PyTorch Tutorial

May 21, 2025

Part 1: Tensor

dtype

1. torch.bool
2. torch.int32, torch.int64
3. torch.float32, torch.float64
4. torch.complex64

dtype

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2. torch.int32, torch.int64
3. torch.float32, torch.float64
4. torch.complex64

Default floating dtpye is torch.float32, which can be modified by torch.set_default_dtype(torch.float64)

```
x = torch.ones(3, 1)
print (x.dtype)

torch.set_default_dtype(torch.float64)
x = torch.ones(3, 1)
print (x.dtype)

```

device

Data can be stored on CPU, GPU, ...

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```
x = torch.ones(3, 1)

# show where the data is
print (x.device)

device = torch.device('cuda')

# move x to GPU
print (x.to(device))

# define a tensor on GPU
y = torch.ones(3, 1, device=device)

```

Part 2: Neural networks

Feedforward neural networks

$$f(x;\theta) = f_L(f_{L-1}(\cdots(f_1(x))\cdots)) \tag{1}$$

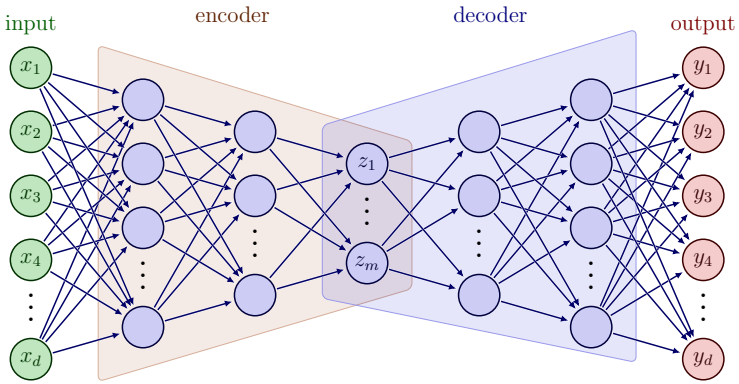
Recursive definition:

$$\begin{aligned} z_0 &= x \\ z_l &= f_l(z_{l-1}) = \varphi(b_l + W_l z_{l-1}), \quad l = 1, 2, \ldots, L-1\,, \\ z_L &= f_L(z_{l-1}) = b_L + W_L z_{L-1}\,. \end{aligned} \tag{2}$$

where

- $z_l, b_l \in \mathbb{R}^{d_l}$, $W_l \in \mathbb{R}^{d_l \times d_{l-1}}$
- φ: activation function
- $\theta = (b_1, b_2, \ldots, b_L, W_1, \ldots, W_L)$

Feedforward neural networks



Building blocks

1. Containers: Sequential, ModuleList
2. nn.Linear
3. Activation: nn.ReLU, nn.Sigmoid, nn.Softplus, nn.Tanh
4. Convolution layers, dropout, recurrent[1]

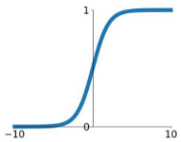
1. `https://docs.pytorch.org/docs/stable/nn.html`

Activation

Activation Functions

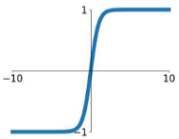
Sigmoid

$\sigma(x) = \frac{1}{1+e^{-x}}$



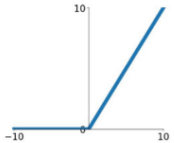
tanh

$\tanh(x)$



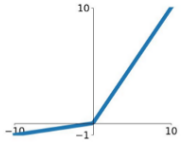
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

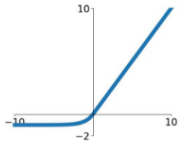


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



torch.nn

```
class MyNet(nn.Module):

    def __init__(self):
        super().__init__()

        self.net = nn.Sequential(
            nn.Linear(1, 3),
            nn.Tanh(),
            nn.Linear(3, 4),
            nn.Tanh(),
            nn.Linear(4, 1),
        )

    def forward(self, x):
        output = self.net(x)
        return output


model = MyNet()
```

torch.nn

A simpler way:

```
model = nn.Sequential(
    nn.Linear(1, 3),
    nn.Tanh(),
    nn.Linear(3, 4),
    nn.Tanh(),
    nn.Linear(4, 1),
)
```

Parameters of the model are PyTorch tensors.

```
# print all (training) parameters of the model
for param in model.parameters():
    print (param)
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Output:

```
Parameter containing:
tensor([[0.1453],
        [0.5682],
        [0.7924]], requires_grad=True)
        ...
```

Model evaluation

Model can be evaluated on mini-batches.

```
x = torch.ones(3, 1)

model(x)
```

Model evaluation

Input tensor and model tensors must have the same dtypes and devices.

```
# both x and tensors in the model have default dtype
↪  torch.float32
x = torch.ones(3, 1)
# works
model(x)

y = torch.ones(3, 1, dtype=torch.float64)
# doesn't work
model(y)
```

Example: positive function

Adding a positive activation to the output layer:

```
class MyNet(nn.Module):

    def __init__(self):
        super().__init__()

        self.net = nn.Sequential(
            nn.Linear(1, 3),
            nn.Tanh(),
            nn.Linear(3, 1),
            nn.Tanh(),
        )

    def forward(self, x):
        output = self.net(x)
        return output

model = MyNet()
```

Example: features as input

Transform input tensor to features before passing to model.

```
class MyNet(nn.Module):

    def __init__(self):
        super().__init__()

        self.net = nn.Sequential(
            nn.Linear(1, 3),
            nn.Tanh(),
            nn.Linear(3, 1),
            nn.Tanh(),
        )

    def forward(self, x):
        output = self.net(torch.sin(x))
        return output

model = MyNet()
```

Part 3: Automatic differentiation

computational graph

Whenever require_grad=True, PyTorch tracks the operations.

```
a = torch.tensor([2.0], requires_grad=True)

s = 0.5 * a ** 2

# requires_grad=True are set for parameters of model
 model = nn.Sequential(
    nn.Linear(1, 3),
    nn.Tanh(),
    nn.Linear(3, 4),
    nn.Tanh(),
    nn.Linear(4, 1),
)
```

computational graph

Backprogration:

```
a = torch.tensor([1.0], requires_grad=True)
b = torch.tensor([2.0])

s = 0.5 * a ** 2 + b

s.backward()
# output: 1 None
print (a.grad, b.grad)
```

computational graph

Gradient of **leaf nodes** will be accumulated in the grad field.

```
a = torch.tensor([1.0], requires_grad=True)

s = 0.5 * a ** 2
s.backward()
# gradient of s
print (a.grad)

s1 = 3 * a
# Gradients of s and s1 will be sumed up.
# To avoid this, write:
# a.grad = None
s1.backward()

print (a.grad)

```

computational graph

Backward propagation will free intermediate values of the graph. To backward twice, add retain_graph=True.

```
a = torch.tensor([1.0], requires_grad=True)

s = 0.5 * a ** 2

# add retain_graph=True to avoid error below
s.backward(retain_graph=True)

s1 = 3 * s
s1.backward()

print (a.grad)

```

computational graph

Avoid gradient computation:

```
a = torch.tensor([1.0], requires_grad=True)

b = torch.tensor([1.5], requires_grad=True)
b.requires_grad = False

s = 0.5 * a ** 2 + b**2
s.backward()
```

computational graph

Detach: remove nodes from computational graph.

```
a = torch.tensor([1.0], requires_grad=True)

b = a
# quadratic in a
s = a * b
s.backward()

b = a.detach()
# linear in a
s = a * b
s.backward()
```

autograd.grad

autograd.grad allows to compute gradients with given tensors.

Example: compute $\int_0^1 |f'(x)|^2 dx$, where $f : \mathbb{R} \to \mathbb{R}$ is the model.

```
x = torch.linspace(0, 1, 101).reshape(-1,1)
  # we need to compute derivative wrt x
x.requires_grad_()

# f
y = model(x)

y_grad_vec = torch.autograd.grad(outputs=y.sum(), inputs=x,
↪  retain_graph=True)[0]

int_val = torch.sum(y_grad_vec**2) * 0.01
```

Part 3: Dataset

different datasets

1. training dataset: training models
2. validation dataset: early stopping
3. test dataset: evaluation of the trained model

dataset splitting

Method 1: torch.utils.data.random_split

```
x = torch.linspace(0, 1, 101).reshape(-1,1)
seed = 42

ratios = [0.8, 0.1, 0.1]

train_data, val_data, test_data =
↪  torch.utils.data.random_split(x, ratios,
↪  generator=torch.Generator().manual_seed(seed))

training_set = x[train_data.indices]
val_set = x[val_data.indices]
test_set = x[test_data.indices]
```

dataset splitting

Method 1: train_test_split from sklearn

```
1 import numpy as np
2 from sklearn.model_selection import train_test_split
3
4 X, y = np.arange(10).reshape((5, 2)), range(5)
5
6 X_train, X_test, y_train, y_test = train_test_split(X, y,
  ↪  test_size=0.33, random_state=42)
7
8 print (X_train.shape, len(y_train))
```

DataLoader

Example 1:

```
1 from torch.utils.data import DataLoader
2
3 x = torch.linspace(0, 1, 101).reshape(-1,1)
4 batch_size = 21
5 data_loader = DataLoader(x, batch_size=batch_size,
  ↪  shuffle=True, drop_last=True)
6
7 for data in data_loader:
8     print (data.shape)
```

DataLoader

Example 2:

```
train_dataset = torchvision.datasets.MNIST(root='./data',
    train=True, transform=transforms.ToTensor(),
    download=True)
test_dataset = torchvision.datasets.MNIST(root='./data',
    train=False, transform=transforms.ToTensor(),
    download=True)

print (train_dataset.data.shape, test_dataset.data.shape)

train_loader = DataLoader(train_dataset, batch_size=1001,
    shuffle=True)
test_loader = DataLoader(test_dataset, batch_size=1001,
    shuffle=True)

for data in test_loader:
    img, label = data
    print (img.shape)
```

Part 3: Training

Optimizer

Optimization objective:

$$\mathcal{L}(\theta) := \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, f(x_n; \theta)).$$

Full gradient: $\nabla_\theta \mathcal{L}(\theta) = \frac{1}{N} \sum_{n=1}^{N} \nabla_\theta \ell(y_n, f(x_n; \theta))$.

SGD:

$$\theta_{t+1} = \theta_t - \frac{\eta_t}{|\mathcal{B}_t|} \sum_{n \in \mathcal{B}_t} \nabla_\theta \ell(y_n, f(x_n; \theta_t))$$

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SGD:

$$\begin{aligned}
\theta_{t+1} =& \theta_t - \frac{\eta_t}{|\mathcal{B}_t|} \sum_{n \in \mathcal{B}_t} \nabla_\theta \ell(y_n, f(x_n; \theta_t)) \\
=& \theta_t - \eta_t \nabla_\theta \mathcal{L}(\theta_t) + \eta_t \left(\nabla_\theta \mathcal{L}(\theta_t) - \frac{1}{|\mathcal{B}_t|} \sum_{n \in \mathcal{B}_t} \nabla_\theta \ell(y_n, f(x_n; \theta_t)) \right) \\
=& \theta_t - \eta_t \nabla_\theta \mathcal{L}(\theta_t) + \eta_t e_t
\end{aligned}$$

Optimizer

SGD:

```
import torch.optim as optim

model = nn.Sequential(nn.Linear(1, 3), nn.Tanh(),
↪  nn.Linear(3, 4))

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

Adam:

```
criterion = nn.MSELoss(reduction='sum')
optimizer = optim.Adam(model.parameters(), lr=0.001)
```

training loop

```
for epoch in range(total_epochs):    # for each epoch

    # loop over all mini-batches
    for data in data_loader:

        y_pred = model(data)
        y = fun(data)

        loss = criterion(y_pred, y)

        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
```