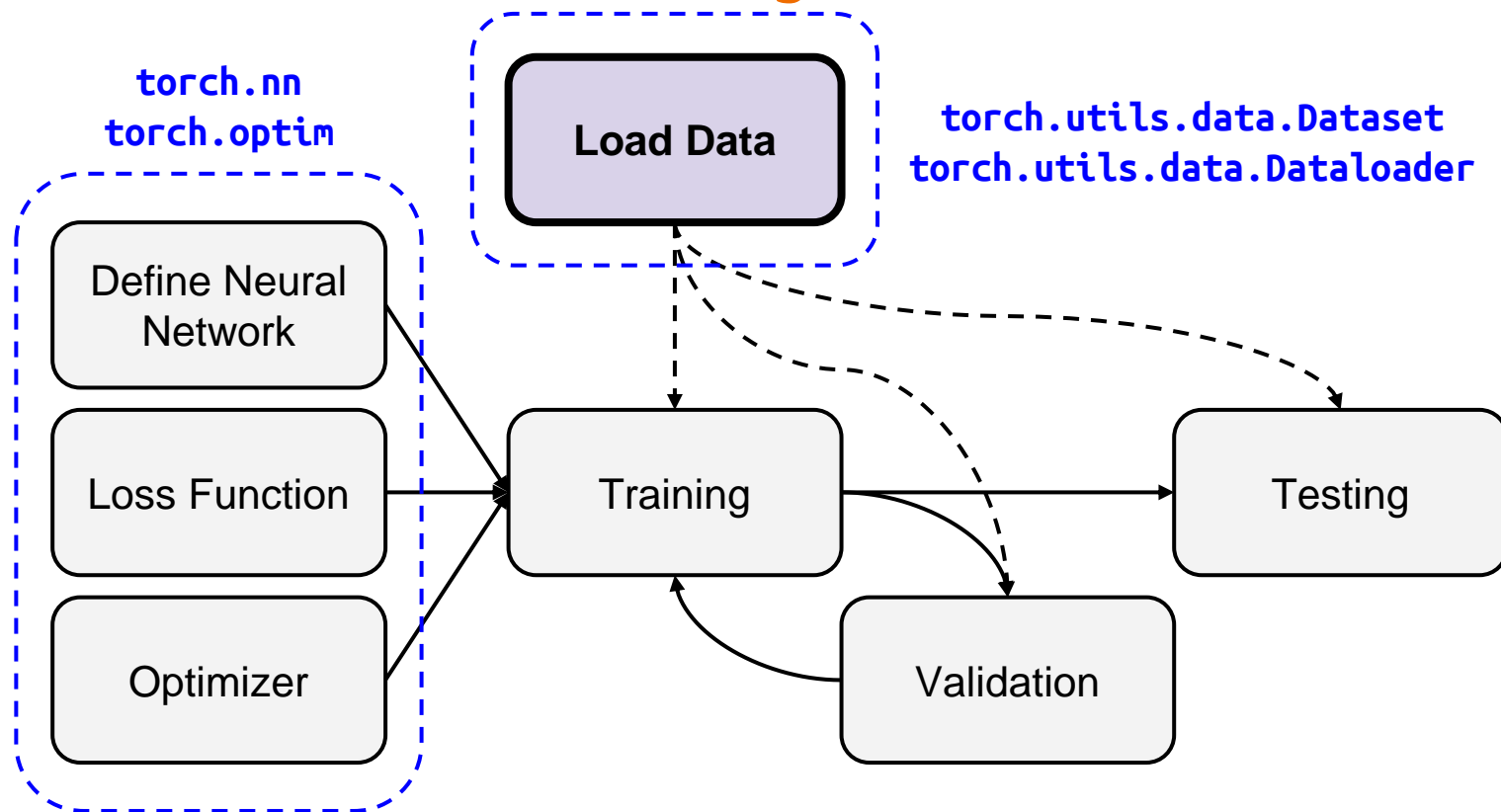
1
$$x = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}$$

2
$$z = \sum_i \sum_j x_{i,j}^2$$

3
$$\frac{\partial z}{\partial x_{i,j}} = 2x_{i,j}$$

4
$$\frac{\partial z}{\partial x} = \begin{bmatrix} 2 & 0 \\ -2 & 2 \end{bmatrix}$$

Overview of the DNN Training Procedure



Dataset & Dataloader

```
from torch.utils.data import Dataset, DataLoader
```

```
class MyDataset(Dataset):
```

```
    def __init__(self, file):  
        self.data = ...
```



Read data & preprocess

```
    def __getitem__(self, index):  
        return self.data[index]
```



Returns one sample at a time

```
    def __len__(self):  
        return len(self.data)
```



Returns the size of the dataset

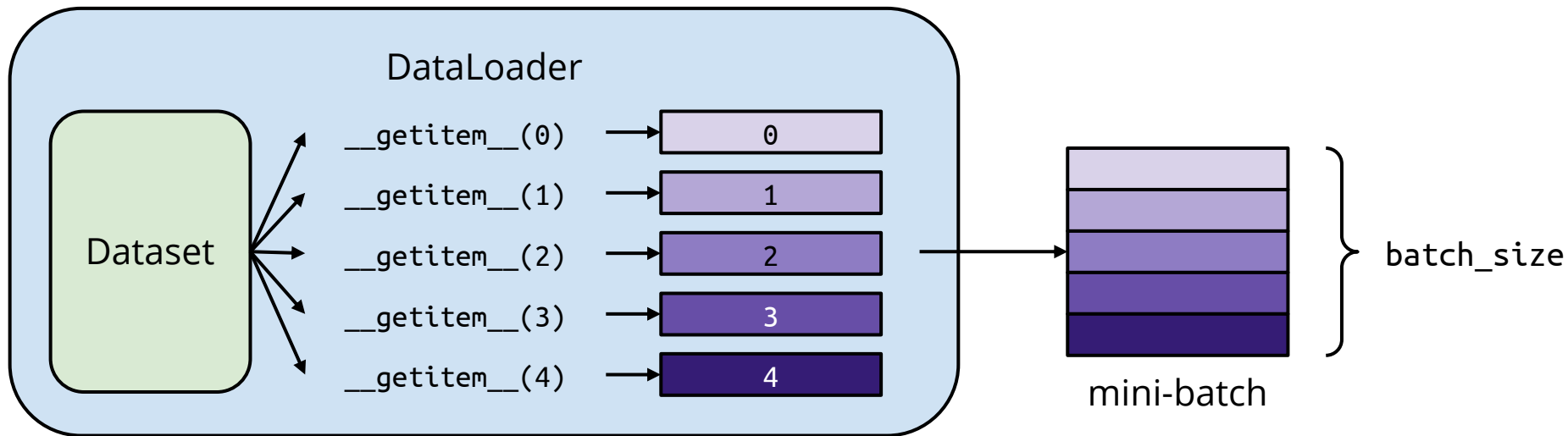
Dataset & Dataloader

```
dataset = MyDataset(file)
```

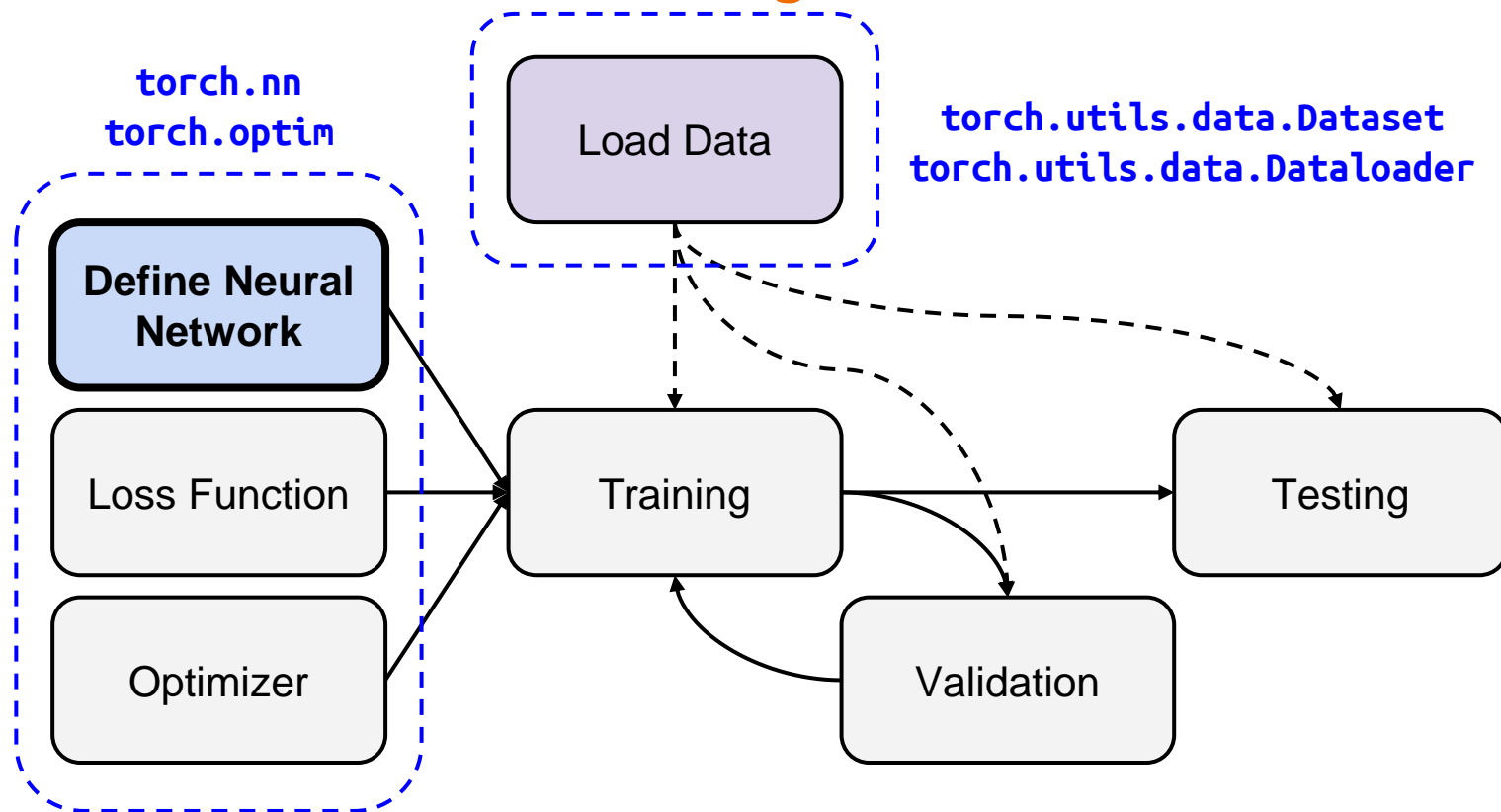
Training: True
Testing: False



```
dataloader = DataLoader(dataset, batch_size, shuffle=True)
```



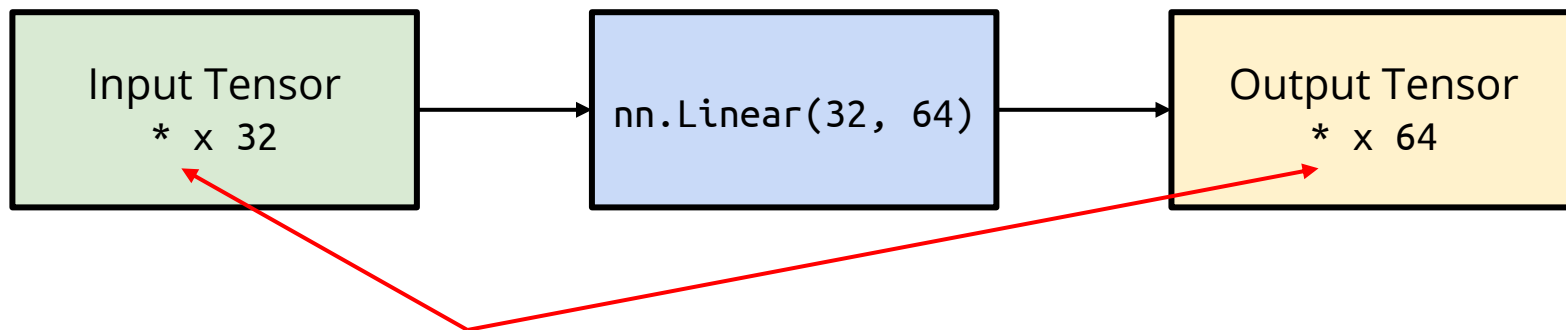
Overview of the DNN Training Procedure



torch.nn -- Neural Network Layers

- Linear Layer (**Fully-connected** Layer)

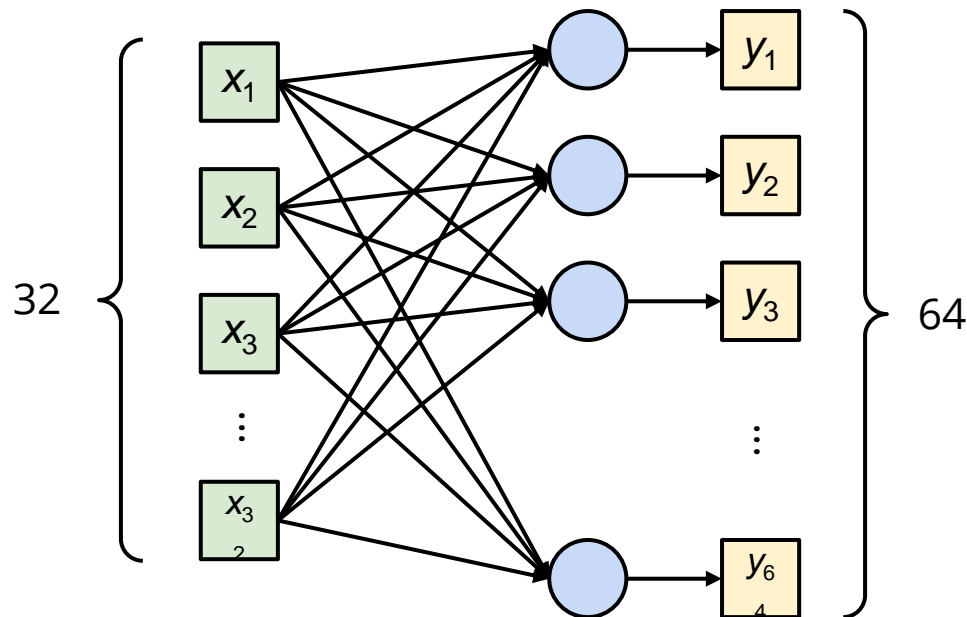
```
nn.Linear(in_features, out_features)
```



can be any shape but the last dimension must be 32
e.g. (10, 32), (10, 5, 32), (1, 1, 3, 32), ...

torch.nn -- Neural Network Layers

- Linear Layer (**Fully-connected** Layer)



$$\begin{matrix} \text{64x32} \\ W \end{matrix} \times \begin{matrix} x \end{matrix} + \begin{matrix} b \end{matrix} = \begin{matrix} y \end{matrix}$$

torch.nn -- Neural Network Layers

- Linear Layer (**Fully-connected** Layer)

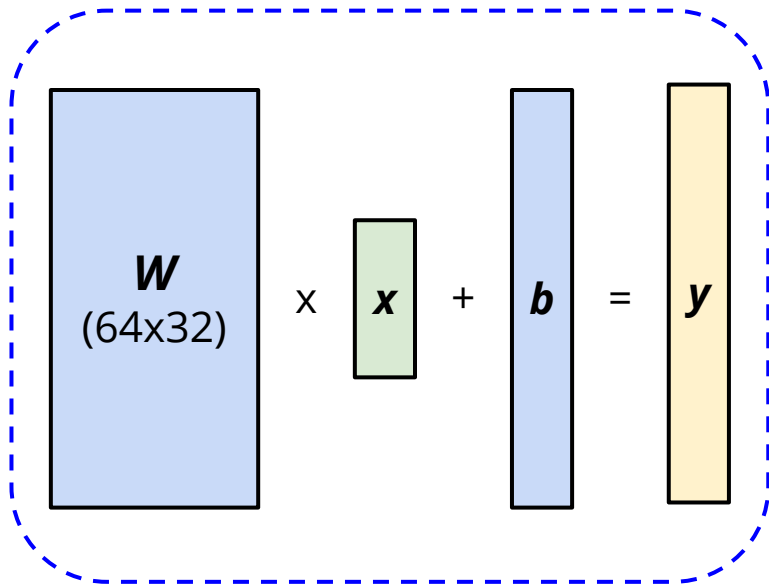
```
>>> layer = torch.nn.Linear(32, 64)
```

```
>>> layer.weight.shape
```

```
torch.Size([64, 32])
```

```
>>> layer.bias.shape
```

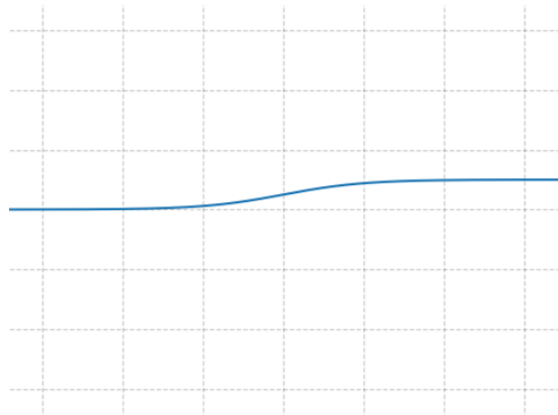
```
torch.Size([64])
```



torch.nn -- Activation Functions

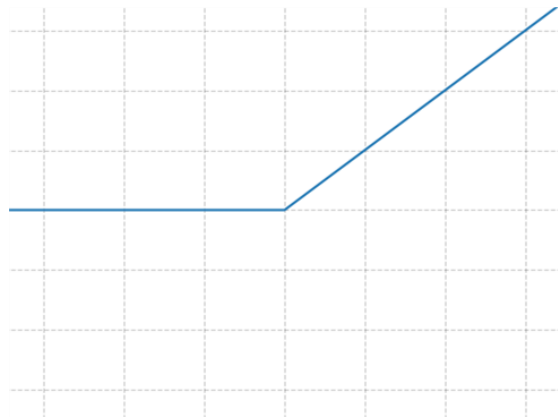
- Sigmoid Activation

`nn.Sigmoid()`

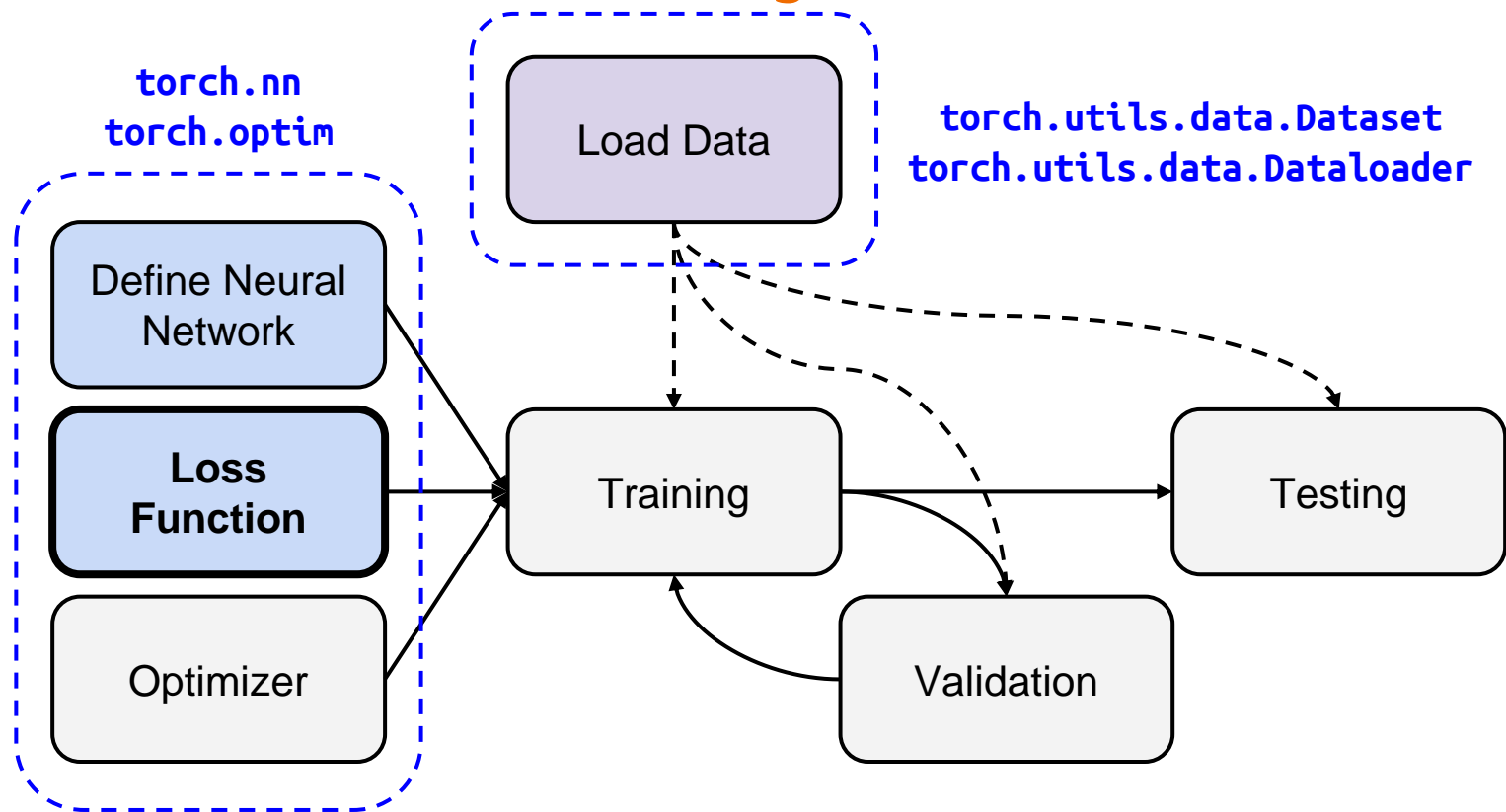


- ReLU Activation

`nn.ReLU()`



Overview of the DNN Training Procedure



torch.nn -- Loss Functions

- Mean Squared Error (for linear regression)

`nn.MSELoss()`

- Cross Entropy (for classification)

`nn.CrossEntropyLoss()`

torch.nn -- Build your own neural network

```
import torch.nn as nn
```

```
class MyModel(nn.Module):  
    def __init__(self):  
        super(MyModel, self).__init__()  
        self.net = nn.Sequential(  
            nn.Linear(10, 32),  
            nn.Sigmoid(),  
            nn.Linear(32, 1)  
        )
```

```
    def forward(self, x):  
        return self.net(x)
```

Initialize your model & define layers

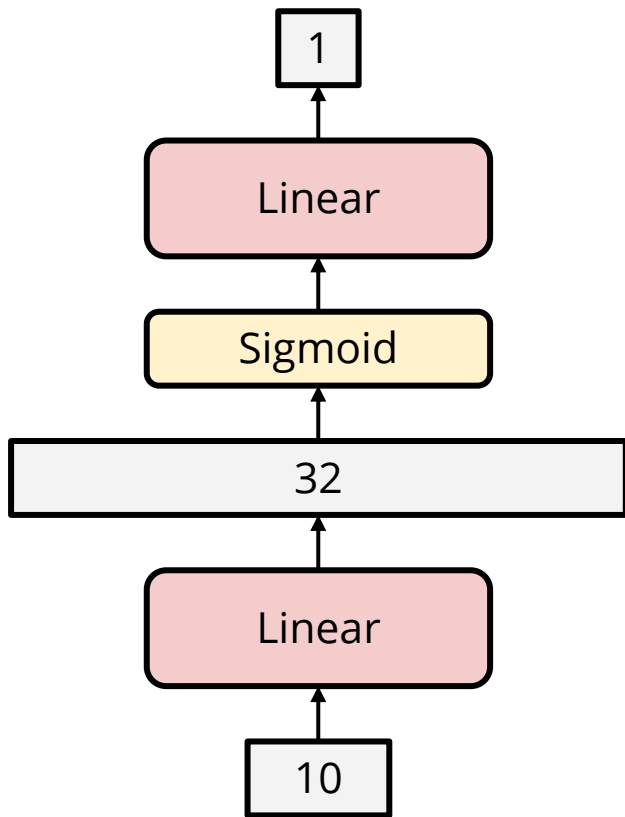
Compute output of your NN

torch.nn -- Build your own neural network

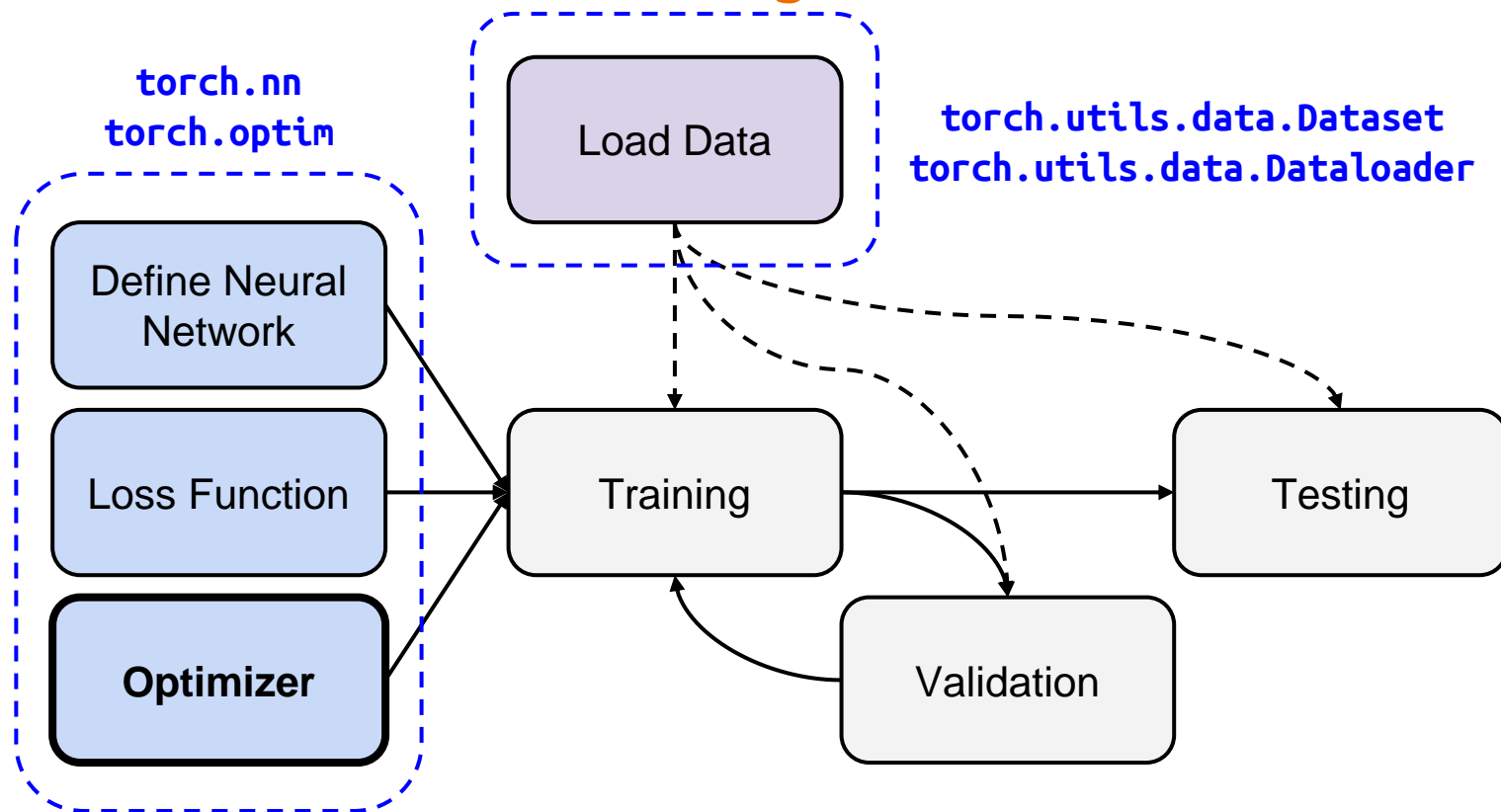
```
import torch.nn as nn

class MyModel(nn.Module):
    def __init__(self):
        super(MyModel, self).__init__()
        self.net = nn.Sequential(
            nn.Linear(10, 32),
            nn.Sigmoid(),
            nn.Linear(32, 1)
        )

    def forward(self, x):
        return self.net(x)
```



Overview of the DNN Training Procedure



torch.optim

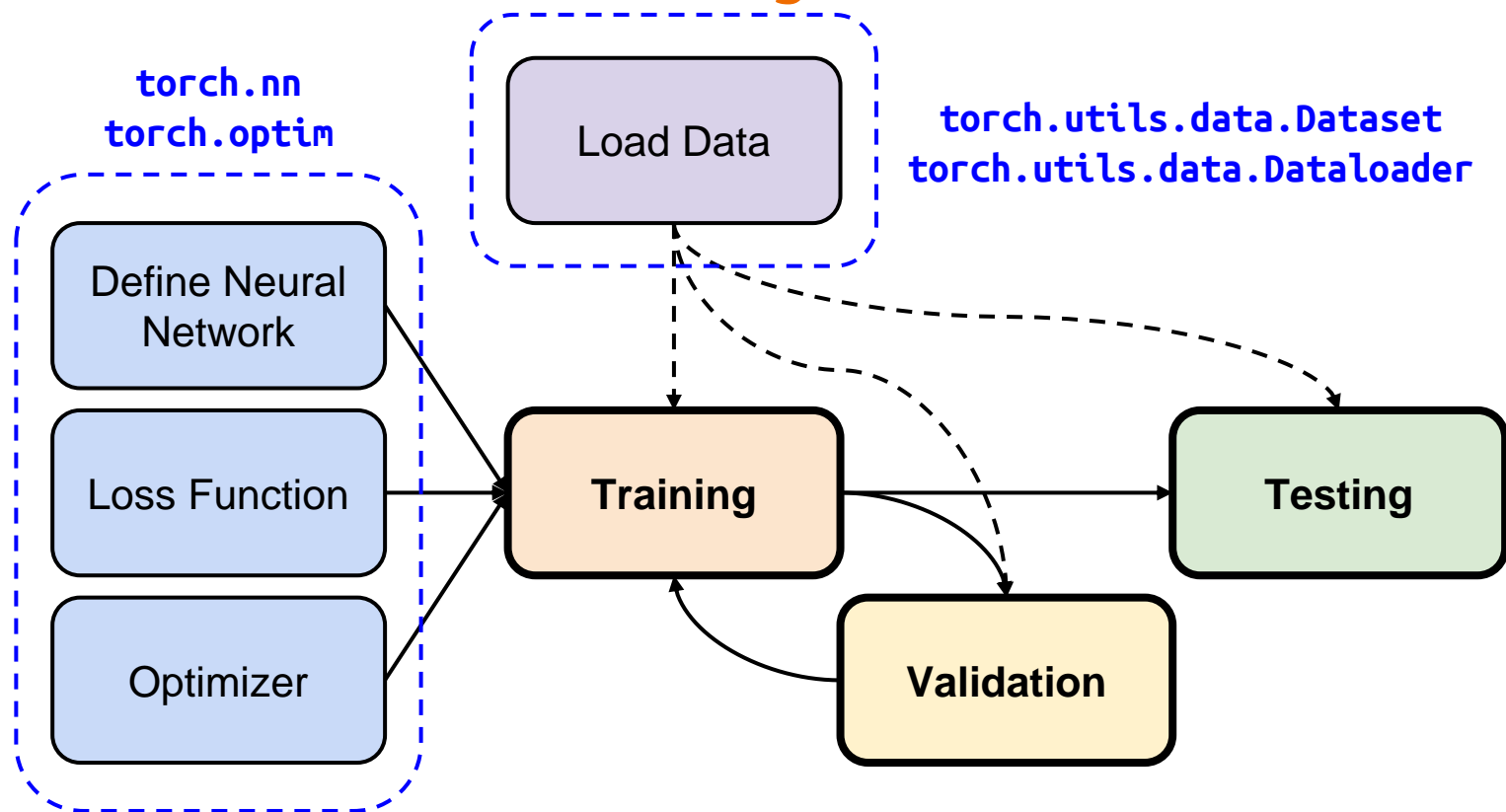
- **Optimization algorithms** for neural networks (gradient descent)
- Stochastic Gradient Descent (SGD)

```
torch.optim.SGD(params, lr, momentum = 0)
```

`model.parameters()`



Overview of the DNN Training Procedure



Neural Network Training

```
dataset = MyDataset(file)
```

read data via MyDataset

```
tr_set = DataLoader(dataset, 16, shuffle=True)
```

put dataset into DataLoader

```
model = MyModel().to(device)
```

construct model and move to device (cpu/cuda)

```
criterion = nn.MSELoss()
```

set loss function

```
optimizer = torch.optim.SGD(model.parameters(), 0.1)
```

set optimizer

Neural Network Training

```
for epoch in range(n_epochs):
```

```
    model.train()
```

```
    for x, y in tr_set:
```

```
        optimizer.zero_grad()
```

```
        x, y = x.to(device), y.to(device)
```

```
        pred = model(x)
```

```
        loss = criterion(pred, y)
```

```
        loss.backward()
```

```
        optimizer.step()
```

```
iterate n_epochs
```

```
set model to train mode
```

```
iterate through the dataloader
```

```
set gradient to zero
```

```
move data to device (cpu/cuda)
```

```
forward pass (compute output)
```

```
compute loss
```

```
compute gradient (backpropagation)
```

```
update model with optimizer
```

Neural Network Evaluation (Validation Set)

```
model.eval()
```

set model to evaluation mode

```
total_loss = 0
```

```
for x, y in dv_set:
```

iterate through the dataloader

```
    x, y = x.to(device), y.to(device)
```

move data to device (cpu/cuda)

```
    with torch.no_grad():
```

disable gradient calculation

```
        pred = model(x)
```

forward pass (compute output)

```
        loss = criterion(pred, y)
```

compute loss

```
        total_loss += loss.cpu().item() * len(x)
```

accumulate loss

```
avg_loss = total_loss / len(dv_set.dataset)
```

compute averaged loss

Neural Network Evaluation (Testing Set)

```
model.eval()
```

set model to evaluation mode

```
preds = []
```

```
for x in tt_set:
```

iterate through the dataloader

```
    x = x.to(device)
```

move data to device (cpu/cuda)

```
    with torch.no_grad():
```

disable gradient calculation

```
        pred = model(x)
```

forward pass (compute output)

```
        preds.append(pred.cpu())
```

collect prediction

Save/Load a Neural Network

- Save

```
torch.save(model.state_dict(), path)
```

- Load

```
ckpt = torch.load(path)  
model.load_state_dict(ckpt)
```

More About PyTorch

- torchaudio
 - speech/audio processing
- torchtext
 - natural language processing
- torchvision
 - computer vision
- skorch
 - scikit-learn + pyTorch

More About PyTorch

- Useful github repositories using PyTorch
 - [Huggingface Transformers](#) (transformer models: BERT, GPT, ...)
 - [Fairseq](#) (sequence modeling for NLP & speech)
 - [ESPnet](#) (speech recognition, translation, synthesis, ...)
 - Many implementation of papers
 - ...

Reference

- <https://pytorch.org/>
- <https://github.com/pytorch/pytorch>
- <https://github.com/wkentaro/pytorch-for-numpy-users>
- <https://blog.udacity.com/2020/05/pytorch-vs-tensorflow-what-you-need-to-know.html>
- <https://www.tensorflow.org/>
- <https://numpy.org/>

Any questions?