Exercise IV Function Approximation

March 31, 2021

I use this exercise as an opportunity to revise the concepts of pytorch. So before using the modules and classes such as `torch.nn`, `torch.optim`, `Dataset`, `DataLoader` to create and train a neural network, I will build a simple network from scratch and then replace each component with the functionality provided by the mentioned modules, gradually. For this, I am using the tutorial provided in the pytorch documentation here: https://pytorch.org/tutorials/beginner/nn_tutorial.html

0.0.1 Dataset setup

I use the MNIST dataset, which consist of images of digits (between 0 to 9)

[1]:
```
from pathlib import Path
import requests

# setup the path to store the data
DATA_PATH = Path("data")
PATH = DATA_PATH / "mnist"

# create the directory
PATH.mkdir(parents = True, exist_ok = True)

URL = "https://github.com/pytorch/tutorials/raw/master/_static/"
FILENAME = "mnist.pkl.gz"

# if file not exist, download
if not (PATH / FILENAME).exists():
        content = requests.get(URL + FILENAME).content
        (PATH / FILENAME).open("wb").write(content)
```

The data is stored in numpy arrays and pickled. The following block of code will read the file and store it in a varaible.

[2]:
```
import pickle
import gzip

with gzip.open((PATH / FILENAME).as_posix(), "rb") as f:
        ((x_train, y_train), (x_valid, y_valid), _) = pickle.load(f,␣
 ↪encoding="latin-1")
```

[3]:
```
print(x_train.shape)
```

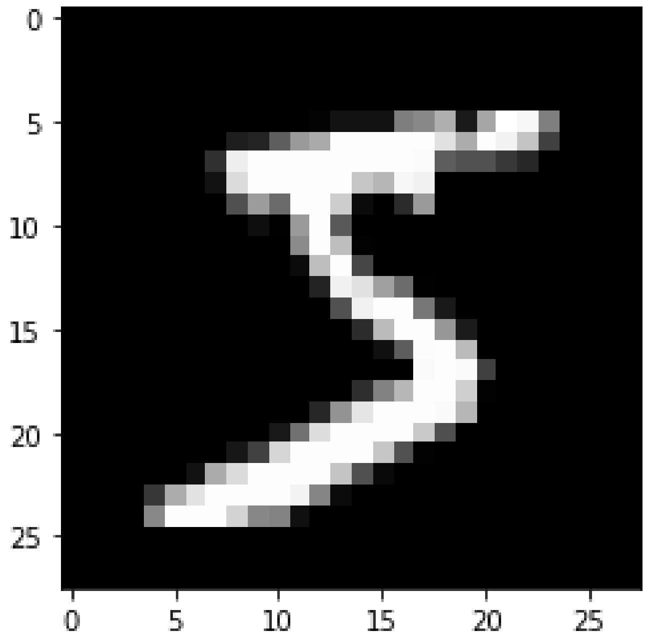
```
(50000, 784)
```

x_train contains 50,000 samples. each sample is a vector of length 784.

[4]:
```
import matplotlib.pyplot as plt
import numpy as np

plt.imshow(x_train[0]. reshape((28,28)), cmap = 'gray')
```

[4]:
```
<matplotlib.image.AxesImage at 0x237daf116d0>
```



pytorch is a replacement to numpy to use the power of a gpu. It uses `torch.tensor` instead of `numpy.array`. So we will convert the data into tensor format.

[5]:
```
import torch

# map numpy array to torch.tensor
x_train, y_train, x_valid, y_valid = map(
    torch.tensor, (x_train, y_train, x_valid, y_valid)
)
# shape of training data
n, c = x_train.shape

print(x_train, y_train)
print(x_train.shape)
print(y_train.min(), y_train.max())
```

```
tensor([[0., 0., 0.,  …, 0., 0., 0.],
        [0., 0., 0.,  …, 0., 0., 0.],
        [0., 0., 0.,  …, 0., 0., 0.],
        …,
        [0., 0., 0.,  …, 0., 0., 0.],
        [0., 0., 0.,  …, 0., 0., 0.],
        [0., 0., 0.,  …, 0., 0., 0.]]) tensor([5, 0, 4,  …, 8, 4, 8])
torch.Size([50000, 784])
tensor(0) tensor(9)
```

0.0.2 NN from scratch

First, we create two tensors for weights and bias. The argument requires_grad = True causes pytorch to record all the oprations doen on the tensor so that it can calculate the gradient during backprop automatically.

[6]:
```
import math
# similar to numpy, generates 2D tensor
weights = torch.randn(784,10)/ math.sqrt(784)
# set requires gradient true
weights.requires_grad_()
# we set requires gradient true while creating the tensor
bias = torch.zeros(10, requires_grad = True)
```

Next, we define our model and activation function. pytorch provides modules for this which will be used later.

[7]:
```
def log_softmax(x):
    return x - x.exp().sum(-1).log().unsqueeze(-1)

# 1 layer network with log_softmax activation
def model(xb):
    return log_softmax(xb @ weights + bias)
```

[8]:
```
# batch size
bs = 64

# example of an forward pass
# minibatch from train set
xb = x_train[0:bs]
# apply our function to batch
preds = model(xb)

print(preds[0], preds.shape)
```

```
tensor([-2.4306, -2.3667, -1.5934, -2.4719, -2.8305, -2.6258, -2.7941, -2.0013,
        -2.2031, -2.3814], grad_fn=<SelectBackward>) torch.Size([64, 10])
```

As we can see, the output is a vector of length 10. Currently, the model is not trained (randomly intialized weights and bias), hence, the output is a gibberish.

We will use neagtive log-liklihood as a loss function.

[9]:
```
def nll(input, target):
    return -input[range(target.shape[0]), target].mean()

loss_func = nll
```

Now, let's check the loss of our model on a minibatch.

[10]:
```
# true value
yb = y_train[0:bs]
print(loss_func(preds, yb))
```

```
tensor(2.4351, grad_fn=<NegBackward>)
```

Accuracy: if a index with the largest value in the output vector matches the target value, the the prediction is correct.

[11]:
```
def accuracy(out, yb):
    preds = torch.argmax(out, dim=1)
    return (preds == yb).float().mean()

print(accuracy(preds, yb))
```

```
tensor(0.0625)
```

0.0.3 training

Process: for each iteration - select a mini-batch of data - use model to make predictions - calculate the loss - `loss.backward()` updates the gradient of the model (weights and bias)

`loss.backward()` adds the gradient to whatever is already stored. So after each batch, we manually set the gradient to zero before the next loop.

[12]:
```
# learning rate
lr = 0.5

epochs = 2 # number of pass through data

for epoch in range(epochs):
    # for each batch (total 782 batches size 64)
    for i in range ((n-1)//bs+1):
        # batch start and end index
        start_i = i*bs
        end_i = start_i +bs
        # current batch
        xb = x_train[start_i:end_i]
        yb = y_train[start_i:end_i]
```

```
        # make prediction
        pred = model(xb)
        # compute loss
        loss = loss_func(pred, yb)

        # compute gradient
        loss.backward()

        # update params and set the gradient to zero
        with torch.no_grad():
            weights -= weights.grad * lr
            bias -= bias.grad * lr
            weights.grad.zero_()
            bias.grad.zero_()
```

That's all. We have created a minimal neural network (actually logistic regression as there is only 1 layer). Next, let's compare the loss before and after training. We expect the loss to decrease.

[13]:
```
print(loss_func(model(xb), yb), accuracy(model(xb), yb))
```

```
tensor(0.0836, grad_fn=<NegBackward>) tensor(1.)
```

0.0.4 use torch modules and library for more cleaner and concise code

nn.functional We can replace our hand written activation and loss function with those from the nn.functional module. This module contains wide variety of loss and activation functions.

[14]:
```
import torch.nn.functional as F

loss_func = F.cross_entropy
```

nn.Module We subclass nn.Module to create a class that holds weights, bias, and a method for forward pass. nn.Module provides a number of attributes and methods useful for downstream tasks.

[15]:
```
from torch import nn

class Mnist_Logistic(nn.Module):
    def __init__(self):
        super().__init__()
        self.weights = nn.Parameter(torch.randn(784,10)/math.sqrt(784))
        self.bias = nn.Parameter(torch.zeros(10))

    def forward(self,xb):
        return xb @ self.weights + self.bias
```

We instantiate the object of our class. The object is callable and executes forward method when called.

[16]:
```
model = Mnist_Logistic()

print(loss_func(model(xb), yb))
```

```
tensor(2.3992, grad_fn=<NllLossBackward>)
```

Previously, we had to update the parameters manually. Now we use `model.parameters()` and `model.zero_grad()` to make those step concise. Also we add the training code inside a fit method.

[17]:
```
def fit():
    for epoch in range(epochs):
        for i in range((n-1)// bs+1):
            start_i = i * bs
            end_i = start_i + bs
            xb = x_train[start_i:end_i]
            yb = y_train[start_i:end_i]
            pred = model(xb)
            loss = loss_func(pred, yb)

            loss.backward()
            with torch.no_grad():
                for p in model.parameters():
                    p -= p.grad*lr
                model.zero_grad()

fit()
```

[18]:
```
# check that our loss has gone down
print(loss_func(model(xb), yb))
```

```
tensor(0.0845, grad_fn=<NllLossBackward>)
```

Next, rather than defining our parameters and network manually, we will use nn.Linear class, which do that for us. pytorch has many predefined layers to simplify the construction of a neural network.

[19]:
```
class Mnist_Logistic(nn.Module):
    def __init__(self):
        super().__init__()
        self.lin = nn.Linear(784, 10)

    def forward(self, xb):
        return self.lin(xb)
```

[20]:
```
# instantiate the model and claculate the loss as before
model = Mnist_Logistic()
print(loss_func(model(xb), yb))
```

```
tensor(2.3474, grad_fn=<NllLossBackward>)
```

[21]:

```python
fit()
print(loss_func(model(xb), yb))
```

```
tensor(0.0817, grad_fn=<NllLossBackward>)
```

torch.optim In our training loop, we manually coded the optimization step, updating one parameter at a time inside the loop. `torch.optim` provides various optimization algorithms such Adam, SGD, etc. We can use .step() method to update parameters.

[22]:

```python
from torch import optim

def fit():
    for epoch in range(epochs):
        for i in range((n - 1) // bs + 1):
            start_i = i * bs
            end_i = start_i + bs
            xb = x_train[start_i:end_i]
            yb = y_train[start_i:end_i]
            pred = model(xb)
            loss = loss_func(pred, yb)

            loss.backward()
            opt.step()
            opt.zero_grad()

# also put model and optimizer in a function
def get_model():
    model = Mnist_Logistic()
    return model, optim.SGD(model.parameters(), lr=lr)

model, opt = get_model()
fit()
print(loss_func(model(xb), yb))
```

```
tensor(0.0825, grad_fn=<NllLossBackward>)
```

Dataset and DataLoader By defining a length and way of indexing, TensorDataset class gives us a way to iterate, index, and slice along the firat dimension of a tensor. This will make it easy to access dependent and independent varaibles in the same line as we train.

[23]:

```python
from torch.utils.data import TensorDataset

train_ds = TensorDataset(x_train, y_train)

# now we can iterate through minibatches in a single line
# xb, yb = train_ds[i*bs : i*bs +bs]
```

```
model, opt = get_model()

for epoch in range(epochs):
    for i in range((n - 1) // bs + 1):
        xb, yb = train_ds[i * bs: i * bs + bs]
        pred = model(xb)
        loss = loss_func(pred, yb)

        loss.backward()
        opt.step()
        opt.zero_grad()

print(loss_func(model(xb), yb))
```

```
tensor(0.0817, grad_fn=<NllLossBackward>)
```

DataLoader manages batches. We crate DataLoader from any Dataset. DataLoader gives us a minibatch automatically, rather than us having to slices the dataset manually.

[24]:
```
from torch.utils.data import DataLoader

train_ds = TensorDataset(x_train, y_train)

# data loader
train_dl = DataLoader(train_ds, batch_size = bs)

# our codes upadate to this
model, opt = get_model()

for epoch in range(epochs):
    # we iterate over batches rather than indexing and slicing
    for xb, yb in train_dl:
        pred = model(xb)
        loss = loss_func(pred, yb)

        loss.backward()
        opt.step()
        opt.zero_grad()

print(loss_func(model(xb), yb))
```

```
tensor(0.0815, grad_fn=<NllLossBackward>)
```

We will now add validation set and assess the performance.

[25]:
```
train_ds = TensorDataset(x_train, y_train)
train_dl = DataLoader(train_ds, batch_size=bs, shuffle=True)

valid_ds = TensorDataset(x_valid, y_valid)
```

```python
valid_dl = DataLoader(valid_ds, batch_size=bs * 2)

model, opt = get_model()

for epoch in range(epochs):
    model.train()
    for xb, yb in train_dl:
        pred = model(xb)
        loss = loss_func(pred, yb)

        loss.backward()
        opt.step()
        opt.zero_grad()

    model.eval()
    with torch.no_grad():
        valid_loss = sum(loss_func(model(xb), yb) for xb, yb in valid_dl)

    print("epoch:", epoch, "loss:" , valid_loss / len(valid_dl))
```

```
epoch: 0 loss: tensor(0.3171)
epoch: 1 loss: tensor(0.2877)
```

We will do some more refactoring for readability of the code. Since we are calculating loss for both training and validation set, we will create a new function loss_batch that computes a loss for one batch. If optimizer is passed, it performs backprop.

[26]:
```python
def loss_batch(model, loss_func, xb, yb, opt=None):
    loss = loss_func(model(xb), yb)

    if opt is not None:
        loss.backward()
        opt.step()
        opt.zero_grad()

    return loss.item(), len(xb)
```

fit perform the training and reports the validation loss.

[27]:
```python
import numpy as np

def fit(epochs, model, loss_func, opt, train_dl, valid_dl):
    for epoch in range(epochs):
        model.train()
        for xb, yb in train_dl:
            loss_batch(model, loss_func, xb, yb, opt)

        model.eval()
```

```
        with torch.no_grad():
            losses, nums = zip(
                *[loss_batch(model, loss_func, xb, yb) for xb, yb in valid_dl]
            )
        val_loss = np.sum(np.multiply(losses, nums)) / np.sum(nums)

        print("epoch:", epoch, "loss:" , valid_loss / len(valid_dl))
```

get_data returns the dataloader for training and validation.

[28]:
```
def get_data(train_ds, valid_ds, bs):
    return (
        DataLoader(train_ds, batch_size=bs, shuffle=True),
        DataLoader(valid_ds, batch_size=bs * 2),
    )
```

Now we can specify the entire process in 3 lines of code

[29]:
```
train_dl, valid_dl = get_data(train_ds, valid_ds, bs)
model, opt = get_model()
fit(epochs, model, loss_func, opt, train_dl, valid_dl)
```

```
epoch: 0 loss: tensor(0.2877)
epoch: 1 loss: tensor(0.2877)
```

0.0.5 Create more advanced NN (CNN)

Now to demonstrate the usage of code, we will create CNN to classify digits using our dataset.

[30]:
```
class Mnist_CNN(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 16, kernel_size=3, stride=2, padding=1)
        self.conv2 = nn.Conv2d(16, 16, kernel_size=3, stride=2, padding=1)
        self.conv3 = nn.Conv2d(16, 10, kernel_size=3, stride=2, padding=1)

    def forward(self, xb):
        xb = xb.view(-1, 1, 28, 28)
        xb = F.relu(self.conv1(xb))
        xb = F.relu(self.conv2(xb))
        xb = F.relu(self.conv3(xb))
        xb = F.avg_pool2d(xb, 4)
        return xb.view(-1, xb.size(1))

lr = 0.1
model = Mnist_CNN()
opt = optim.SGD(model.parameters(), lr=lr, momentum=0.9)
```

```
fit(epochs, model, loss_func, opt, train_dl, valid_dl)
```

```
epoch: 0 loss: tensor(0.2877)
epoch: 1 loss: tensor(0.2877)
```

nn.Sequential Sequential module provides a handy way to create a model. Sequencial object runs each of the modules contained within it in a sequencial manner. We can create a custom layer from a function and use it when defining the network with sequencial.

[31]:
```
# define a custome layer
class Lambda(nn.Module):
    def __init__(self, func):
        super().__init__()
        self.func = func

    def forward(self, x):
        return self.func(x)


def preprocess(x):
    return x.view(-1, 1, 28, 28)

# define a model with Sequential
model = nn.Sequential(
    Lambda(preprocess),
    nn.Conv2d(1, 16, kernel_size=3, stride=2, padding=1),
    nn.ReLU(),
    nn.Conv2d(16, 16, kernel_size=3, stride=2, padding=1),
    nn.ReLU(),
    nn.Conv2d(16, 10, kernel_size=3, stride=2, padding=1),
    nn.ReLU(),
    nn.AvgPool2d(4),
    Lambda(lambda x: x.view(x.size(0), -1)),
)

opt = optim.SGD(model.parameters(), lr=lr, momentum=0.9)

fit(epochs, model, loss_func, opt, train_dl, valid_dl)
```

```
epoch: 0 loss: tensor(0.2877)
epoch: 1 loss: tensor(0.2877)
```

GPU! Finally we can use GPU to train fastera and use .to(dev) method to send tensor to GPU.

[32]:
```
# create the device object
dev = torch.device("cuda") if torch.cuda.is_available() else torch.device("cpu")
```

In the above code, we use preprocessing layer within our network. Rather, we can write a wrapper to the dataloader to do the preprocessing. Thia way we can abstarct our model to use with different shape of datasets.

[33]:
```
def preprocess(x, y):
    return x.view(-1, 1, 28, 28).to(dev), y.to(dev)

class WrappedDataLoader:
    def __init__(self, dl, func):
        self.dl = dl
        self.func = func

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

    def __iter__(self):
        batches = iter(self.dl)
        for b in batches:
            yield (self.func(*b))

train_dl, valid_dl = get_data(train_ds, valid_ds, bs)
train_dl = WrappedDataLoader(train_dl, preprocess)
valid_dl = WrappedDataLoader(valid_dl, preprocess)

model = nn.Sequential(
    nn.Conv2d(1, 16, kernel_size=3, stride=2, padding=1),
    nn.ReLU(),
    nn.Conv2d(16, 16, kernel_size=3, stride=2, padding=1),
    nn.ReLU(),
    nn.Conv2d(16, 10, kernel_size=3, stride=2, padding=1),
    nn.ReLU(),
    nn.AdaptiveAvgPool2d(1),
    Lambda(lambda x: x.view(x.size(0), -1)),
)

model.to(dev)
opt = optim.SGD(model.parameters(), lr=lr, momentum=0.9)

fit(epochs, model, loss_func, opt, train_dl, valid_dl)
```

```
epoch: 0 loss: tensor(0.2877)
epoch: 1 loss: tensor(0.2877)
```

The code shown is the final code that we need to create and train neural network.

stochastic_gradient_descent_example from class.

[34]:
```
# training data (plotted at the end of this file)
train = np.array([[-2,-10], [-1,-5], [0, 0], [1,5], [2,10]])
x_train = torch.Tensor(train[:, 0])
```

```
y_train = torch.Tensor(train[:, 1])
```

[35]:
```
# for stochastic gradient descent, create batches
batch_size = 1

# dataset and dataloader
train_ds = TensorDataset(x_train, y_train)
train_dl = DataLoader(train_ds, batch_size=batch_size, shuffle=True)
```

[36]:
```
import numpy as np

# fit method for training

def loss_batch(model, loss_func, xb, yb, opt=None):
    loss = loss_func(model(xb), yb)

    if opt is not None:
        loss.backward()
        opt.step()
        opt.zero_grad()

    return loss.item(), len(xb)

def fit(epochs, model, loss_func, opt, train_dl):
    for epoch in range(epochs):
        # train the model
        model.train()
        for xb, yb in train_dl:
            loss_batch(model, loss_func, xb, yb, opt)

        # evaluate on the train set
        model.eval()
        with torch.no_grad():
            losses, nums = zip(
                *[loss_batch(model, loss_func, xb, yb) for xb, yb in train_dl]
            )
        val_loss = np.sum(np.multiply(losses, nums)) / np.sum(nums)

        print("epoch:", epoch, "loss:" , valid_loss / len(valid_dl))
```

[37]:
```
# create model
model = nn.Sequential(
    nn.Linear(1,64),
    nn.ReLU(),
    nn.Linear(64,64),
    nn.ReLU(),
    nn.Linear(64, 1)
```

```
)

alpha = 0.001
opt = optim.SGD(model.parameters(), lr=alpha)
loss_func = nn.MSELoss()
epochs = 40

# fit the model
fit(epochs, model, loss_func, opt, train_dl)
```

```
epoch: 0 loss: tensor(0.2877)
epoch: 1 loss: tensor(0.2877)
epoch: 2 loss: tensor(0.2877)
epoch: 3 loss: tensor(0.2877)
epoch: 4 loss: tensor(0.2877)
epoch: 5 loss: tensor(0.2877)
epoch: 6 loss: tensor(0.2877)
epoch: 7 loss: tensor(0.2877)
epoch: 8 loss: tensor(0.2877)
epoch: 9 loss: tensor(0.2877)
epoch: 10 loss: tensor(0.2877)
epoch: 11 loss: tensor(0.2877)
epoch: 12 loss: tensor(0.2877)
epoch: 13 loss: tensor(0.2877)
epoch: 14 loss: tensor(0.2877)
epoch: 15 loss: tensor(0.2877)
epoch: 16 loss: tensor(0.2877)
epoch: 17 loss: tensor(0.2877)
epoch: 18 loss: tensor(0.2877)
epoch: 19 loss: tensor(0.2877)
epoch: 20 loss: tensor(0.2877)
epoch: 21 loss: tensor(0.2877)
epoch: 22 loss: tensor(0.2877)
epoch: 23 loss: tensor(0.2877)
epoch: 24 loss: tensor(0.2877)
epoch: 25 loss: tensor(0.2877)
epoch: 26 loss: tensor(0.2877)
epoch: 27 loss: tensor(0.2877)
epoch: 28 loss: tensor(0.2877)
epoch: 29 loss: tensor(0.2877)
epoch: 30 loss: tensor(0.2877)
epoch: 31 loss: tensor(0.2877)
epoch: 32 loss: tensor(0.2877)
epoch: 33 loss: tensor(0.2877)
epoch: 34 loss: tensor(0.2877)
epoch: 35 loss: tensor(0.2877)
epoch: 36 loss: tensor(0.2877)
```

```
epoch: 37 loss: tensor(0.2877)
epoch: 38 loss: tensor(0.2877)
epoch: 39 loss: tensor(0.2877)
```

[38]:
```python
# test the model
D=np.arange(-2,2,.1).reshape((40,1))
R=model(torch.Tensor(D)).detach().numpy()

from matplotlib import pyplot as plt
plt.plot(x_train,y_train,'gx',D,R,'r-')
```

[38]:
```
[<matplotlib.lines.Line2D at 0x237cbbae4f0>,
 <matplotlib.lines.Line2D at 0x237cbbae5e0>]
```