Lab1. PyTorch Basics

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Outline

- Background: What is PyTorch?
- Tensors
- Training & Testing a Classification Model in Pytorch
  - Dataset & Dataloader
  - torch.nn: Models & Loss Functions
  - torch.optim: Optimization Process

Goals of this Lab

- Learn the basic concepts of PyTorch
- Tensors
    - Get proficient at handling PyTorch Tensors
- Training & Testing Models in PyTorch
    - Know how a Logistic Regression model is trained and evaluated
- Work with Kaggle Notebooks

Prerequisites

- We assume you are already familiar with…

1. **Python3**
   - if-else, loop, function, file IO, class, ...
   - refs: link1, link2, link3
2. **Linear Classifiers**
   - Logistic Regression
   - Loss / Optimization

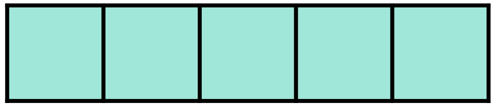
Some knowledge of **NumPy** will also be useful!

What is PyTorch?

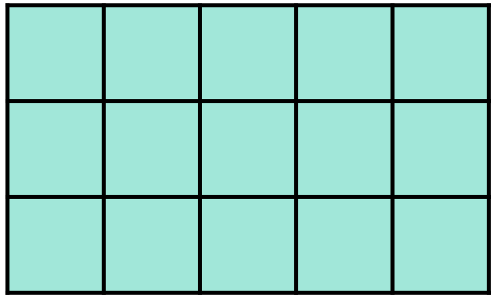
- An **machine learning framework** in Python.
- Two main features:
  - N-dimensional **Tensor** computation (like NumPy) on **GPUs**
  - **Automatic differentiation** for training deep neural networks

Tensors

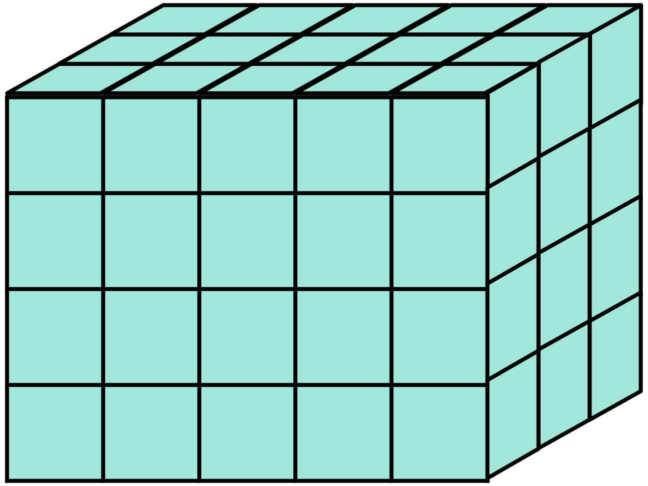
- High-dimensional matrices (arrays)



1-D tensor
e.g. audio

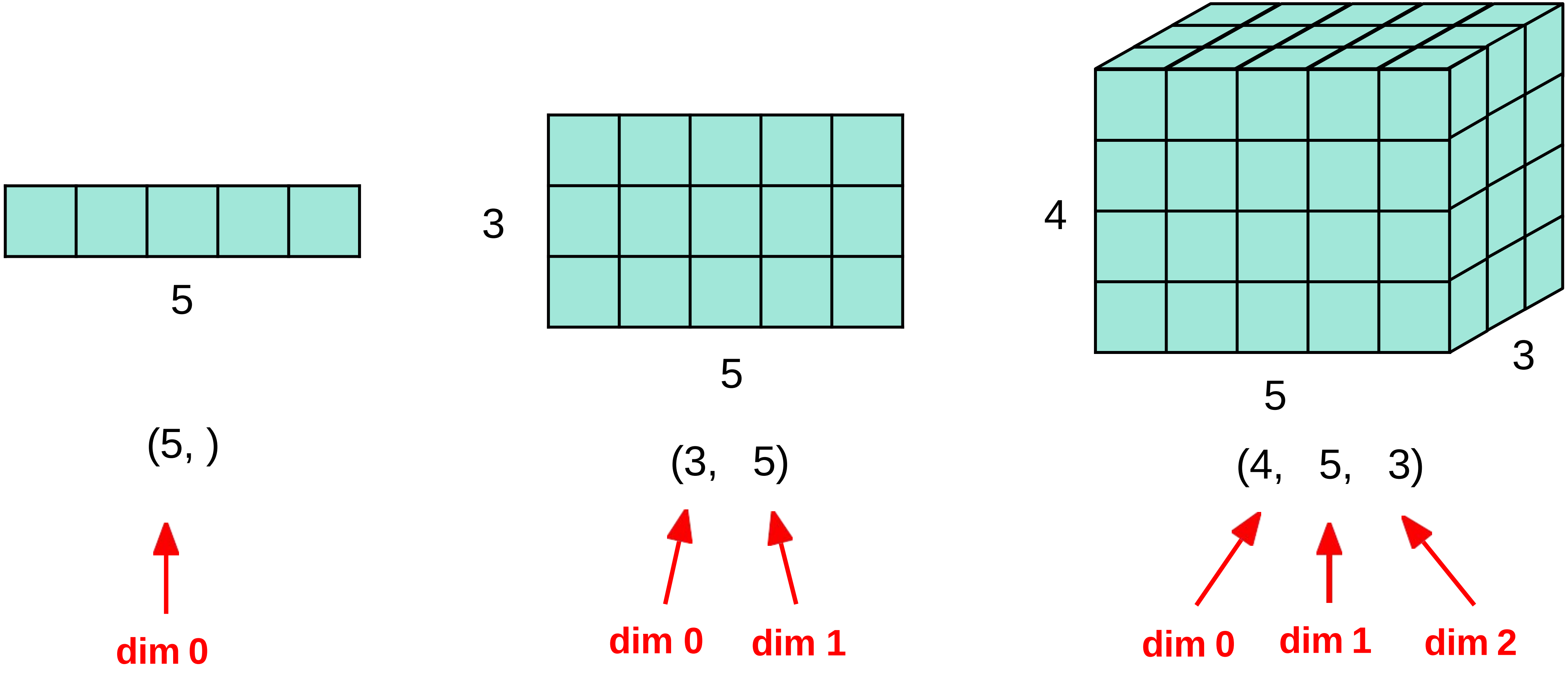


2-D tensor
e.g. black&white images



3-D tensor
e.g. RGB images

Tensors – Shape of Tensors



Note: dim in PyTorch == axis in NumPy

Tensors – Creating Tensors

- Directly from data (list or numpy.ndarray)

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

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

- Tensor of constant zeros & ones

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

shape

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

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

Tensors – Common Operations

Common arithmetic functions are supported, such as:

- Addition

$$z = x + y$$

- Subtraction

$$z = x - y$$

- Power

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

- Summation

$$y = x.\mathbf{sum()}$$

- Mean

$$y = x.\mathbf{mean()}$$

Tensors – Common Operations

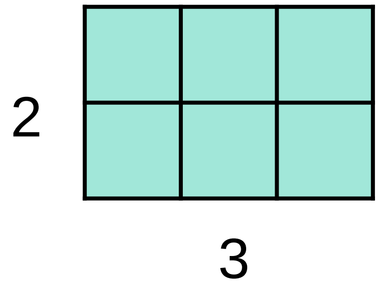
- **Transpose**: transpose two specified dimensions

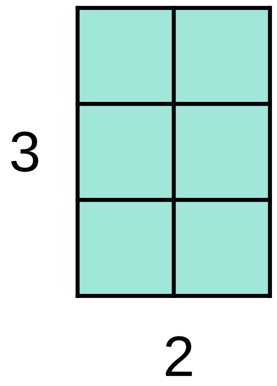
```
>>> x = torch.zeros([2, 3])

>>> x.shape
torch.Size([2, 3])

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

>>> x.shape
torch.Size([3, 2])
```





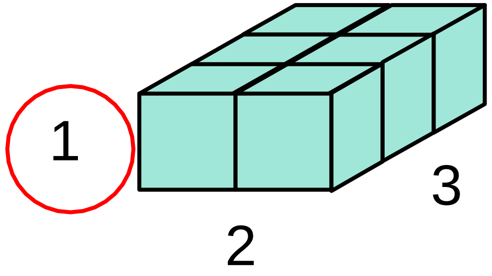
Tensors – Common Operations

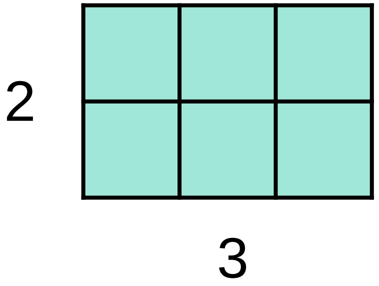
- **Squeeze**: remove the specified dimension with length = 1

```
>>> 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])
```

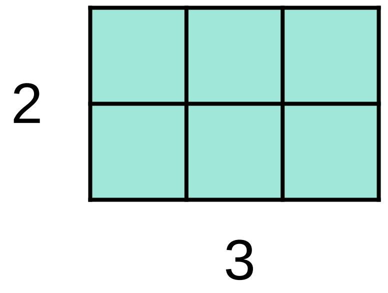


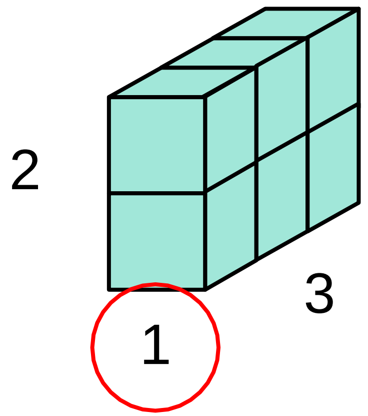


Tensors – Common Operations

- **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])
```

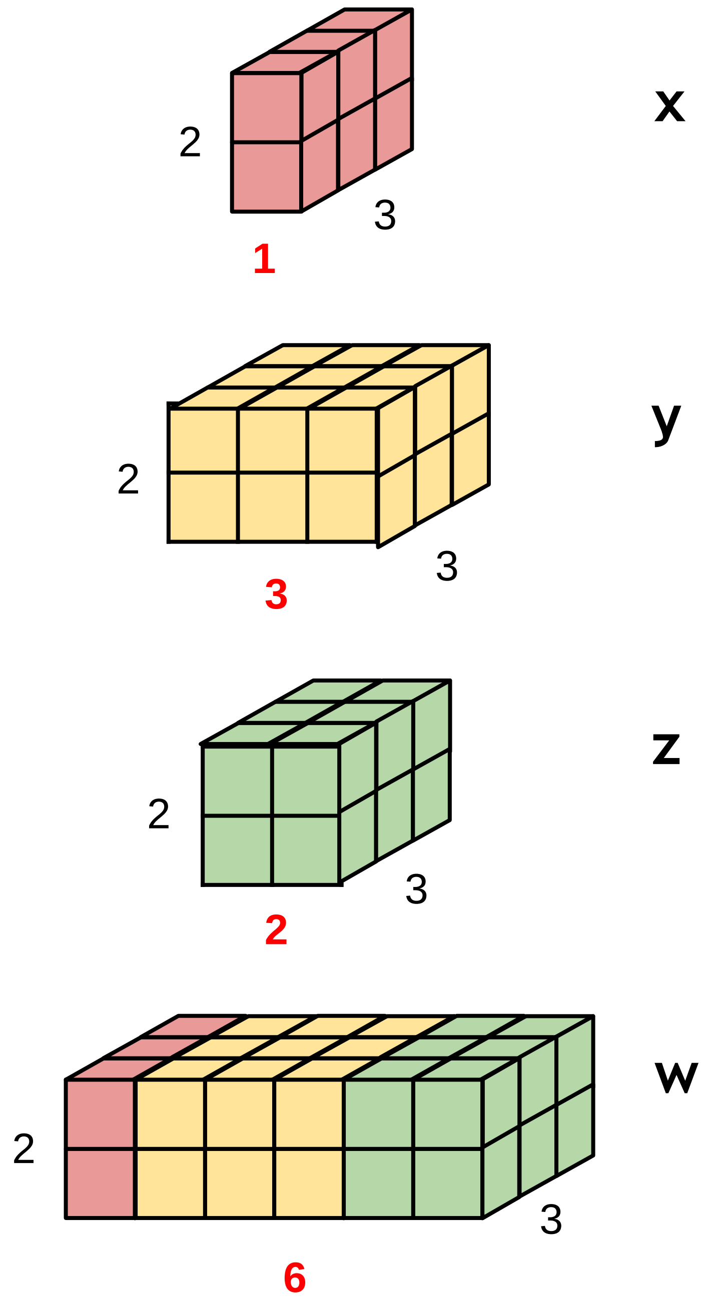




Tensors – Common Operations

- **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])
```



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

Tensors – Device

- Tensors & modules will be computed with **CPU** by default

  Use **.to()** to move tensors to appropriate devices.
- CPU

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

- GPU

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

Tensors – Device (GPU)

- Check if your computer has NVIDIA GPU

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

- Multiple GPUs: specify

```
'cuda:0', 'cuda:1', 'cuda:2', ...
```

- Why use GPUs?
  - Parallel computing with more cores for arithmetic calculations
  - See [What is a GPU and do you need one in deep learning?]()

Tensors – Gradient Calculation

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

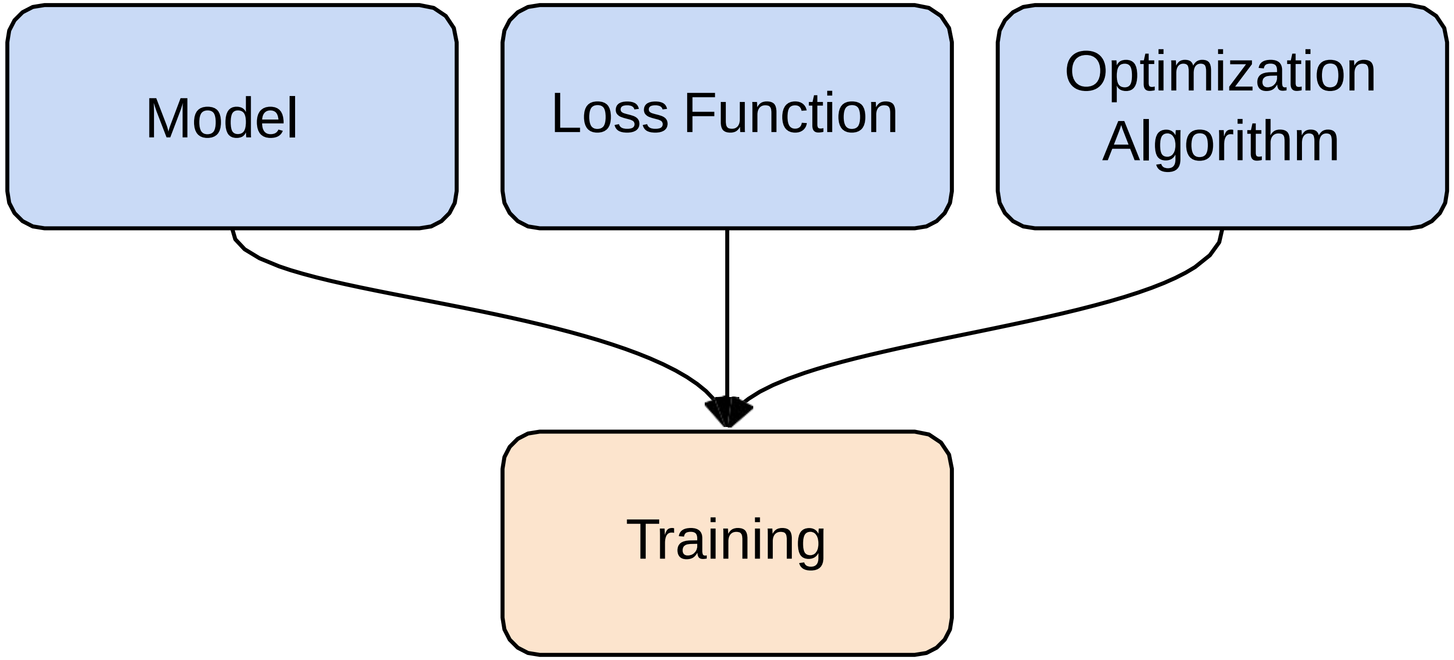
2 $z = \sum_i \sum_j x_{i,j}^2$

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

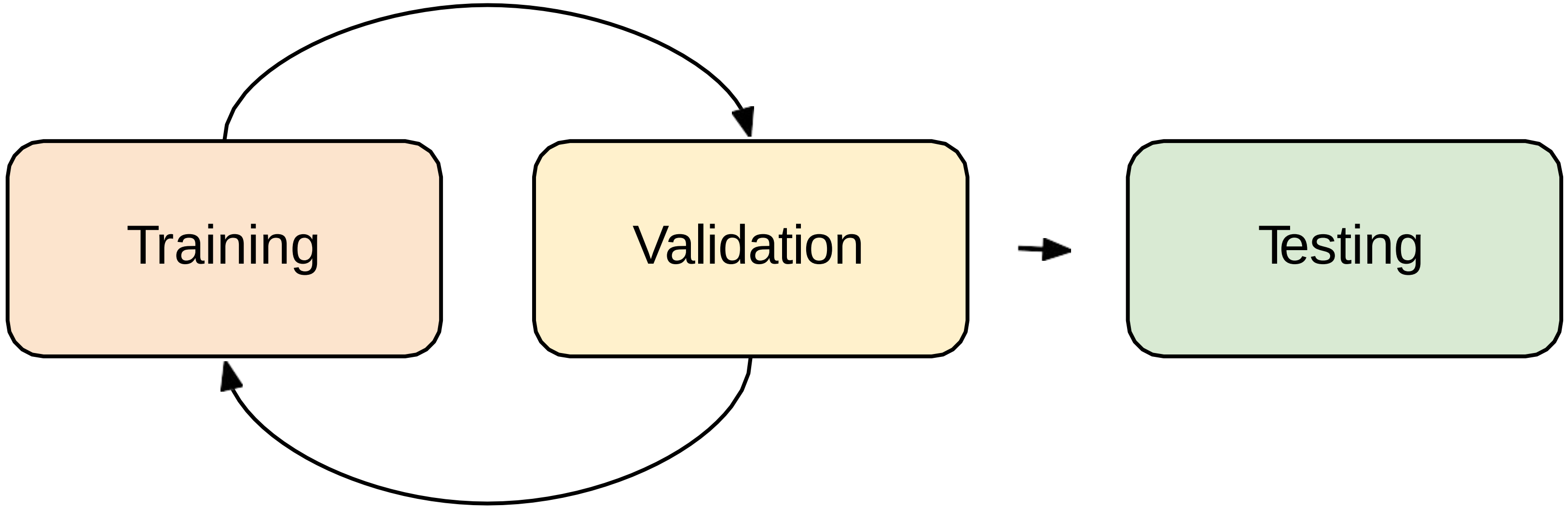
4 $\frac{\partial z}{\partial x} = \begin{bmatrix} 2 & 0 \\ -2 & 2 \end{bmatrix}$

See here to learn about gradient calculation.

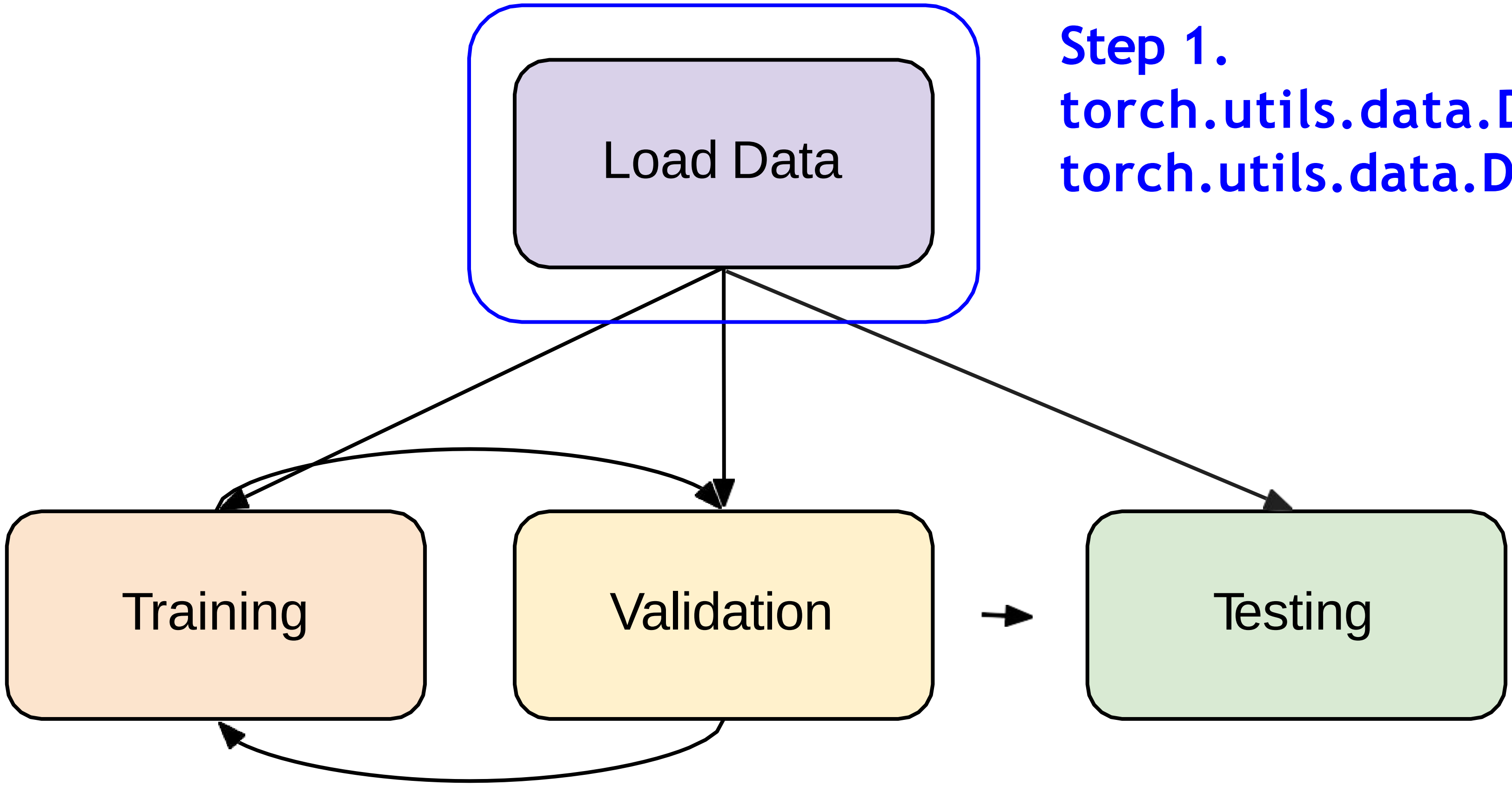
Training a Model



Training & Testing Models



Training & Testing Models



Step 1.
torch.utils.data.Dataset &
torch.utils.data.DataLoader

Dataset & Dataloader

- `Dataset`: stores data samples and expected values
- `Dataloader`: groups data in batches, enables multiprocessing

- `dataset = MyDataset(file)`
- `dataloader = DataLoader(dataset, batch_size, shuffle=True)`

Training: True
Testing: False

More info about batches and shuffling here.

Dataset & Dataloader

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

class MyDataset(Dataset):
    def init (self, file):
        self.data = ...

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

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

Read data & preprocess

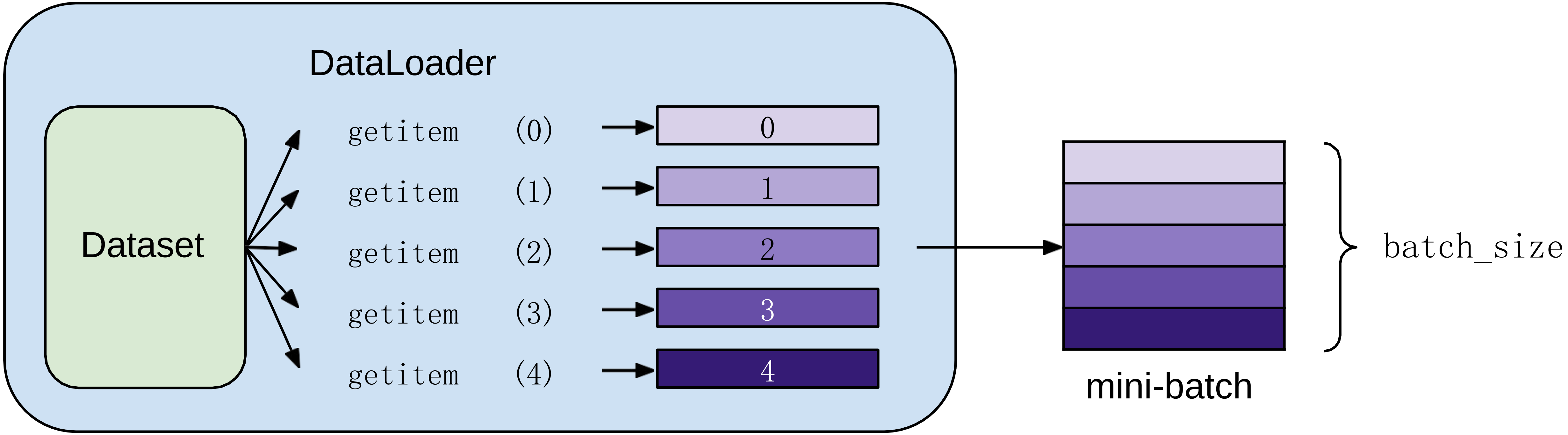
Returns one sample at a time

Returns the size of the dataset

Dataset & Dataloader

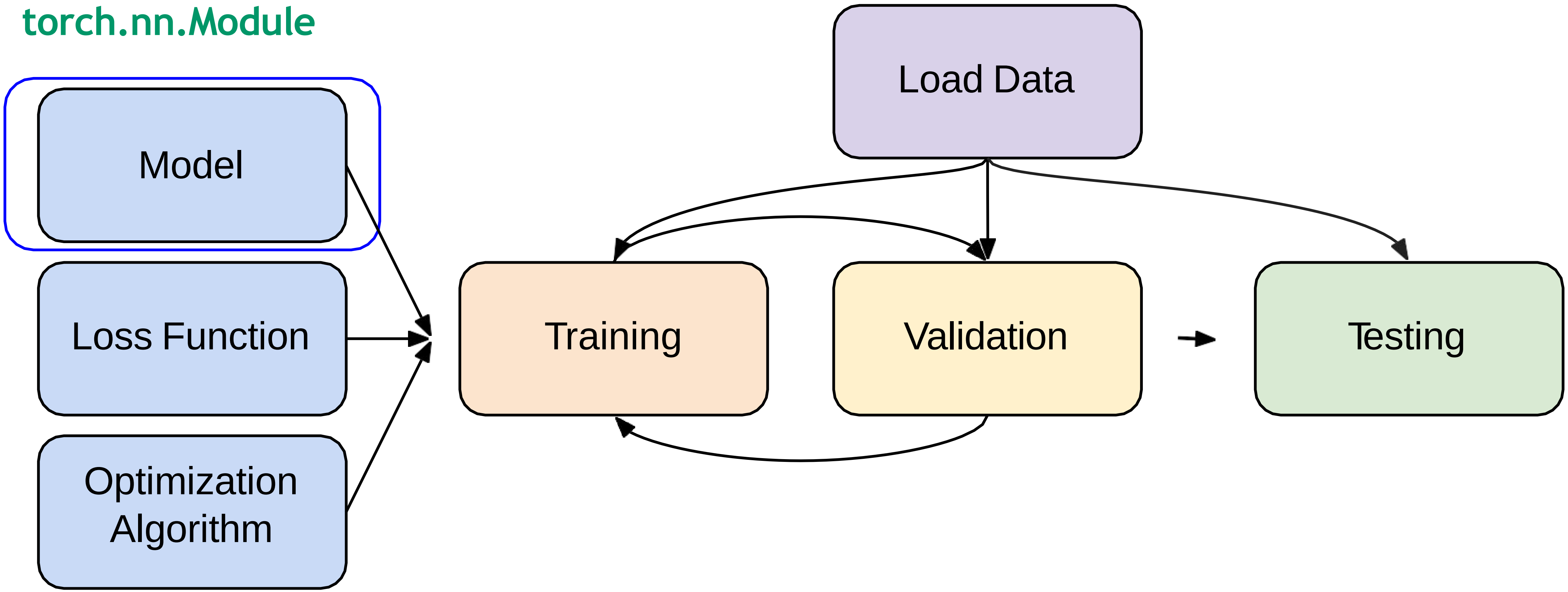
```
dataset = MyDataset(file)

dataloader = DataLoader(dataset, batch_size=5, shuffle=False)
```



Training & Testing Models

Step 2.
torch.nn.Module

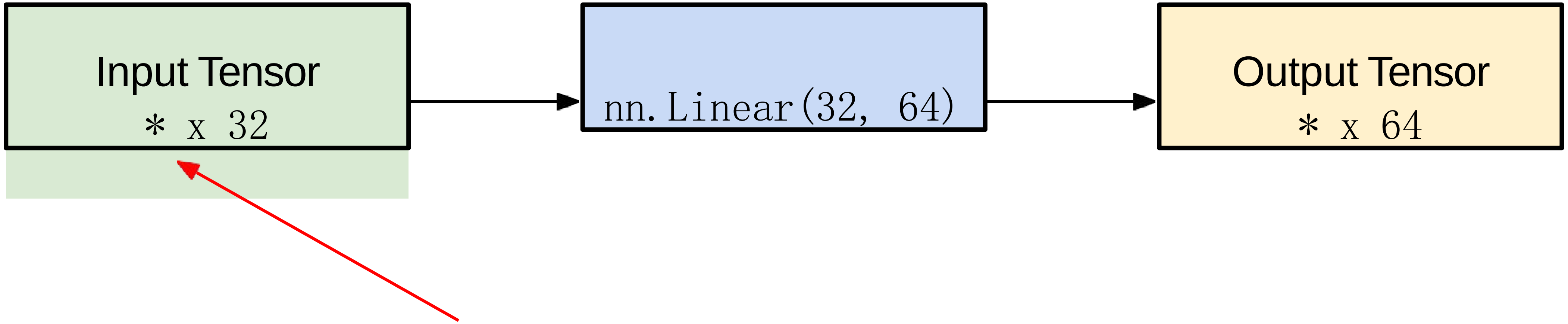


torch.nn – Network Layers

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

  `nn.Linear(in_features, out_features)`

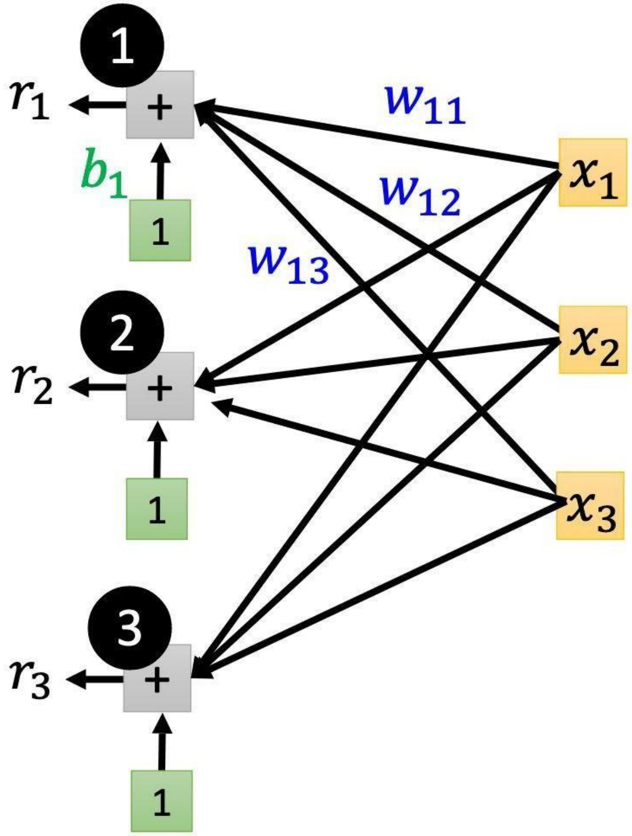
- We use this for our Logistic Regression Model

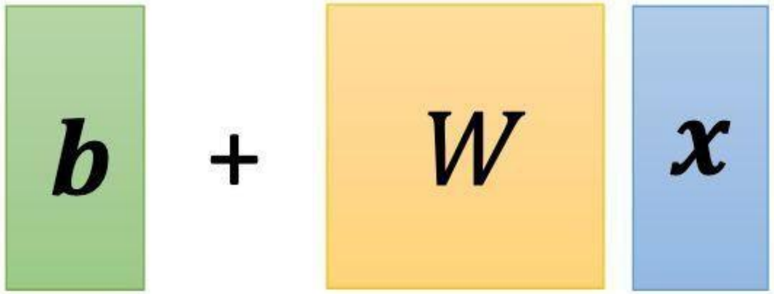


can be any shape (but last dimension must be 32)
e.g. (10, 32), (10, 5, 32), (1, 1, 3, 32), ...

torch.nn – Network Layers

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

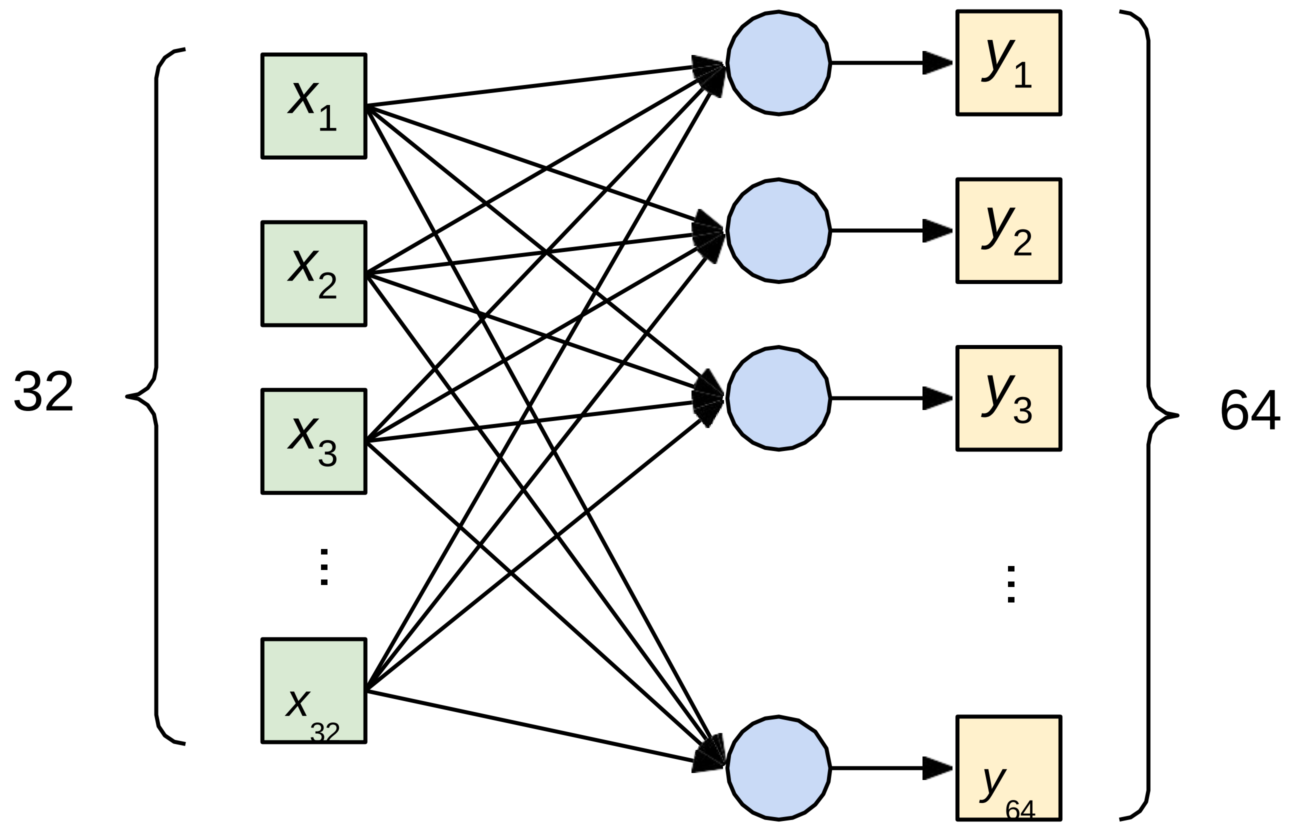


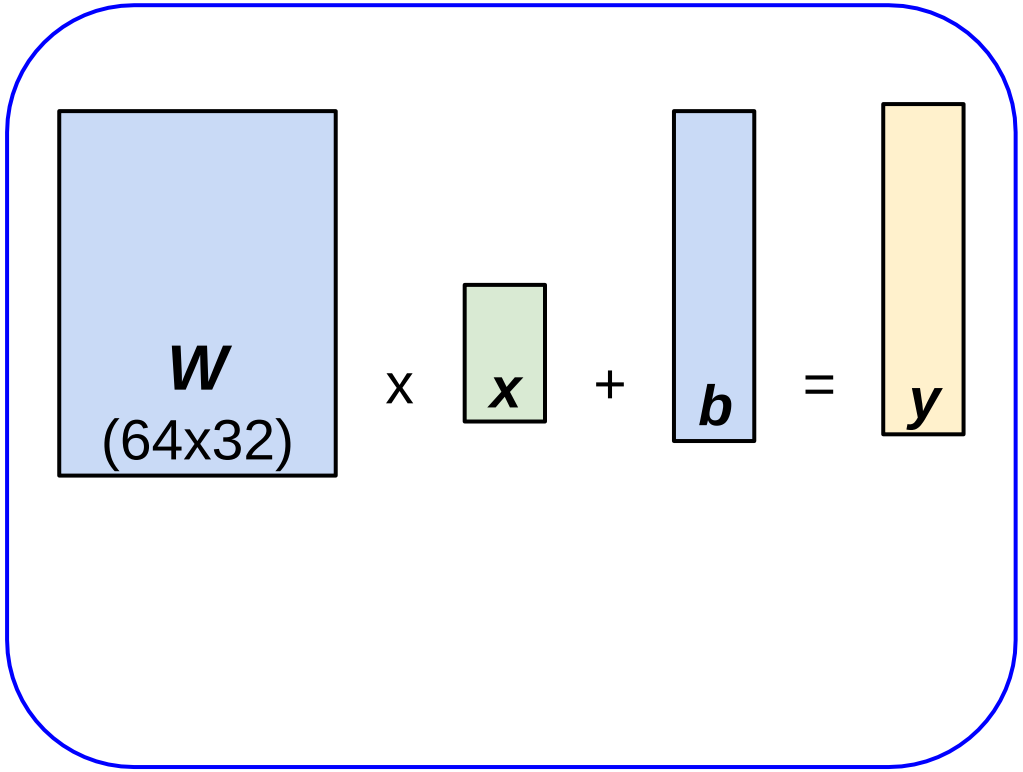


ref: [last year's lecture video]()

torch.nn – Network Layers

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

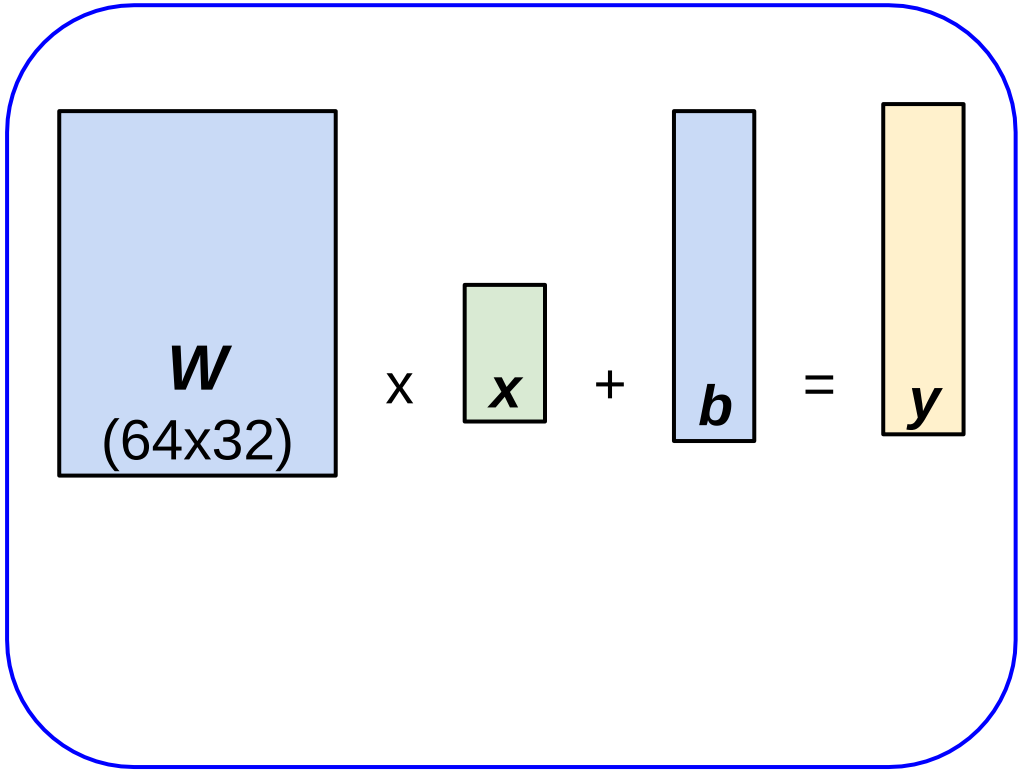




torch.nn – Network Parameters

- 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 – Non-Linear Activation Functions

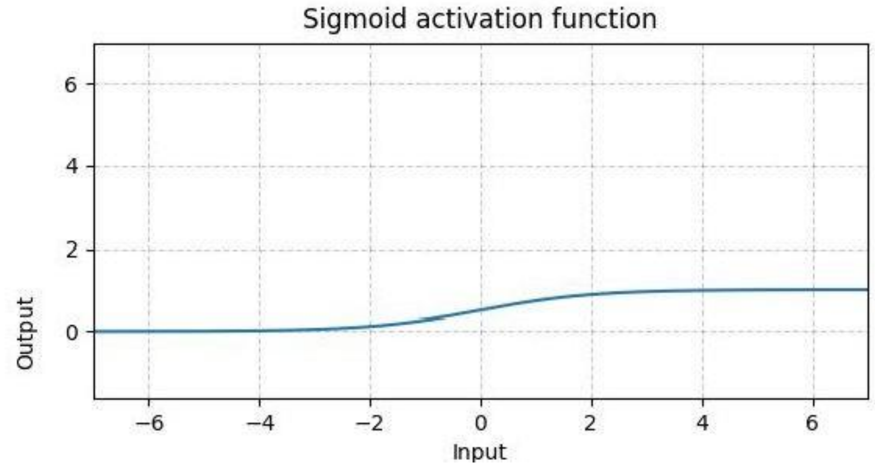
- These are for more complex Neural Networks, which will be introduced in the future lessons.

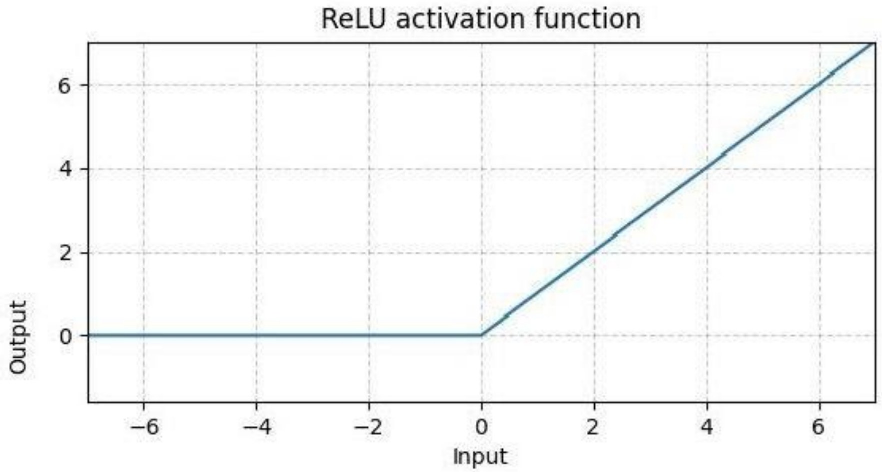
- Sigmoid Activation

```
nn.Sigmoid()
```

- ReLU Activation

```
nn.ReLU()
```

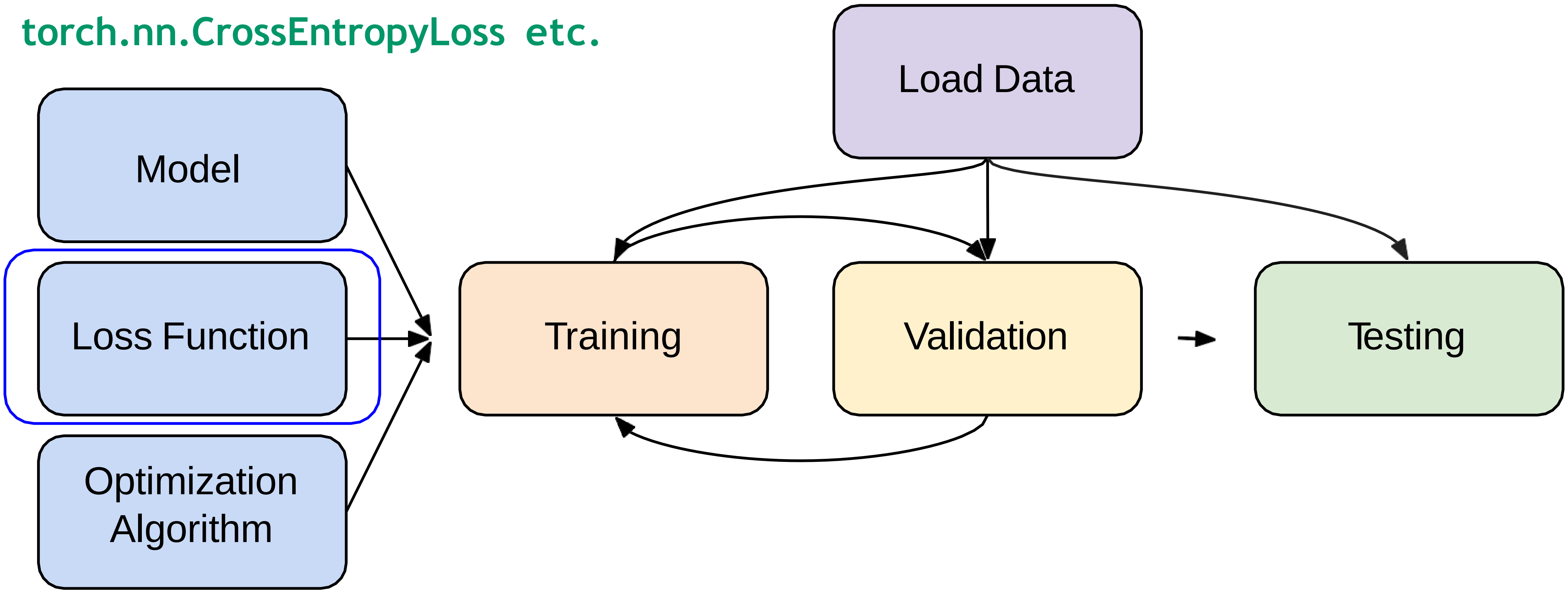




See here to learn about why we need activation functions.

Training & Testing Models

Step 3.
torch.nn.MSELoss
torch.nn.CrossEntropyLoss etc.



torch.nn – Loss Functions

- Mean Squared Error (for regression tasks)

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

- Cross Entropy (for classification tasks, a Multi-class Version of Logistic Regression)

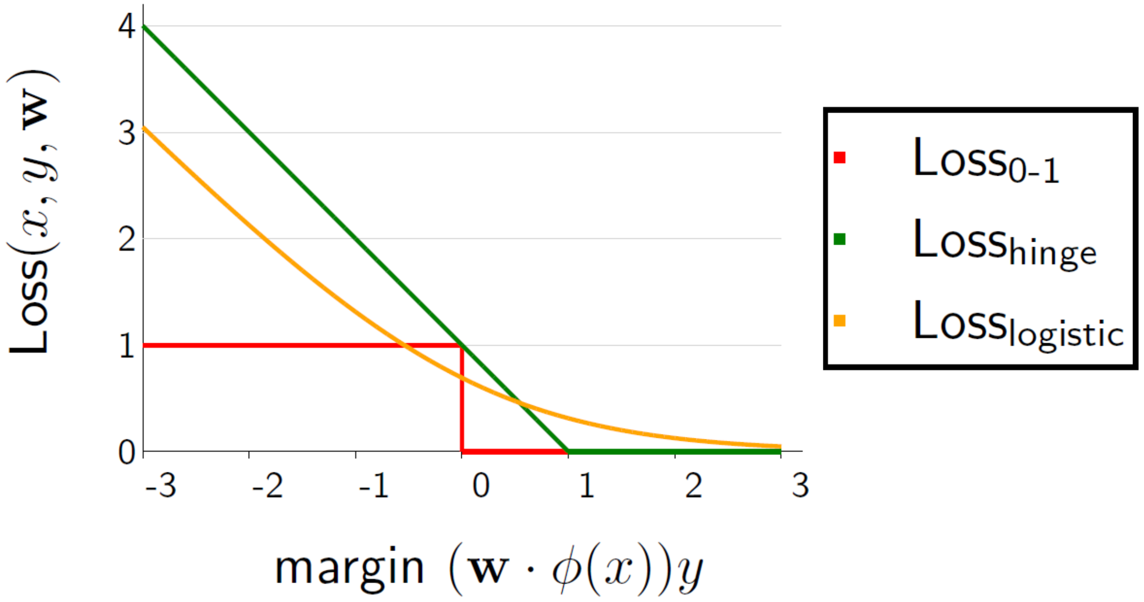
  ```
  criterion = nn.CrossEntropyLoss()
  ```

- `loss = criterion(model_output, expected_value)`

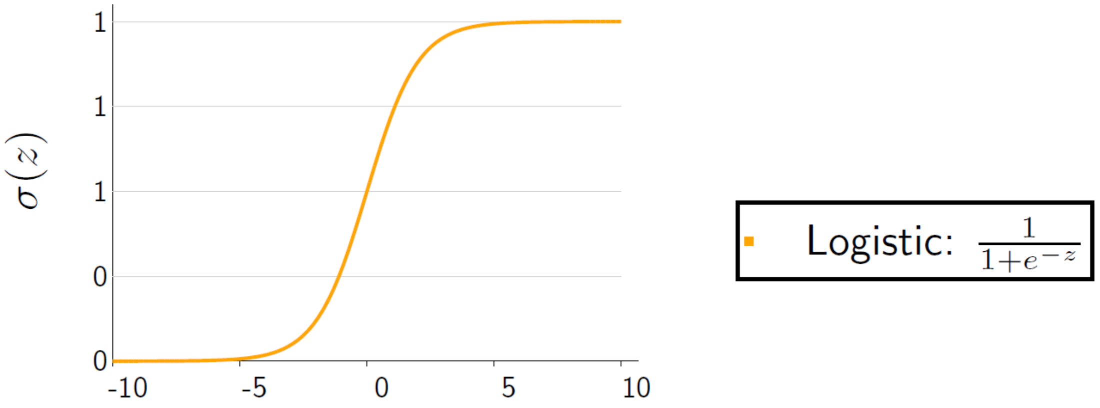
Logistic Regression – For 2 classes (binary classification)

逻辑回归

$$\text{Loss}_{\text{logistic}}(x, y, \mathbf{w}) = \log(1 + e^{-(\mathbf{w}\cdot\phi(x))y})$$



逻辑回归的另外一个角度



Logistic Regression, Softmax, Cross Entropy

- Logistic Regression
- Softmax

$$\mathrm{softmax}(\boldsymbol{v}) = \frac{1}{\sum_{k=1}^{K} e^{v_k}} \begin{bmatrix} e^{v_1} \\ e^{v_2} \\ \vdots \\ e^{v_K} \end{bmatrix}.$$

Equivalent to the multi-class version of Log. Func.

▪ Logistic: $\frac{1}{1+e^{-z}}$

- Cross Entropy Loss – the multi-class version of Log. Reg.

$$H(\boldsymbol{P}, \boldsymbol{Q}) = -\sum_{i=1}^{K} p_i \log(q_i),$$

loss = nn.CrossEntropyLoss(model_output, expected_value)

P: one-hot ground truth labels like (0, 1, 0)

model_output: (2.0, 3.0, 0.0)

Softmax

Q: (0.26, 0.71, 0.04)

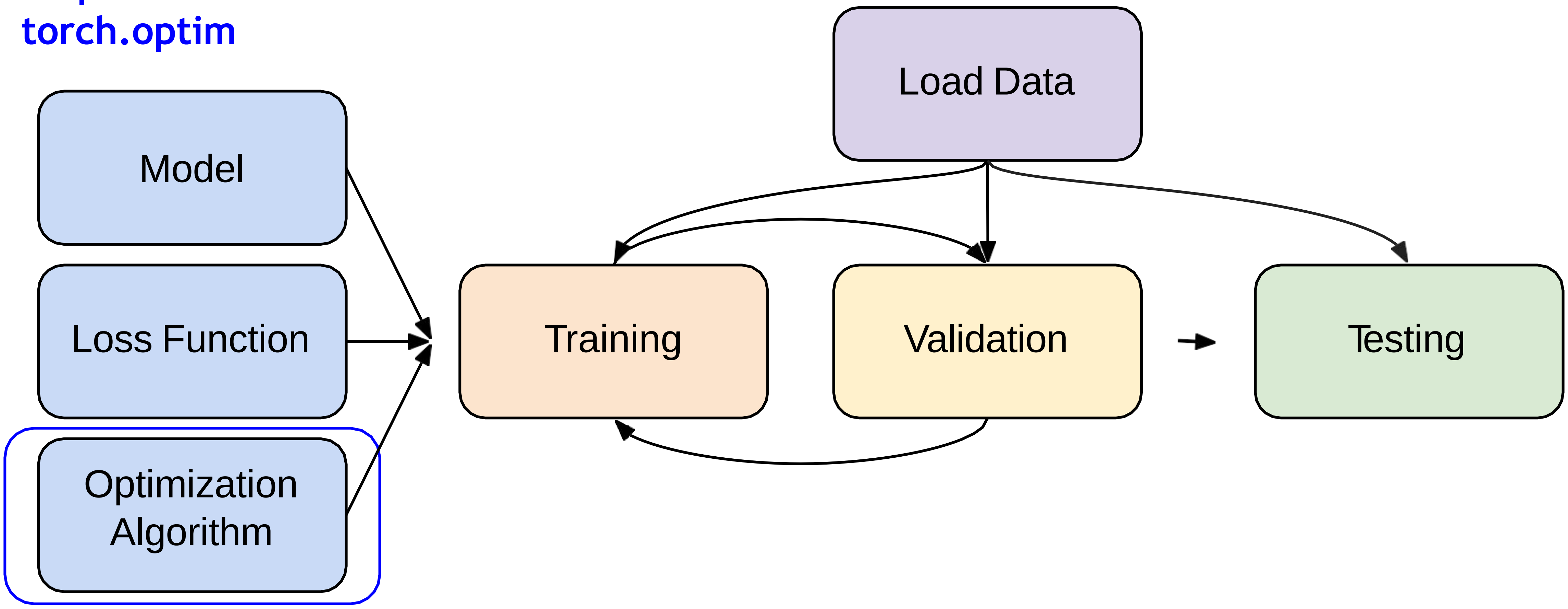
Calculate H(P, Q)

Consider 3 classes

For Detailed Explanation: here

Training & Testing Models

Step 4.
torch.optim



torch.optim

- Gradient-based **optimization algorithms** that adjust network parameters to reduce error. (See Adaptive Learning Rate lecture video)

- E.g. Stochastic Gradient Descent (SGD)

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

torch.optim

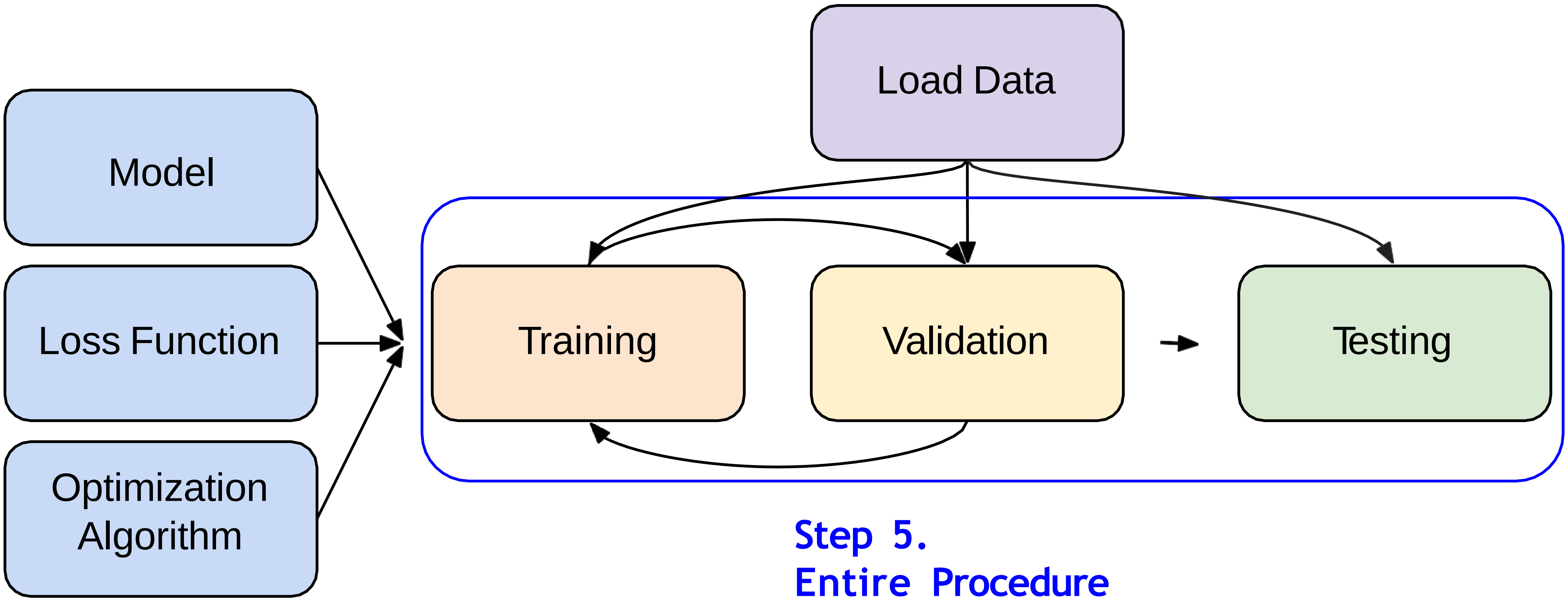
```
optimizer = torch.optim.SGD(model.parameters(), lr, momentum = 0)
```

- For every batch of data:

1. Call `optimizer.zero_grad()` to reset gradients of model parameters.
2. Call `loss.backward()` to backpropagate gradients of prediction loss.
3. Call `optimizer.step()` to adjust model parameters.

See official documentation for more optimization algorithms.

Training & Testing Models



Step 5.
Entire Procedure

Training Setup – Linear Regression

X (input): 1, 2, …, 10
Y (output): 2, 4, …, 20

```
dataset = MyDataset(file)
```
read data via MyDataset

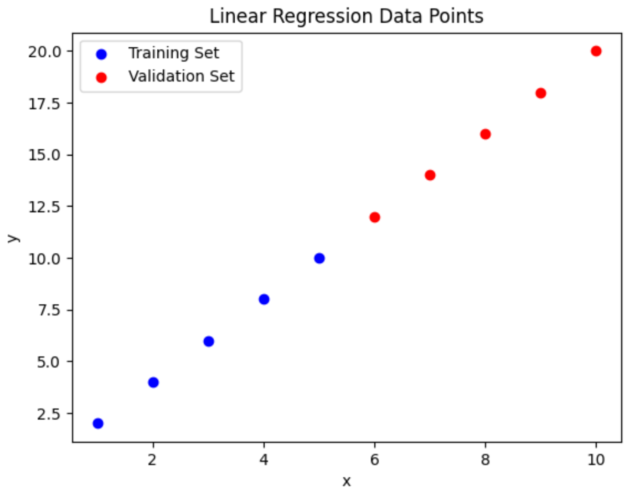
```
tr_set = DataLoader(dataset, batch_size=2, shuffle=True)
```
put dataset into Dataloader

```
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

Linear(1, 1): w & b
Give model an x, output is wX+b



Training Loop – Linear Regression

- 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

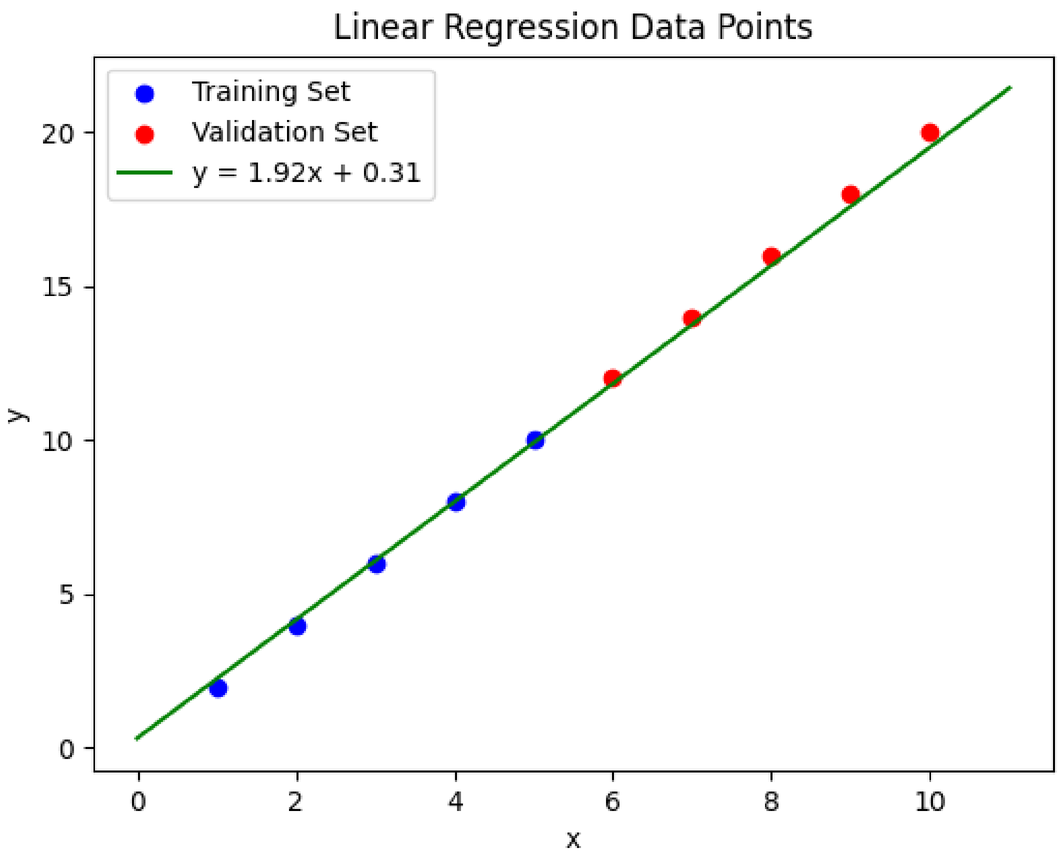
$wX + b$

$||wX + b - Y||_2$

We use MSELoss here for regression.

Training Loop – Linear Regression

- After training, we get the model: w=1.92, b=0.31

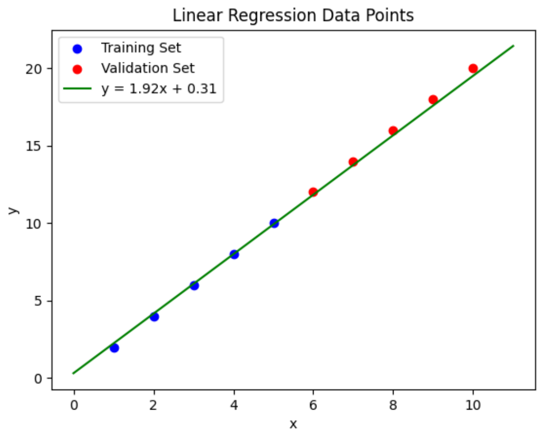


Validation / Testing Loop

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

$1.92X + 0.31$

Preds is [11.8, 13.8, 15.7, 17.6, 19.5]
Y is [12, 14, 16, 18, 20]



Notice - model.eval(), torch.no_grad()

- **model.eval()**
  Changes behaviour of some model layers, such as dropout and batch normalization.

- **with torch.no_grad()**
  Prevents calculations from being added into gradient computation graph.
  Usually used to prevent accidental training on validation/testing data.

Save / Load Trained Models

- Save

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

- Load

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

More About PyTorch

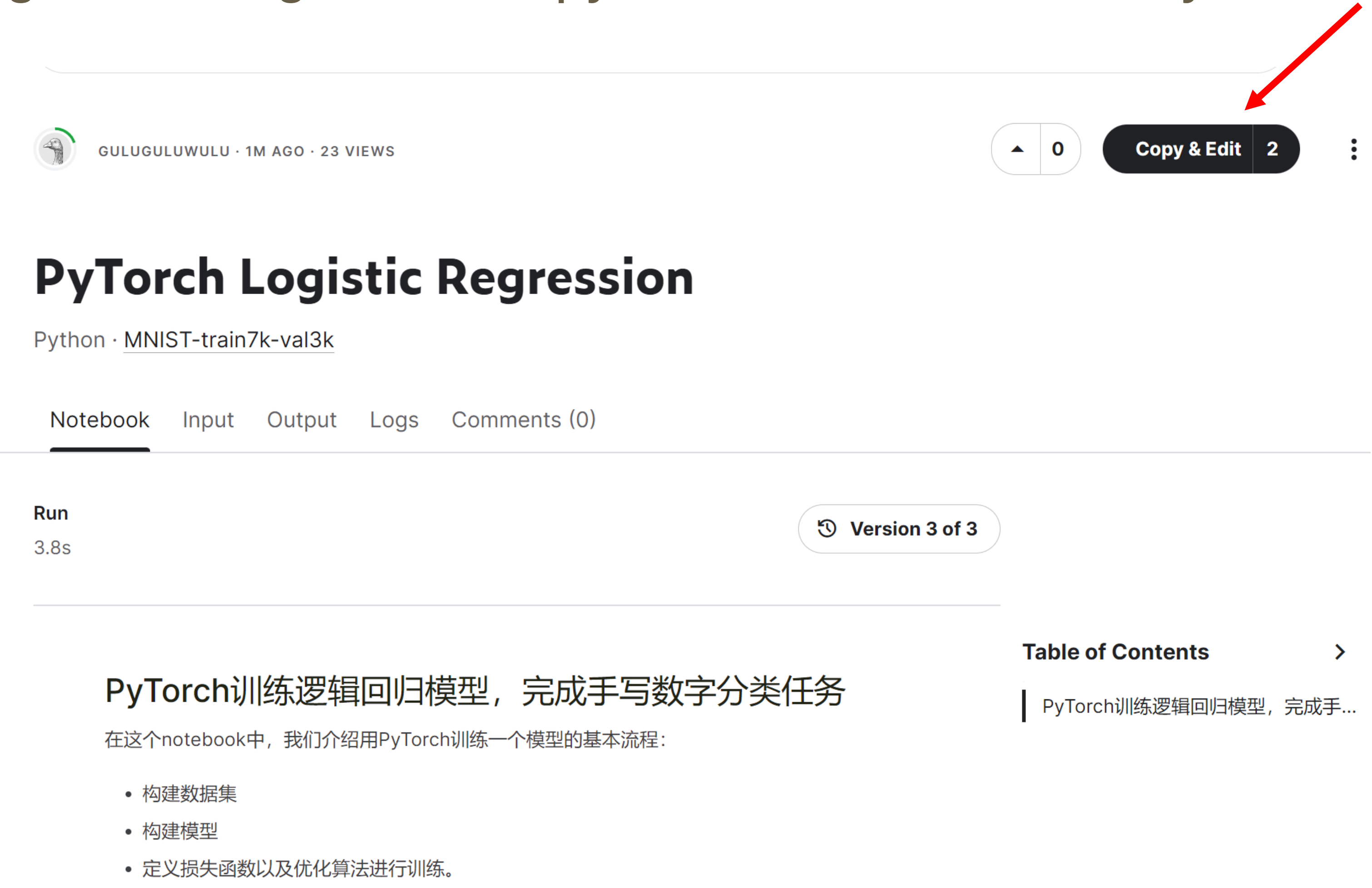
- Additional packages
  - torchvision for Computer Vision
  - torchaudio for Audio
- Useful github repositories using PyTorch
  - Huggingface Transformers (transformer models: BERT, GPT, ...)
  - Fairseq (sequence modeling for NLP & speech)
  - ESPnet (speech recognition, translation, synthesis, ...)
  - Most implementations of recent deep learning papers
  - ...

Homework Specifics

- Two parts:
- Ctrl + 点击访问链接
  - PyTorch Tensors: kaggle link
  - PyTorch Logistic Regression: kaggle link

Homework Specifics

- Use Kaggle – 1. Login and Copy the two notebooks to your own account



Homework Specifics

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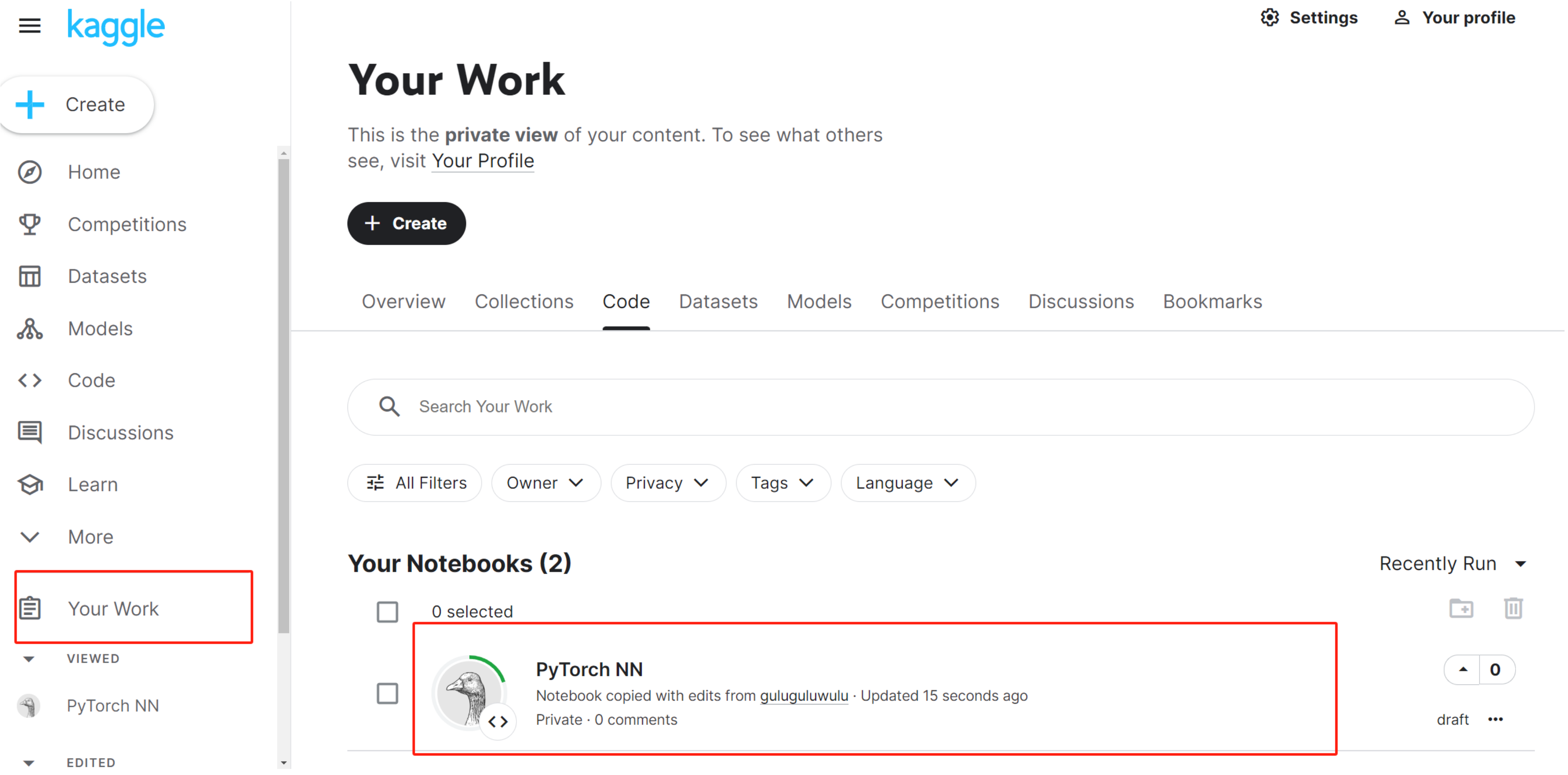
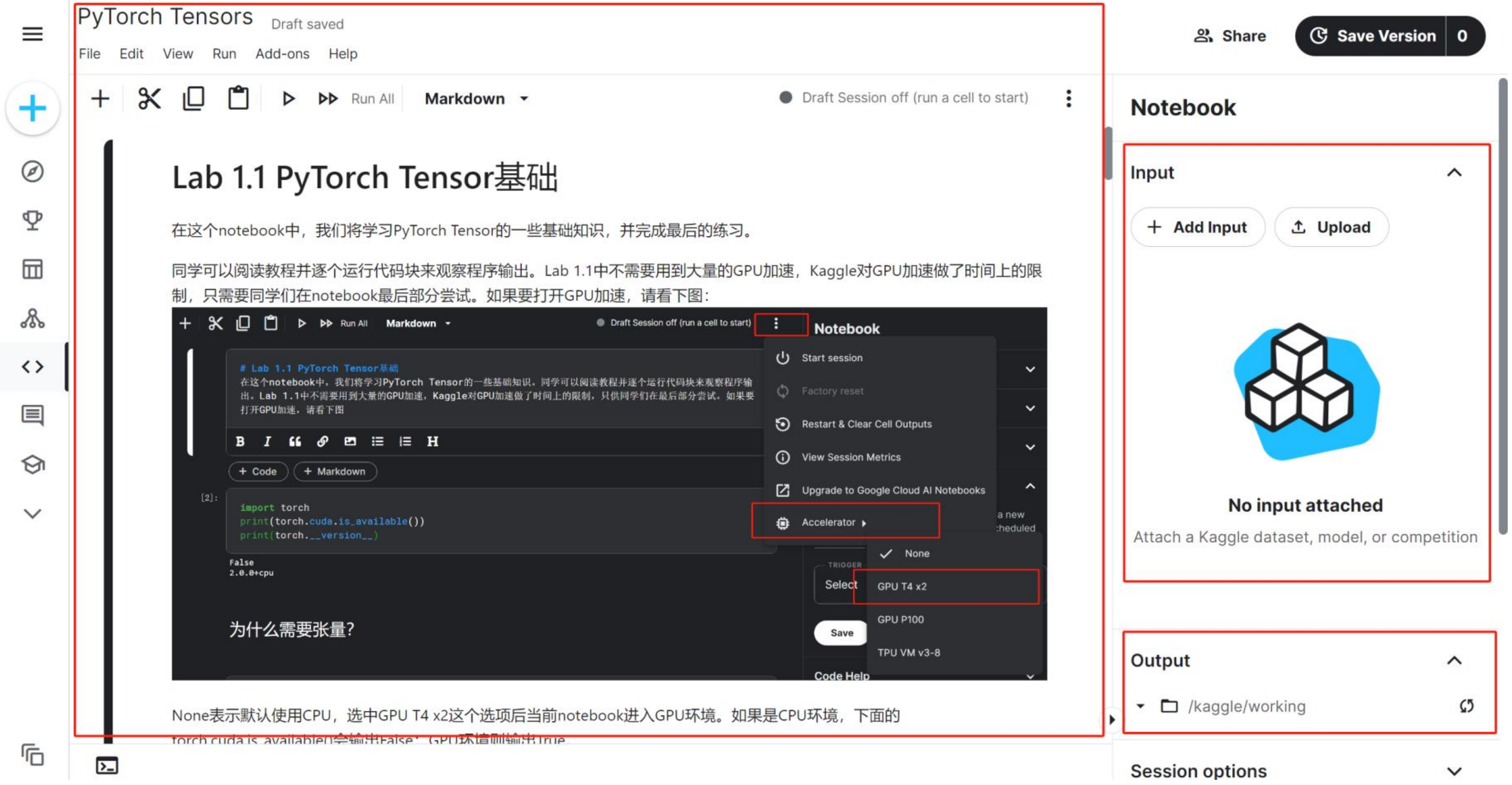


Homework Specifics

- Use Kaggle – 2. Notebook provides a Python environment, where Kaggle installs the PyTorch package for us by default.

正文：教程+可运行的代码块

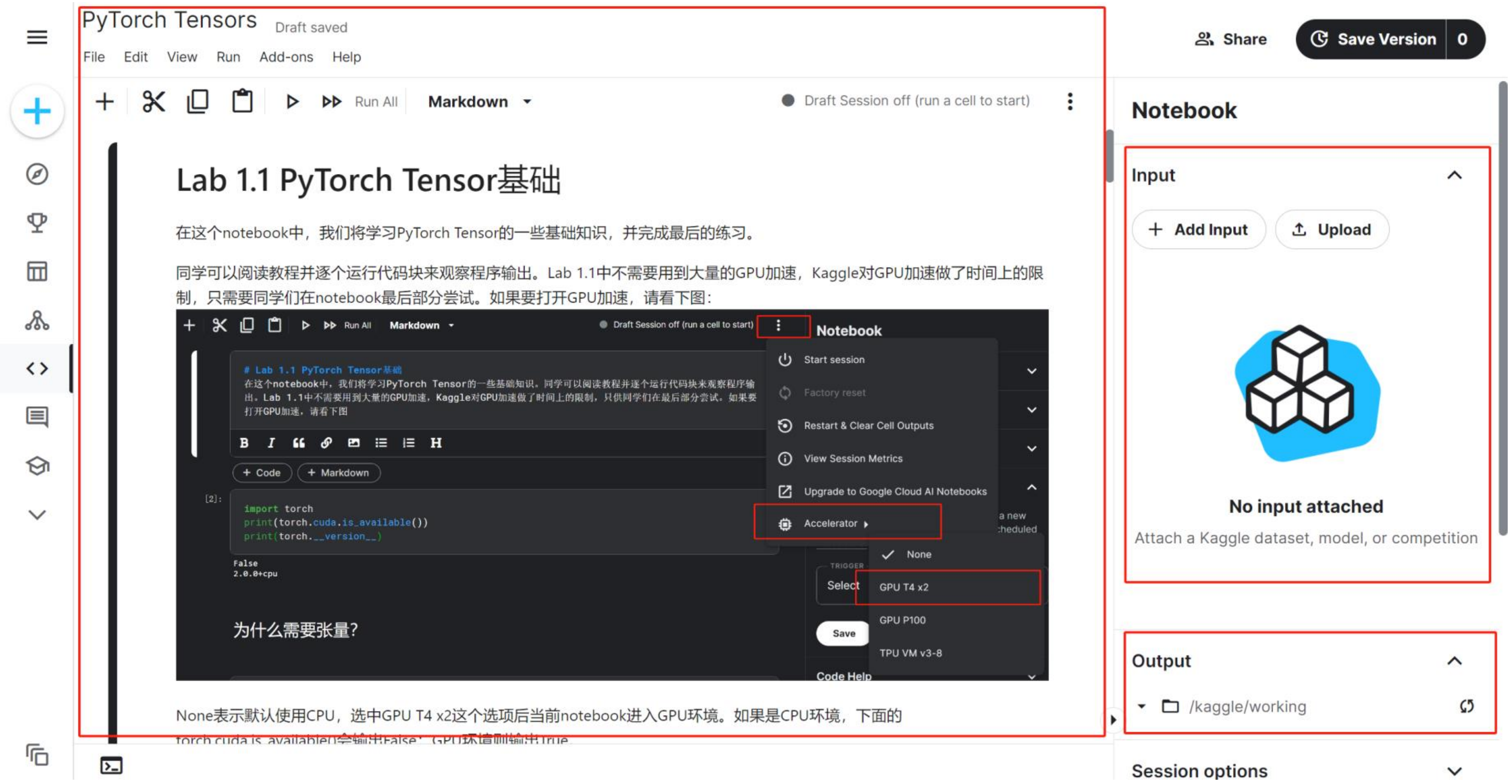


输入

输出

Homework Specifics

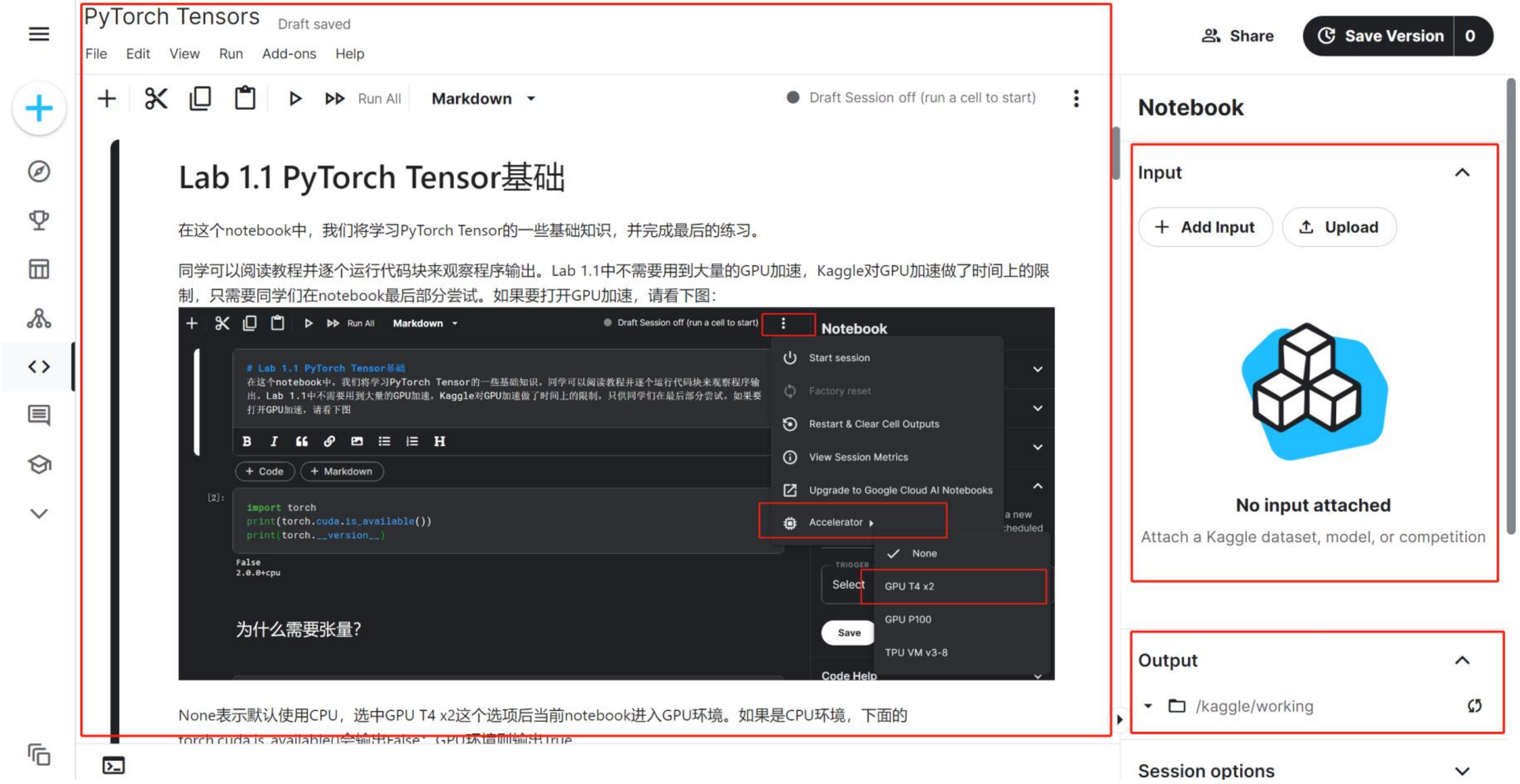
- Use Kaggle – 2. Notebook



输入：可以存放notebook所挂载的数据集，供模型的训练推理使用。

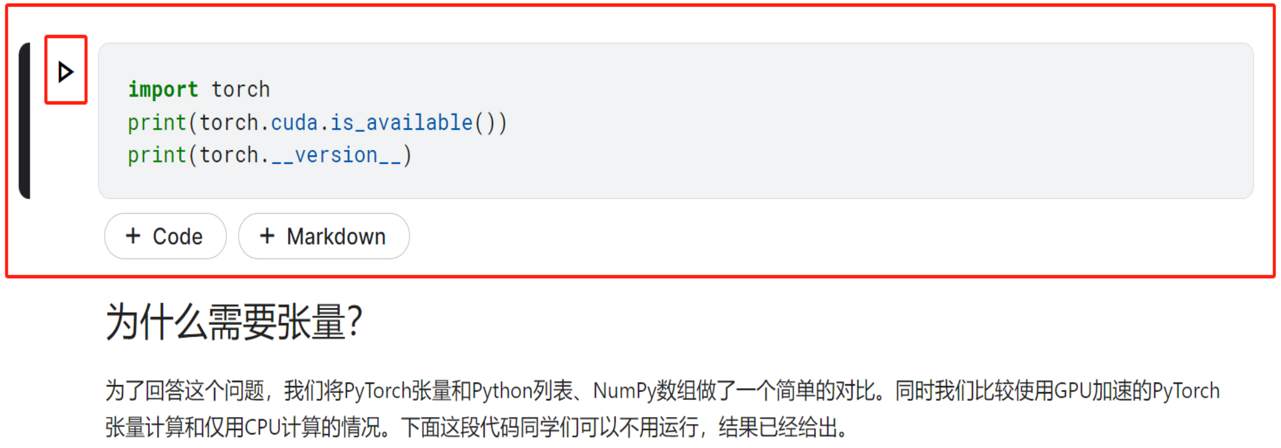
Homework Specifics

- Use Kaggle – 2. Notebook



输出：当前环境一个临时的文件区域，你的代码可以把一些输出存放在Output。例如训练得到的模型权重文件。

Homework Specifics



- Use Kaggle – 3. Running a code block in Notebook

- 点击箭头运行
- 代码块可以修改

- 同一个notebook中，命名空间共享：
  - 我在前一个代码块中做了import torch的操作，并运行该代码块。该notebook下的import操作就完成了，那么下一个代码块中即使不显式地再次import，也可以调用torch.xxx。
  - 前一个代码块声明变量a=1，并运行。那么在下一个代码块中我依然能访问到变量a。

Homework Specifics

- 阅读两个notebook中的教程
- 运行教程里的代码块，观察输出
- **完成PyTorch Tensor部分练习**

作业有五道题，完成四题即可满分（25*4），多做不加分（做错了也不扣分），填入空缺代码并通过测试用例。

提交：

- **DDL: 3.31, 23:59；晚交一天扣10分**
- 完成**PyTorch Tensor**练习。完成后，先运行你所完成练习的代码块，再下载(File -> Download Notebook) .ipynb文件 （如果不运行，ipynb文件中无法看到你的代码块输出）
- 把ipynb文件命名为学号_姓名.ipynb，上传到elearning。
- 禁止抄袭，鼓励大家在各自的小组助教群提问

Thanks!

Any questions?