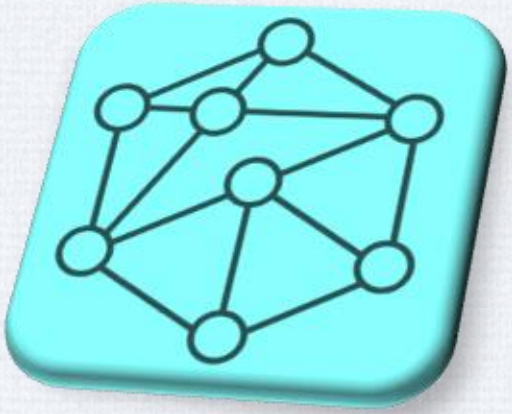
Network Training

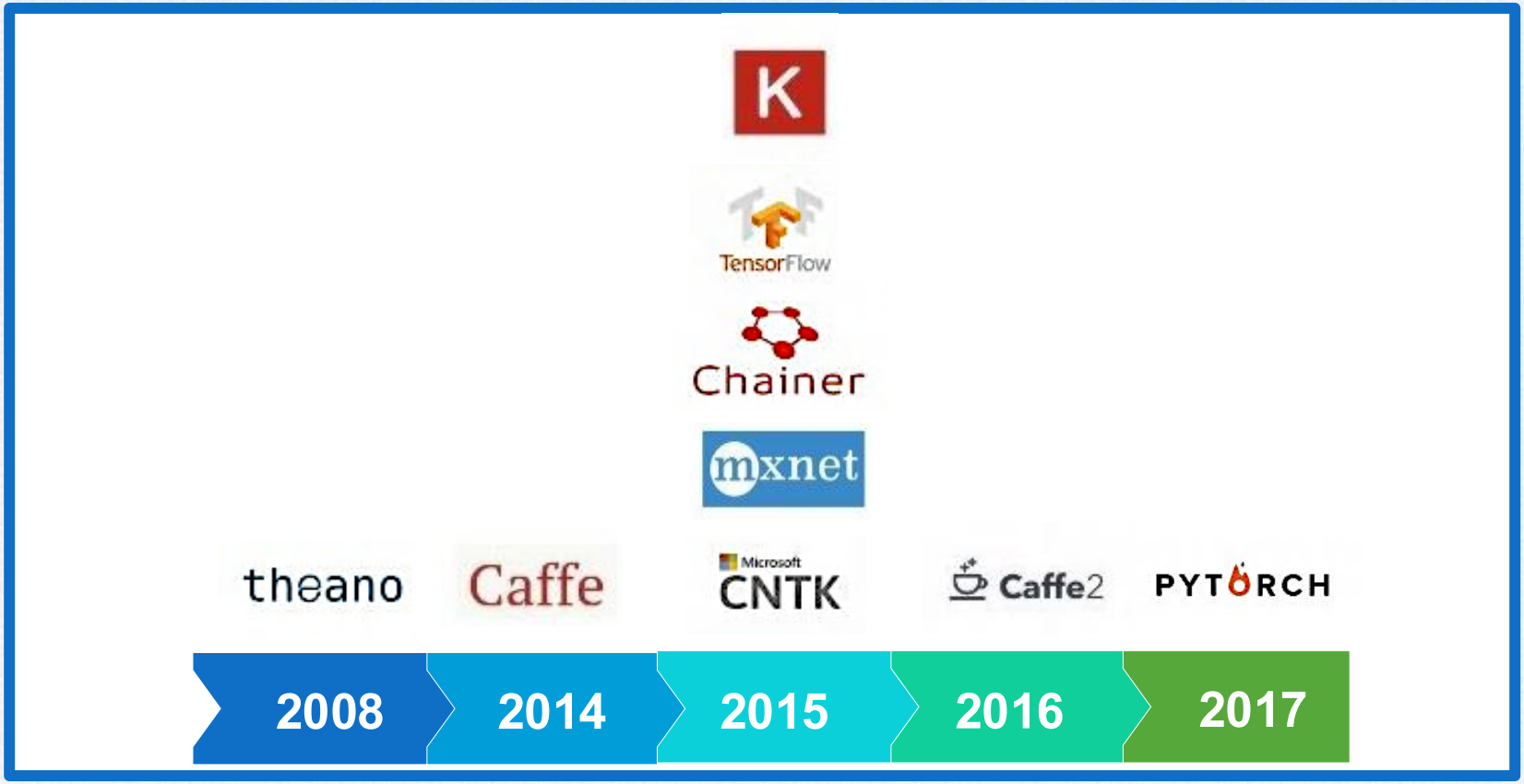


Venkatakrishnan V K

ECE 208/408 – The Art of Machine Learning

Zhiyao Duan

Popular Deep Learning Frameworks



Computational Graph

What is a Graph?

Graph is a structure containing –

Set of **vertices/nodes** **(V)**

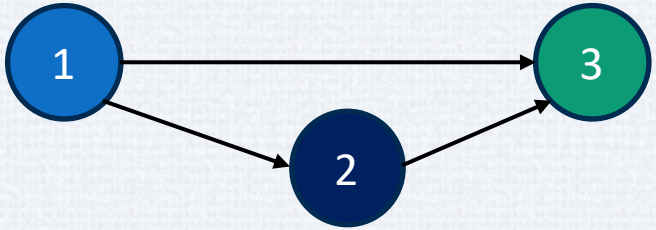
Set of **edges** **(E)** (connecting the vertices)

GRAPH!

$G = \{V, E\}$

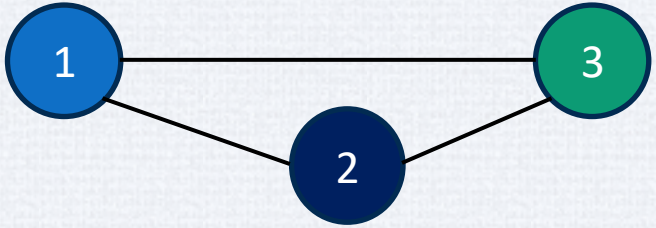
Directed Graph

Consists of edges pointing from one vertex to another vertex.



Undirected Graph

Consists of bidirectional edges



Computational Graph

What is a Computational Graph?

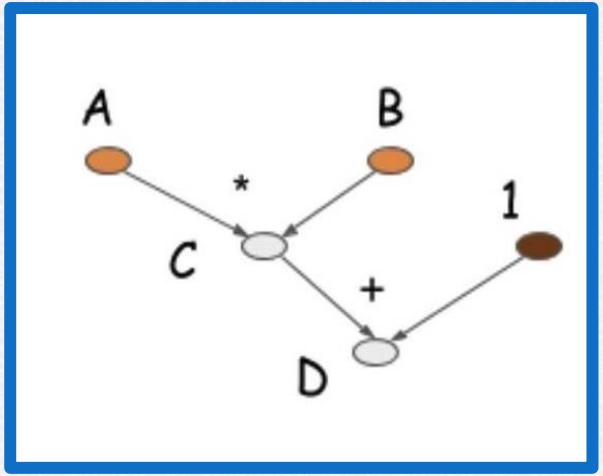
- A **directed** graph used to describe **mathematical expressions**

- **Forward** pass/propagation
  To compute the **output** of the network/graph

- **Backward** pass/propagation
  To compute the **gradients/derivatives**

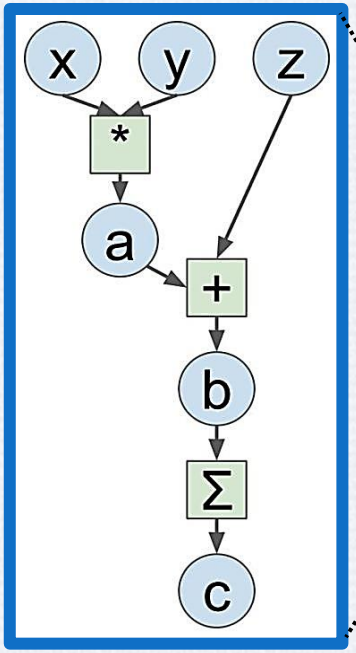
```
C = A * B
D = C + 1
```

```
import numpy as np
a = np.ones(10)
b = np.ones(10) * 2
c = b * a
d = c + 1
```



Tensor

Computational Graph



NumPy

```
import numpy as np
np.random.seed(0)

N, D = 3, 4

x = np.random.randn(N, D)
y = np.random.randn(N, D)
z = np.random.randn(N, D)
```

INITIALIZE

```
a = x * y
b = a + z
c = np.sum(b)
```

FORWARD PASS

```
grad_c = 1.0
grad_b = grad_c * np.ones((N, D))
grad_a = grad_b.copy()
grad_z = grad_b.copy()
grad_x = grad_a * y
grad_y = grad_a * x
```

BACKWARD PASS

Tensor

Computational Graph

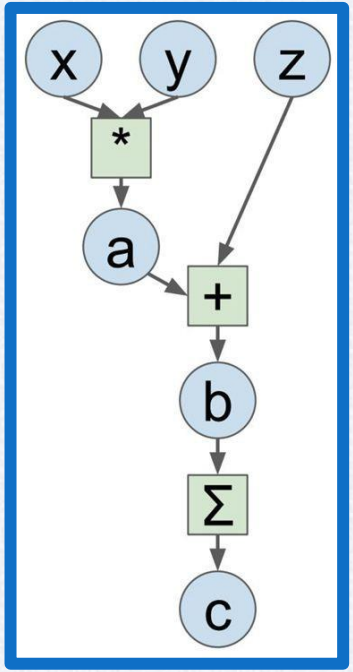
1. Define a tensor with gradient required
2. This tensor will be added to the computational graph

PyTorch

```
import torch

N, D = 3, 4

x = torch.randn(N, D, requires_grad = True)
y = torch.randn(N, D, requires_grad = True)
z = torch.randn(N, D, requires_grad = True)
```

Tensor

Computational Graph



The **forward pass** is similar to `numpy`.

These are **PyTorch** functions!

`*, +, torch.sum()`

These functions will build the dependency between tensors.

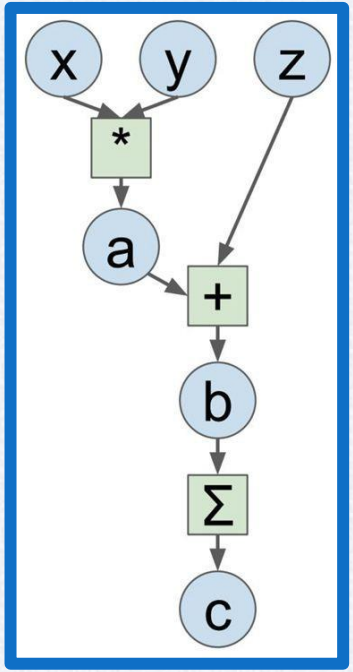
PyTorch

```
import torch

N, D = 3, 4

x = torch.randn(N, D, requires_grad = True)
y = torch.randn(N, D, requires_grad = True)
z = torch.randn(N, D, requires_grad = True)
```

```
a = x * y
b = a + z
c = torch.sum(b)
```

Tensor

Computational Graph



PyTorch is capable of performing **automatic differentiation** (due to the computational graphs)!

`c.backward()`:

1. Calculates the derivatives of `c` with respect to the inputs.
2. Writes the gradient to the `grad` attribute of `x, y, z`.

PyTorch

```
import torch

N, D = 3, 4

x = torch.randn(N, D, requires_grad = True)
y = torch.randn(N, D, requires_grad = True)
z = torch.randn(N, D, requires_grad = True)
```

```
a = x * y
b = a + z
c = torch.sum(b)
```

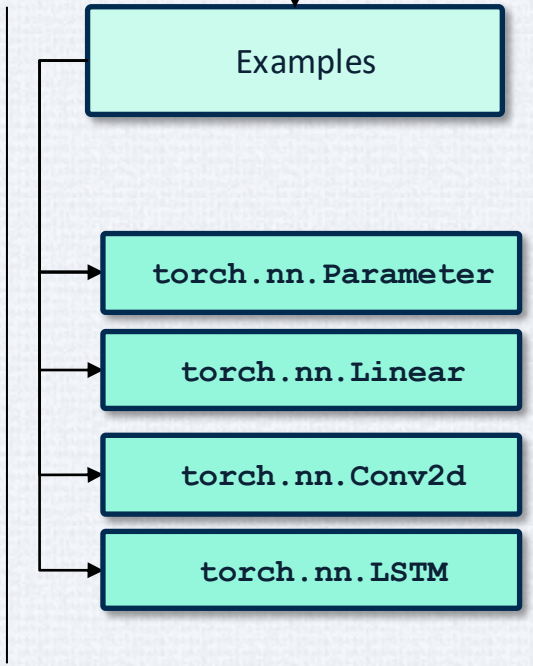
```
c.backward()

print(x.grad)
print(y.grad)
print(z.grad)
```

Module

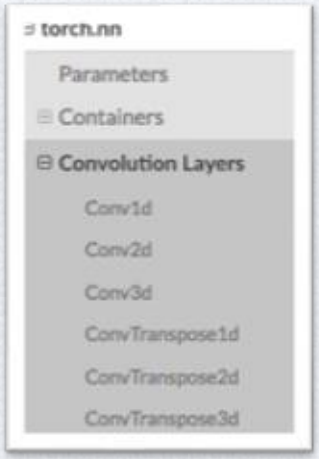
It consists of the fundamental building blocks for **creating any Neural Network**.

It often has the following:

- **Weight Attribute**: Store the weights.
- **Weight Initialization method**: Initializing the weight.
- **Forward method:** The computation build in the forward part.
- **Backward :** This part is invisible to users but is implemented by PyTorch already inside `torch.nn.Module`.
- **Buffer Attribute**: Weights but don't require grad.

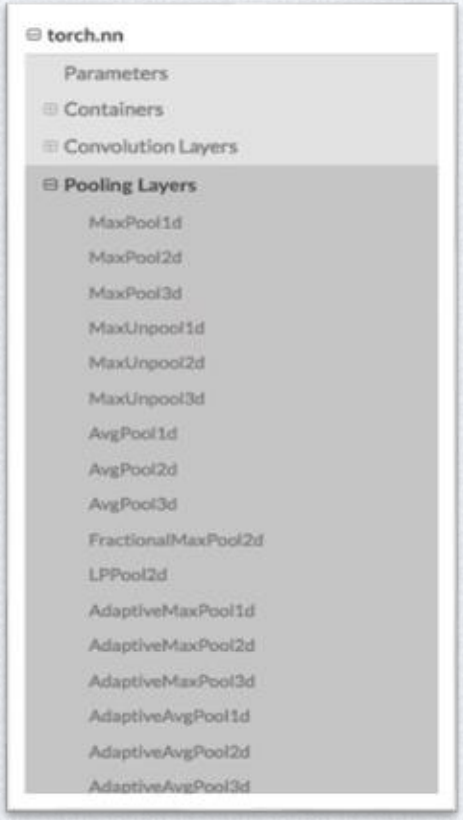


Module



Other Layers:

Dropout,
Linear,
Normalization
Layer



Pytorch: Two levels of Abstraction

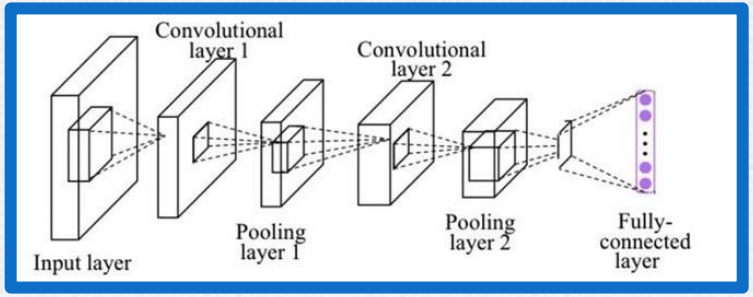
Tensor:

- If **Tensor.requires_grad==False**, it is imperative `ndarray`, but no gradient will be computed
- If **Tensor.requires_grad==True**, it is a node in a computational graph; stores data and gradient

Module:

Neural Network layer(s); store learnable weights.

Module




```
class Net(nn.Module):

    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(1, 10, kernel_size=5)
        self.conv2 = nn.Conv2d(10, 20, kernel_size=5)
        self.mp = nn.MaxPool2d(2)
        self.fc = nn.Linear(320, 10) # 320 -> 10

    def forward(self, x):
        in_size = x.size(0)
        x = F.relu(self.mp(self.conv1(x)))
        x = F.relu(self.mp(self.conv2(x)))
        x = x.view(in_size, -1) # flatten the tensor
        x = self.fc(x)
        return F.log_softmax(x)
```

Define a CNN

- Network class is a neural network defined by the user that inherits from `torch.nn.Module`
- Initialize the basic layer variables in the constructor function `__init__()`.
- Define the `forward()` method to build your computational graph.
- When you call a module, it will automatically call the forward method of the module.

Check the Model Structure

Torchinfo · PyPI

```
from torchinfo import summary

model = Net()
batch_size = 16
summary(model, input_size=(batch_size, 1, 28, 28))

==========================================================================================
Layer (type:depth-idx)                   Output Shape              Param #
==========================================================================================
Net                                      [16, 10]                  --
├─Conv2d: 1-1                            [16, 10, 24, 24]          260
├─MaxPool2d: 1-2                         [16, 10, 12, 12]          --
├─Conv2d: 1-3                            [16, 20, 8, 8]            5,020
├─MaxPool2d: 1-4                         [16, 20, 4, 4]            --
├─Linear: 1-5                            [16, 10]                  3,210
==========================================================================================
Total params: 8,490
Trainable params: 8,490
Non-trainable params: 0
Total mult-adds (M): 7.59
==========================================================================================
Input size (MB): 0.05
Forward/backward pass size (MB): 0.90
Params size (MB): 0.03
Estimated Total Size (MB): 0.99
==========================================================================================
```

Dataset and Dataloader

```
class CustomImageDataset(Dataset):
    def __init__(self, annotations_file, img_dir, transform=None, target_transform=None):
        self.img_labels = pd.read_csv(annotations_file)
        self.img_dir = img_dir
        self.transform = transform
        self.target_transform = target_transform

    def __len__(self):
        return len(self.img_labels)

    def __getitem__(self, idx):
        img_path = os.path.join(self.img_dir, self.img_labels.iloc[idx, 0])
        image = read_image(img_path)
        label = self.img_labels.iloc[idx, 1]
        if self.transform:
            image = self.transform(image)
        if self.target_transform:
            label = self.target_transform(label)
        sample = {"image": image, "label": label}
        return sample
```

Dataset and Dataloader

The `Dataset` retrieves our dataset's features and labels one sample at a time.

While training a model, we typically want to pass samples in mini-batches, reshuffle the data at every epoch to reduce model overfitting, and use Python's `multiprocessing` to speed up data retrieval.

`DataLoader` is an iterable that abstracts this complexity for us in an easy API.

```
from torch.utils.data import DataLoader

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

Define a Loss Function and Optimizer

Input `net.parameters()` to `optim.SGD`, so the gradient descent will be applied to the parameters of the CNN model we defined earlier.

`CrossEntropyLoss()` is also a module.

```
import torch.optim as optim

criterion = nn.CrossEntropyLoss()
optimizer = optim.SGD(net.parameters(), lr=0.001, momentum=0.9)
```

`Adam` optimizer is recommended. Reference to GBC Ch. 8.5

Train a Neural Network

1. Set the model to the training mode.
2. It inform layers such as `Dropout` and `BatchNorm`

```
def train(dataloader, model, loss_fn, optimizer):
    size = len(dataloader.dataset)
    model.train()
    for batch, (X, y) in enumerate(dataloader):
        X, y = X.to(device), y.to(device)

        # Compute prediction error
        pred = model(X)
        loss = loss_fn(pred, y)

        # Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if batch % 100 == 0:
            loss, current = loss.item(), (batch + 1) * len(X)
            print(f"loss: {loss:>7f}  [{current:>5d}/{size:>5d}]")
```

https://stackoverflow.com/questions/51433378/what-does-model-train-do-in-pytorch

Train a Neural Network

1. Iterate the dataloader to get mini-batches of data
2. Shift the tensors to GPU if available

```python
def train(dataloader, model, loss_fn, optimizer):
    size = len(dataloader.dataset)
    model.train()
    for batch, (X, y) in enumerate(dataloader):
        X, y = X.to(device), y.to(device)

        # Compute prediction error
        pred = model(X)
        loss = loss_fn(pred, y)

        # Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if batch % 100 == 0:
            loss, current = loss.item(), (batch + 1) * len(X)
            print(f"loss: {loss:>7f}  [{current:>5d}/{size:>5d}]")
```

Train a Neural Network

1. Equivalent to calling `model.forward(X)`
2. Compute the loss using the loss function

```
def train(dataloader, model, loss_fn, optimizer):
    size = len(dataloader.dataset)
    model.train()
    for batch, (X, y) in enumerate(dataloader):
        X, y = X.to(device), y.to(device)

        # Compute prediction error
        pred = model(X)
        loss = loss_fn(pred, y)

        # Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if batch % 100 == 0:
            loss, current = loss.item(), (batch + 1) * len(X)
            print(f"loss: {loss:>7f}  [{current:>5d}/{size:>5d}]")
```

Train a Neural Network

```python
def train(dataloader, model, loss_fn, optimizer):
    size = len(dataloader.dataset)
    model.train()
    for batch, (X, y) in enumerate(dataloader):
        X, y = X.to(device), y.to(device)

        # Compute prediction error
        pred = model(X)
        loss = loss_fn(pred, y)

        # Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if batch % 100 == 0:
            loss, current = loss.item(), (batch + 1) * len(X)
            print(f"loss: {loss:>7f}  [{current:>5d}/{size:>5d}]")
```

Set the gradients to zero before computing the gradients

https://stackoverflow.com/questions/48001598/why-do-we-need-to-call-zero-grad-in-pytorch

Train a Neural Network

`loss.backward()` calculates all the gradient of loss w.r.t parameters with the help of the computational graph

```python
def train(dataloader, model, loss_fn, optimizer):
    size = len(dataloader.dataset)
    model.train()
    for batch, (X, y) in enumerate(dataloader):
        X, y = X.to(device), y.to(device)

        # Compute prediction error
        pred = model(X)
        loss = loss_fn(pred, y)

        # Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if batch % 100 == 0:
            loss, current = loss.item(), (batch + 1) * len(X)
            print(f"loss: {loss:>7f}  [{current:>5d}/{size:>5d}]")
```

Train a Neural Network

```python
def train(dataloader, model, loss_fn, optimizer):
    size = len(dataloader.dataset)
    model.train()
    for batch, (X, y) in enumerate(dataloader):
        X, y = X.to(device), y.to(device)

        # Compute prediction error
        pred = model(X)
        loss = loss_fn(pred, y)

        # Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if batch % 100 == 0:
            loss, current = loss.item(), (batch + 1) * len(X)
            print(f"loss: {loss:>7f}  [{current:>5d}/{size:>5d}]")
```

1. The `optimizer.step()` updates the model parameters defined optimizer.
2. If SGD without momentum, then it is defined as –

   `ws = ws - lr*ws.grad`

Train a Neural Network

```python
def train(dataloader, model, loss_fn, optimizer):
    size = len(dataloader.dataset)
    model.train()
    for batch, (X, y) in enumerate(dataloader):
        X, y = X.to(device), y.to(device)

        # Compute prediction error
        pred = model(X)
        loss = loss_fn(pred, y)

        # Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if batch % 100 == 0:
            loss, current = loss.item(), (batch + 1) * len(X)
            print(f"loss: {loss:>7f}  [{current:>5d}/{size:>5d}]")
```

`loss.item()` is to convert a `torch.float` type scalar into float

Save and Load the Trained Network

When the training reaches the end or some particular conditions (for example the highest precision in the validation set), we would like to save the current parameters of the model.

For more information, please check:
Saving and Loading Models - PyTorch Tutorials

Save:

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

Load:

```
model = TheModelClass(*args, **kwargs)
model.load_state_dict(torch.load(PATH))
model.eval()
```

Save and Load the Trained Network: Takeaways

- When loading models, use `map_location='cpu'` in most cases to conserve VRAM.
- In distributed training, ensure that checkpoints are saved only on the master process.
- To resume training, *include the optimizer state in the checkpoint*. For inference purposes, omit the optimizer state to reduce storage requirements.

PyTorch Tutorials

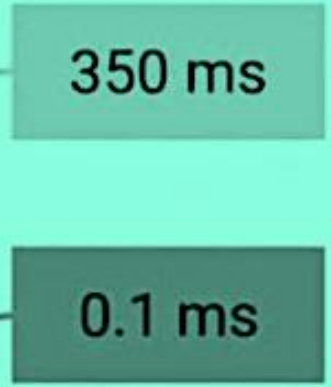
https://pytorch.org/tutorials/beginner/basics/quickstart_tutorial.html

http://cs231n.stanford.edu/slides/2022/discussion_4_pytorch.pdf

https://pytorch.org/tutorials/beginner/blitz/cifar10_tutorial.html

GPU Acceleration

```python
import numpy as np
import torch

# Task: compute matrix multiplication C = AB
d = 3000

# using numpy
A = np.random.rand(d, d).astype(np.float32)
B = np.random.rand(d, d).astype(np.float32)
C = A.dot(B)

# using torch with gpu
A = torch.rand(d, d).cuda()
B = torch.rand(d, d).cuda()
C = torch.mm(A, B)
```



https://transfer.d2.mpi-inf.mpg.de/rs_hetty/hlcv/Pytorch_tutorial.pdf

Using GPU

Bluehive:

BluehiveInfo.pdf

Google Colab: Runtime / change runtime type

```
device = 'cuda' if torch.cuda.is_available() else 'cpu'
```

Move Tensors and Modules to GPU: `.cuda()` or `.to(device)`

Monitor GPU usage: `nvidia-smi` *or* *gpustat · PyPI*

How to prevent **overfitting** when training Deep Neural Networks?

Three Perspectives

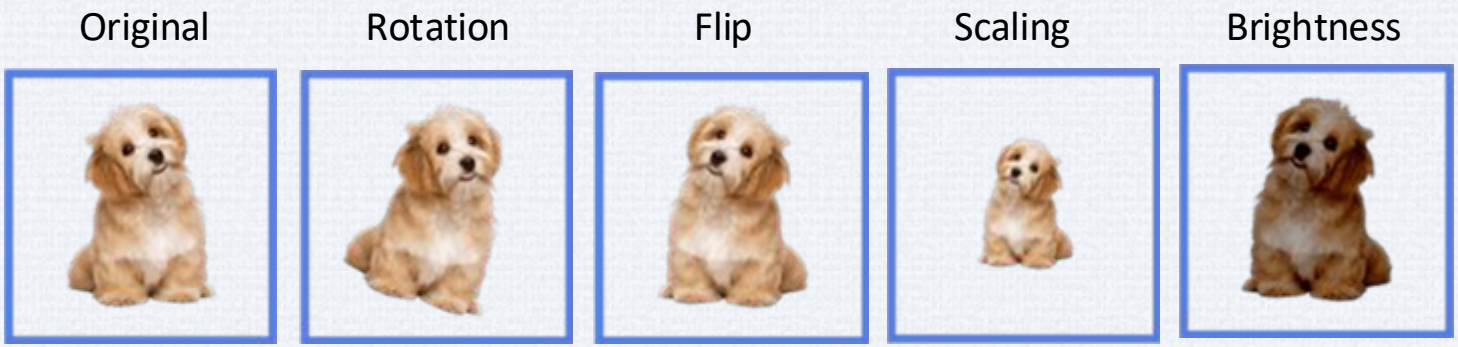
Data

Model

Training strategies

Data Augmentation

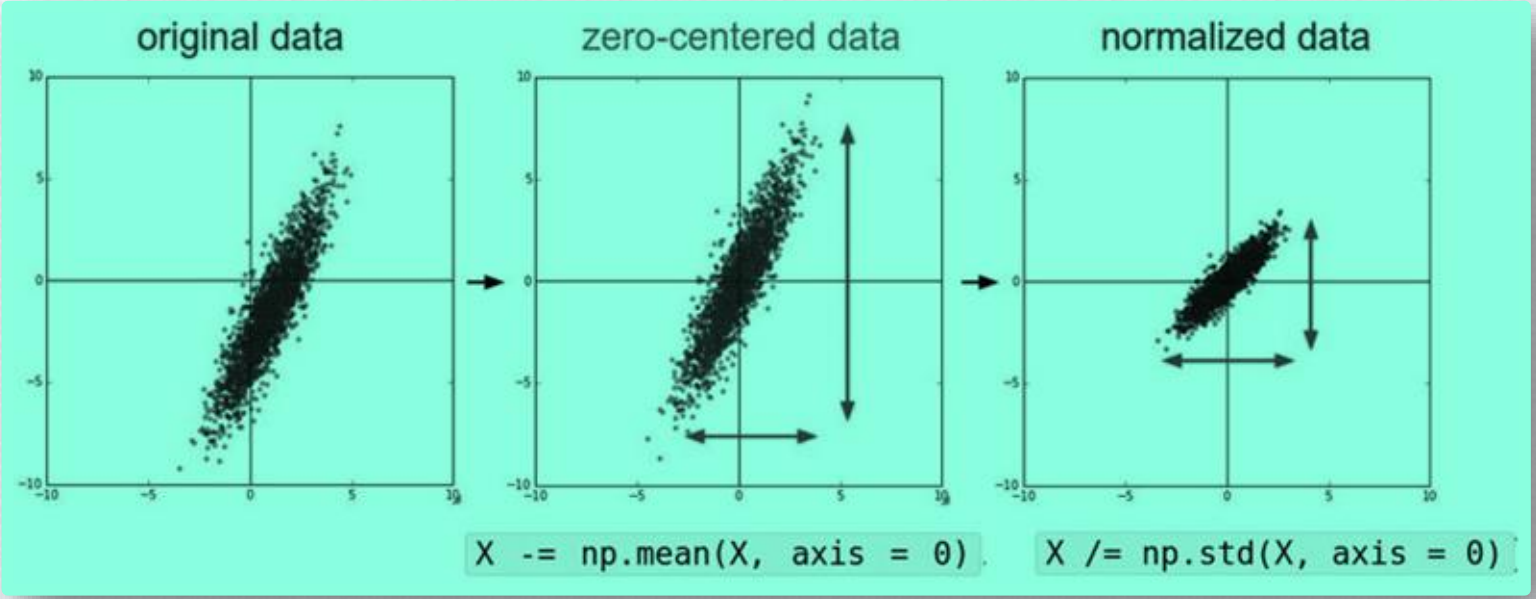
Augment the Training Data



https://www.baeldung.com/cs/ml-data-augmentation

Data Preprocessing

Make the optimization more stable and easier

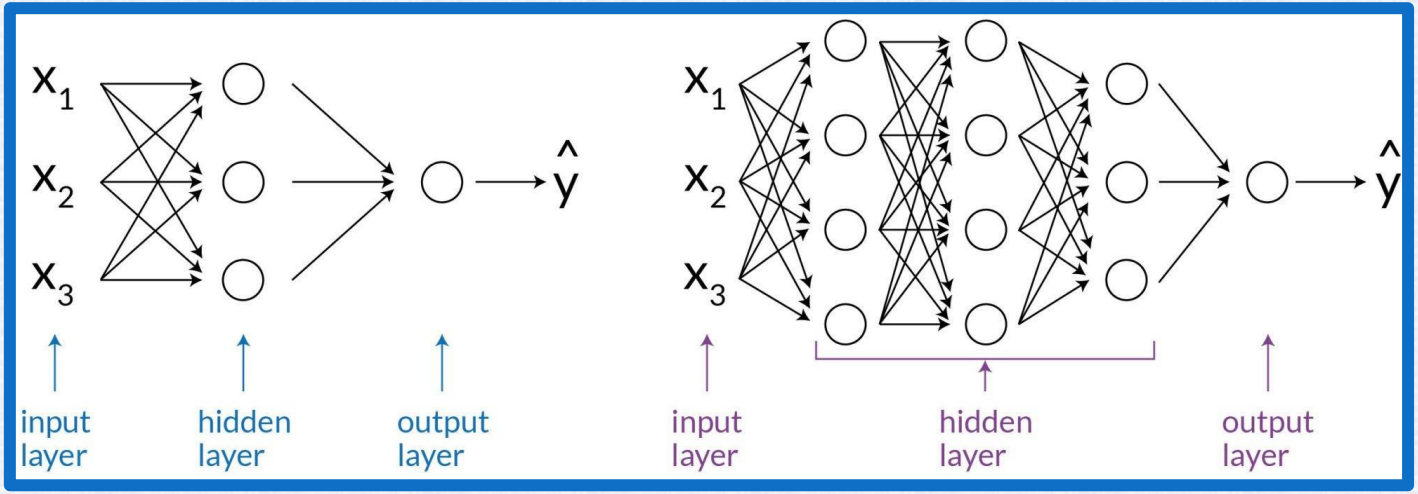


http://cs231n.stanford.edu/slides/2022/lecture_7_ruohan.pdf

Reduce Model Complexity

Reduce the number of layers or neurons in the network

Use simpler activation functions.



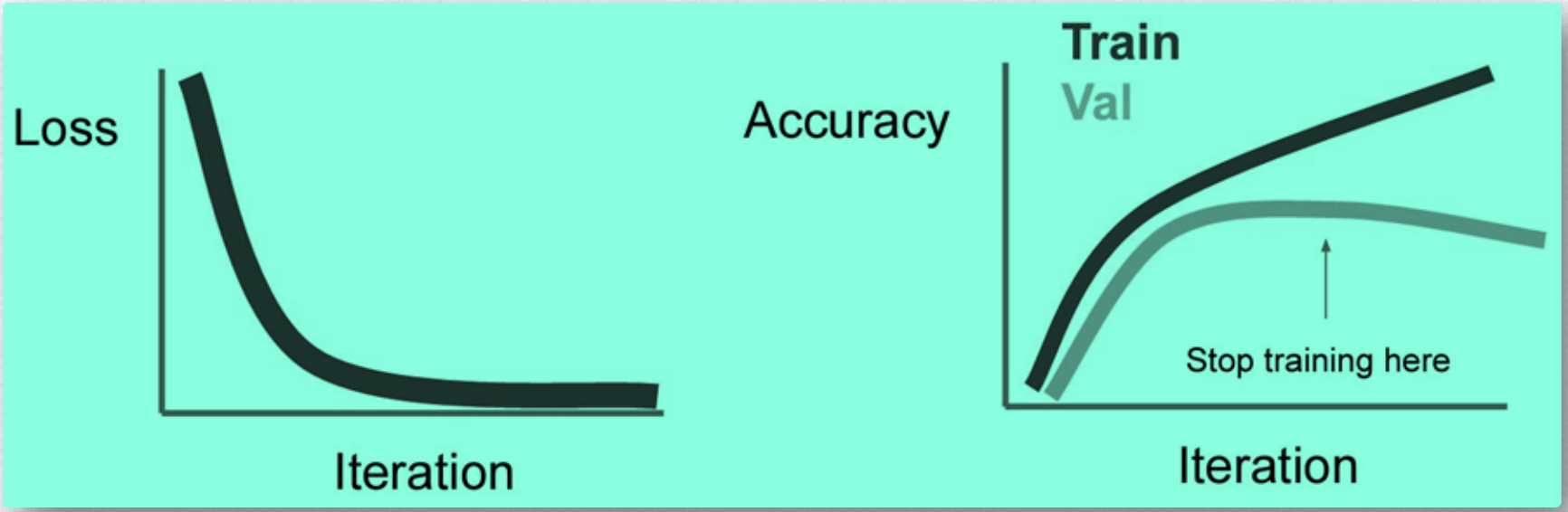
https://www.druva.com/blog/understanding-neural-networks-through-visualization/

Add Regularization term to the Loss Function

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \underbrace{J(\boldsymbol{\theta}; \mathbf{X}, \mathbf{y})}_{\text{(i)}} + \underbrace{\lambda}_{\text{(iii)}} \underbrace{R(\boldsymbol{\theta})}_{\text{(ii)}} .$$

- Fit the training data
- The regularization term R(θ), such as L1 or L2 norm of the weights.
- Hyperparameter λ for controlling the trade-off

Early Stopping



Tools for observing learning curves: *tensorboard, wandb*

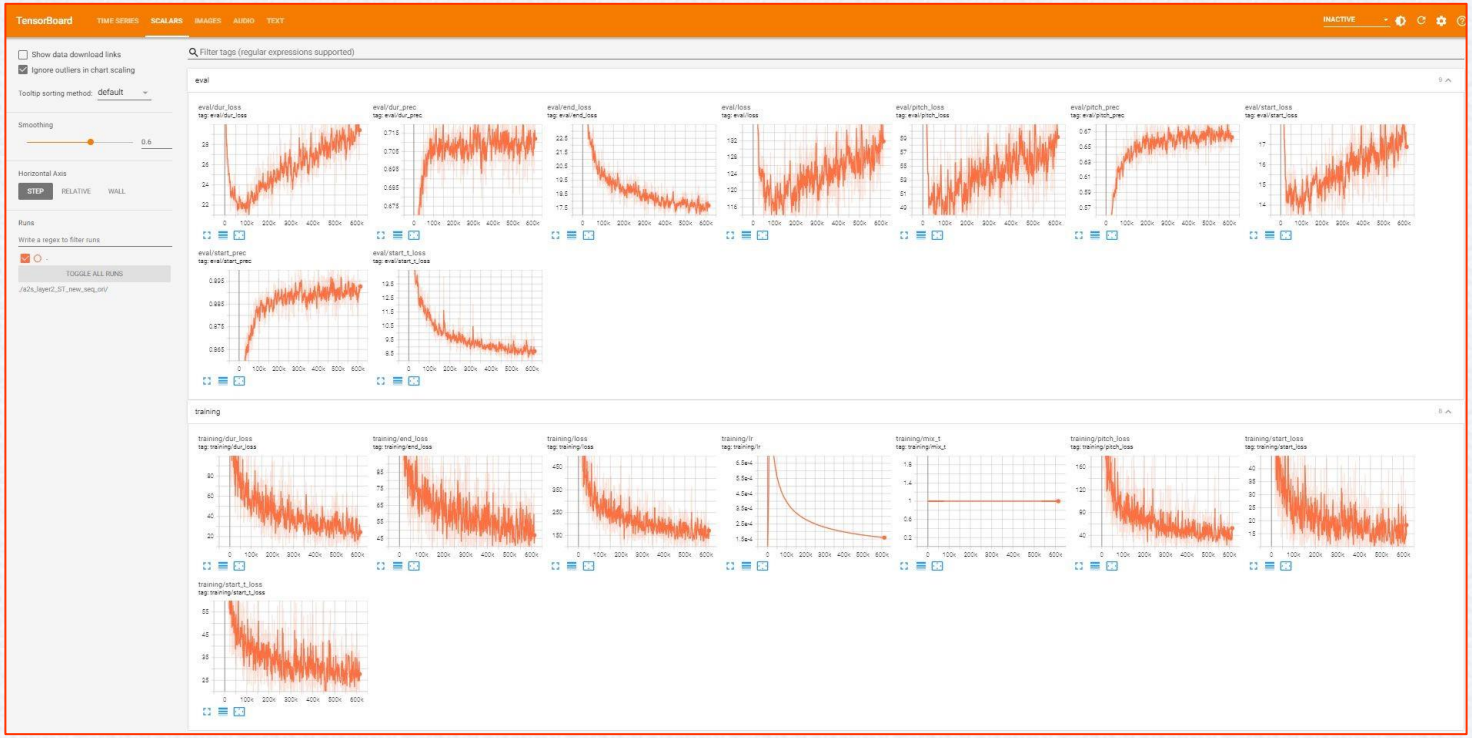
Tensorboard

- Install `tensorboard` with `pip` or `conda`
- Add code in your training script:

```
1 from torch.utils.tensorboard import SummaryWriter
2
3 writer = SummaryWriter("path/to/logdir")
4
5 # record scaler
6 writer.add_scalar("tag/title", x, steps)
7
8 # record picture
9 add_image("tag/title", img_tensor, steps)
10 # shape of img_tensor: (3, H, W)
11
12 # More examples at: https://pytorch.org/docs/stable/tensorboard.html
```

- Run "`tensorboard --logdir path/to/logdir`" with command line and it will provide you a link to access the tensorboard web application. You can also launch it in the jupyter notebook if you need.

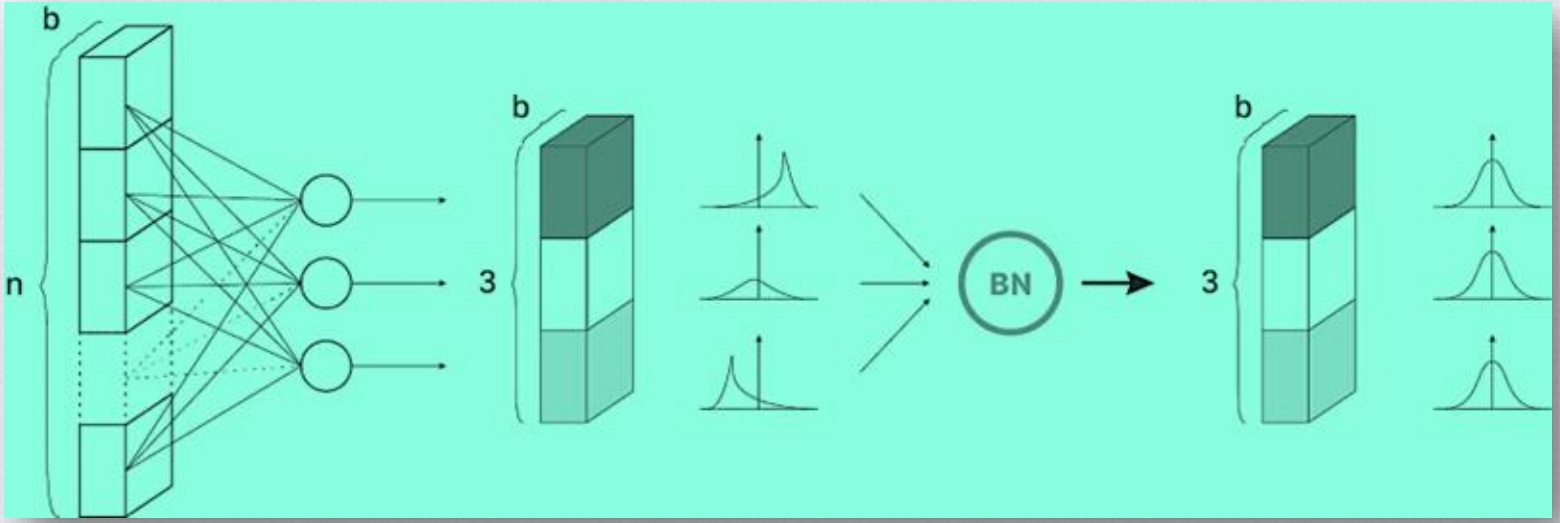
Tensorboard



Batch Normalization

During training, it normalizes the activation values across the batch.

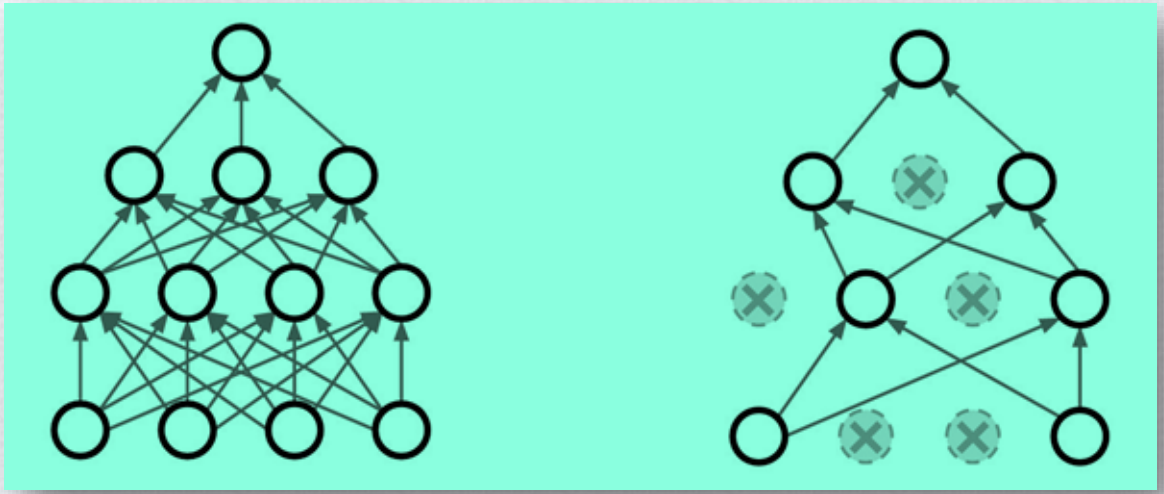
During testing, it uses the mean and variance values determined in the training.



https://towardsdatascience.com/batch-normalization-in-3-levels-of-understanding-14c2da90a338

Dropout

During training, in each forward pass, randomly set some neurons to zero. Probability of dropping is a hyperparameter; 0.5 is common



At test time,neurons are active, but we scale the activations; Multiply by dropout probability

How to choose hyperparameters when training Deep Neural Networks?

Choose Hyperparameters

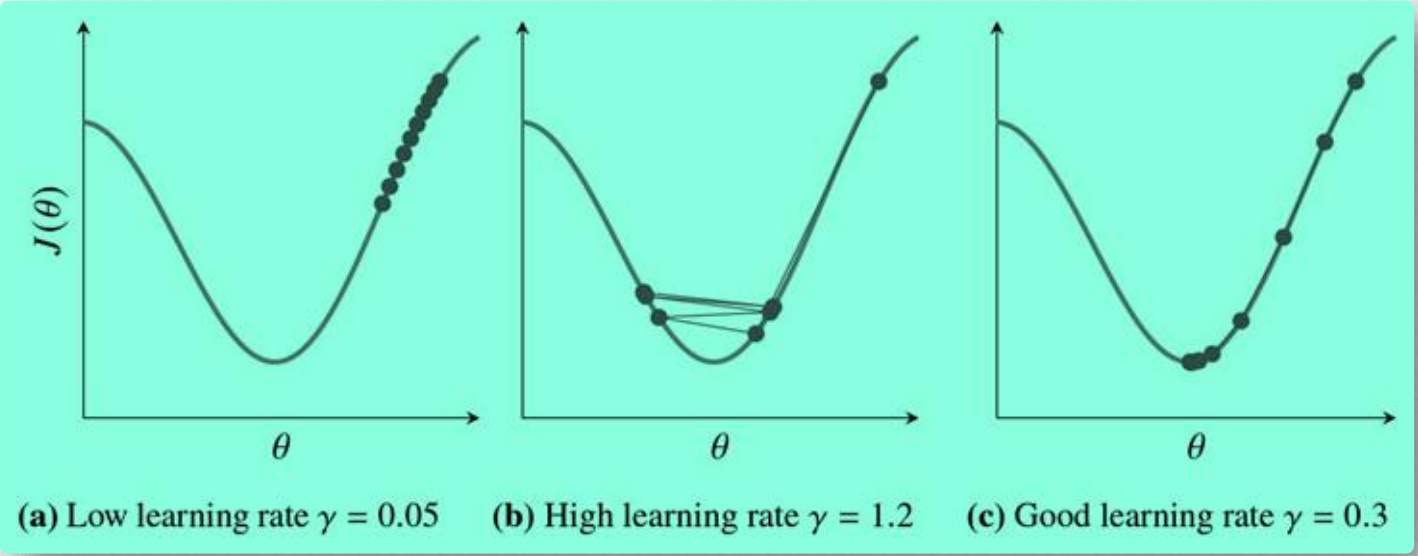
- Choose the batch size according to your device.

- Start with a learning rate that makes training loss go down.

If not, overfit a small batch of samples to debug.

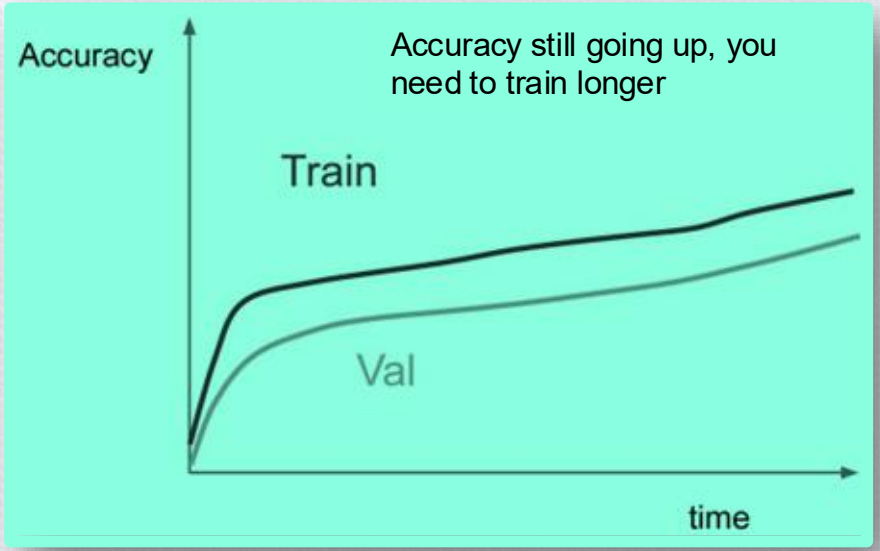
- Look at the learning curves (loss and metrics).

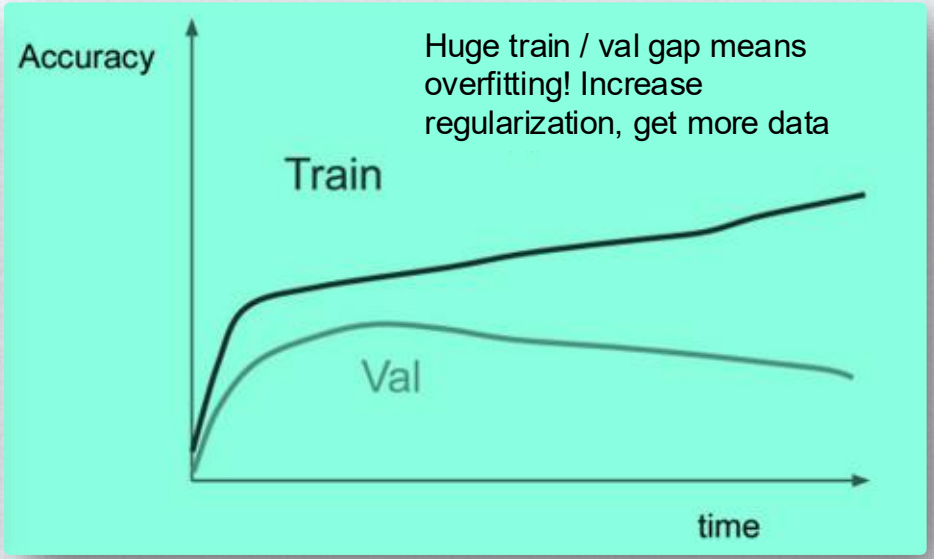
Learning Rate



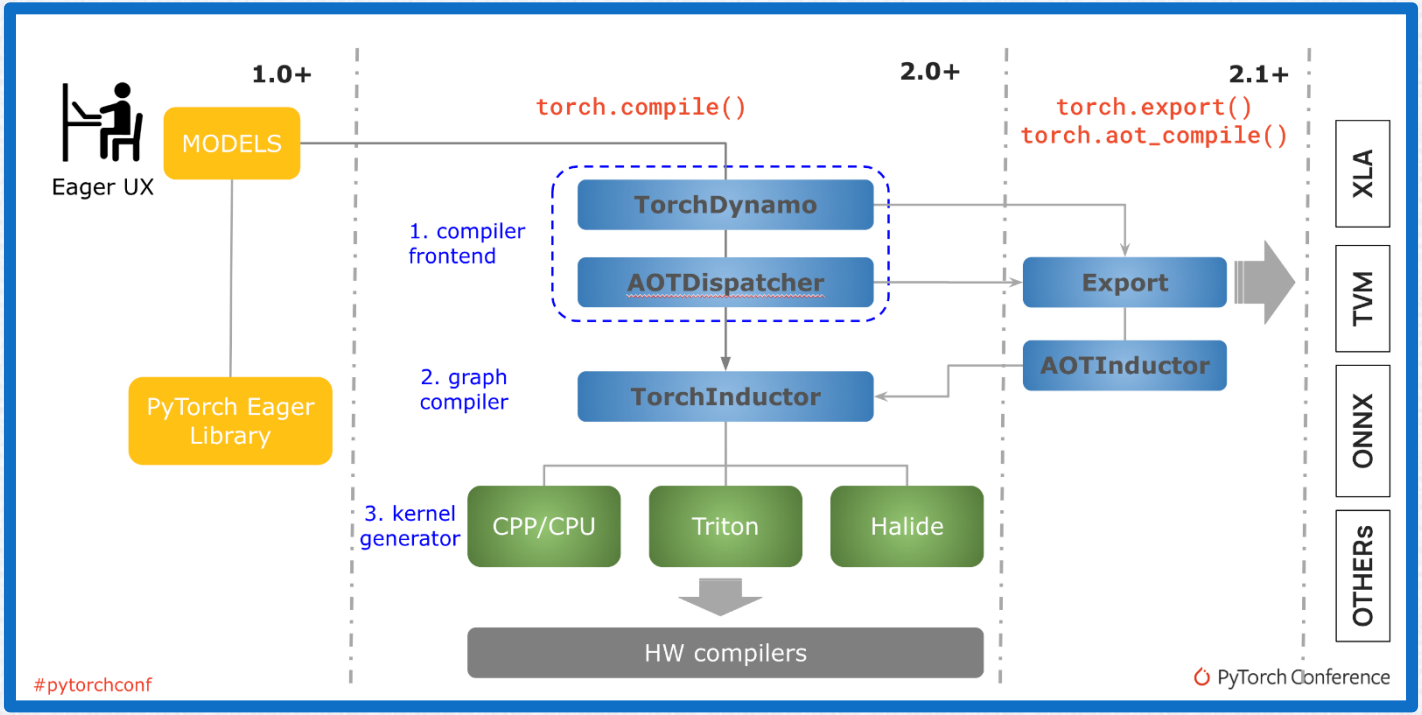
LWLS Figure 5-7

Learning Curves





Training Acceleration: torch.compile

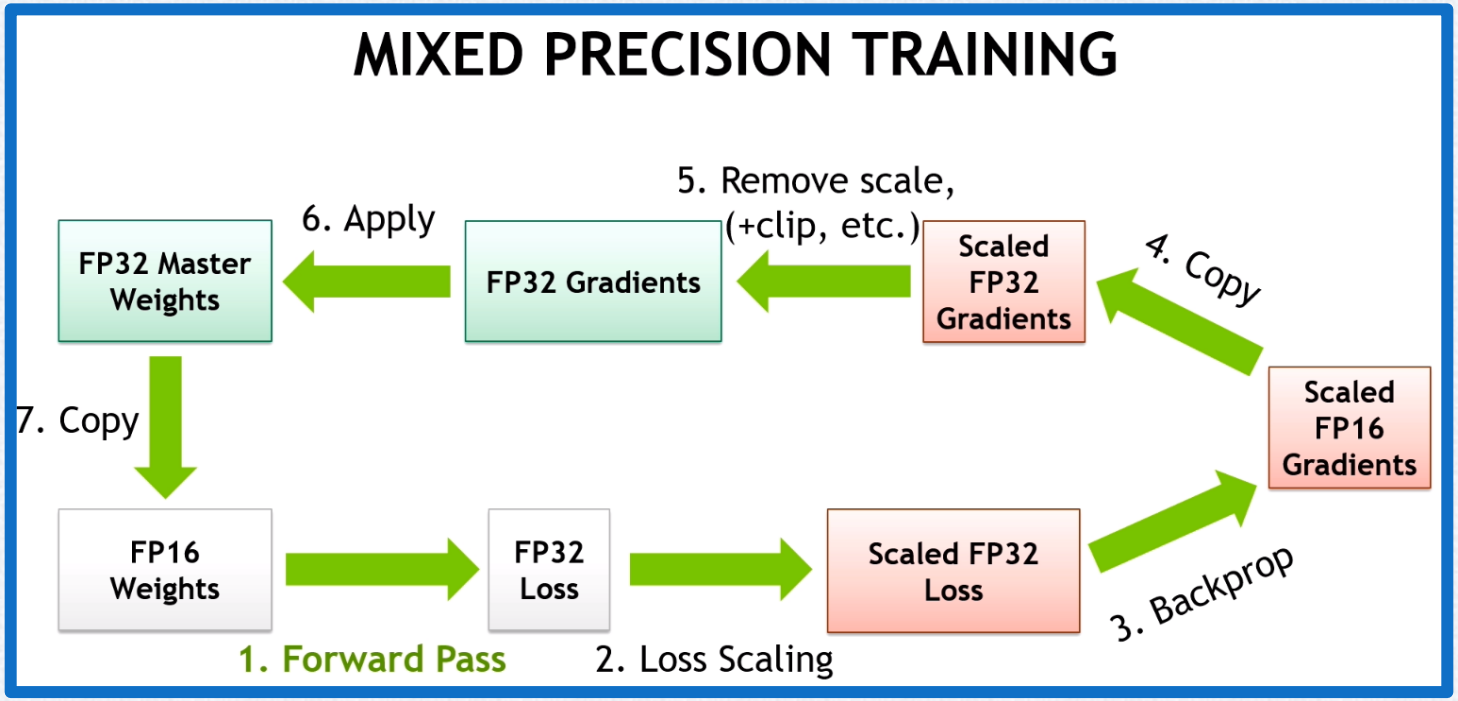


Eager to Static

Training Acceleration: torch.compile

```
def foo(x, y):
    a = torch.sin(x)
    b = torch.cos(y)
    return a + b
opt_foo1 = torch.compile(foo)
print(opt_foo1(torch.randn(10, 10), torch.randn(10, 10)))
```

Training Acceleration: Mixed Precision Training



Training Acceleration: Mixed Precision

```
# Creates model and optimizer in default precision
model = Net().cuda()
optimizer = optim.SGD(model.parameters(), ...)

# Creates a GradScaler once at the beginning of training.
scaler = GradScaler()

for epoch in epochs:
    for input, target in data:
        optimizer.zero_grad()

        # Runs the forward pass with autocasting.
        with autocast(device_type='cuda', dtype=torch.float16):
            output = model(input)
            loss = loss_fn(output, target)

        # Scales loss.  Calls backward() on scaled loss to create scaled gradients.
        # Backward passes under autocast are not recommended.
        # Backward ops run in the same dtype autocast chose for corresponding forward ops.
        scaler.scale(loss).backward()

        # scaler.step() first unscales the gradients of the optimizer's assigned params.
        # If these gradients do not contain infs or NaNs, optimizer.step() is then called,
        # otherwise, optimizer.step() is skipped.
        scaler.step(optimizer)

        # Updates the scale for next iteration.
        scaler.update()
```

Lecture Wrap up

We covered **PyTorch** basics. Practice with homework 6.

Preventing **overfitting** in Deep Neural Networks requires a combination of techniques, including using more data, regularization, early stopping, reducing model complexity, dropout, batch normalization, etc.

Use learning curves to tune **hyperparameters**.