COMP 691 Assignment 1

Xiang Chen Zhu , Student ID: 40216952

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Note: The Jupyter notebook is attached at the end. There are some hyperlinks that you can click to jump to that specific page. Like this: Jump to Jupyter

1 Problem 1

Exercise 1. *Derive expressions*

Solution.

$$\frac{\partial J}{\partial W_1} = \frac{1}{N}\sum_{i=1}^{N} sign(\hat{y^i} - y^i) * w_2 \odot (1 - \tanh(b_1 + W_1 \cdot x^i)^2) \cdot x^{i^\top}$$

$$\frac{\partial J}{\partial w_2} = \frac{1}{N}\sum_{i=1}^{N} sign(\hat{y^i} - y^i) * \tanh(b_1 + W_1 \cdot x^i)$$

$$\frac{\partial J}{\partial b_1} = \frac{1}{N}\sum_{i=1}^{N} sign(\hat{y^i} - y^i) * w_2 \odot (1 - \tanh(b_1 + W_1 \cdot x^i)^2)$$

$$\frac{\partial J}{\partial b_2} = \frac{1}{N}\sum_{i=1}^{N} sign(\hat{y^i} - y^i)$$

Exercise 2. *Implement in PyTorch*

Solution. See the Jupyter notebook.Jump to Jupyter

Exercise 3. *Train this model on the sklearn California Housing Prices datasets.*

Solution. See the Jupyter notebook.Jump to Jupyter

2 Problem 2

Exercise 4. *Use torch tensors to write a function which computes the Jacobian, using backward mode automatic differentiation.*

Solution. See the Jupyter notebook. Jump to Jupyter

Exercise 5. *Use torch tensors to write a function which computes the Jacobian, using forward mode automatic differentiation.*

Solution. See the Jupyter notebook.Jump to Jupyter

Exercise 6. *Benchmark*

Solution. See the Jupyter notebook. Jump to Jupyter

Exercise 7. *Briefly discuss the theoretical speed comparisons of (b) and (c)*

Solution. Backward results in M^2 multiply operations and forward results in M^3 operations when calculating the gradient. But backward has fewer operations at the cost of needed to run forward pass one time and store intermediate values. Therefore, the size of M has to be sufficiently large to compensate for it. If we simply use the $D = 2, K = 30, P = 10$ values in (a) for (b) and (c), then the difference is not much and in fact forward could be even faster than backward, due backward need to perform a forward pass at first.

However, if we increase the size of M, then the backward will be significantly faster than the forward. With more depth (L) the difference could be drastic. Therefore for deep learning tasks with multiple layers and large matrix sizes, it's more favor to use backward mode due to the computational saving cost.

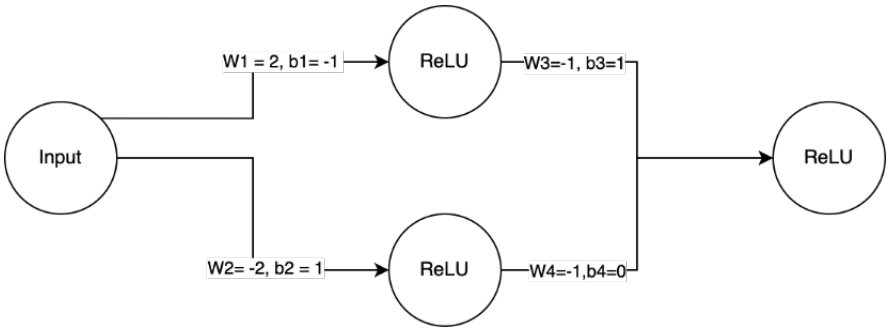
3 Problem 3

Exercise 8. $f(x) = \begin{cases} 2x & 0 \leq x \leq \frac{1}{2} \\ 2(1-x) & \frac{1}{2} \leq x \leq 1 \\ 0 & otherwise \end{cases}$

Solution. The function can be written as

$$\boxed{NN(x) = ReLU\left(w_3 * ReLU\left(w_1 x + b_1\right) + b_3 + w_4 * ReLU\left(w_2 * x + b_2\right) + b_4\right)}$$

which have parameters like the image below:



So essentially it becomes:

$$\boxed{ReLU\left(-ReLU\left(2x-1\right)-ReLU\left(-2x+1\right)+1\right)}$$

The logic for arriving at this expression is as follows. We can easily tell from the function that we want should be positive between $(0, 1)$ and 0 elsewhere. Therefore, naturally, we can come up with two ReLU expressions.

$$ReLU(2x), ReLU(1-2x)$$

However, within $0 < x < 1$ these two functions intersect at $x = \frac{1}{4}$. We would like to let them intersect at $x = 1/2$ since the constraints given diverged that point. Therefore we can shift the first expression to right by 1 unit. Now we have

$$ReLU(2x-1) + ReLU(1-2x)$$

This function is opening upwards with a minimum point at $x = 1/2$. If we flip it over x-axis, we can have it opening downwards. But after flipping , we need to make sure that the maximum point is at $y = 1$ (from the original expression).

To do that we simply add +1 to shift it upward on y-axis. And now the only thing we need to do is to apply ReLU again to make negative value are bounded by 0. So we have it at the end.

$$\boxed{ReLU\left(-ReLU\left(2x-1\right)-ReLU\left(-2x+1\right)+1\right)}$$

We can justify it by testing. When $x < 0$, obviously $-ReLU(2x-1)$ will equal to 0, and $ReLU(-2x+1)$ will be a positive number that is > 1, therefore $1 - ReLU(-2x+1) < 0$, and the whole equation yield 0 after the final ReLU.

When $0 \leq x \leq \frac{1}{2}$, $-ReLU(2x-1)$ will still equal to 0, and $ReLU(-2x+1)$ will be a positive number, therefore $1 - ReLU(-2x+1) = 1 - (-2x+1) = 2x$.

When $\frac{1}{2} \leq x \leq 1$, $-ReLU(2x-1)$ will a negative number ≥ -1, and $ReLU(-2x+1)$ will be 0, therefore $1 - ReLU(2x+1) = 1 - (2x-1) = 2(1-x)$.

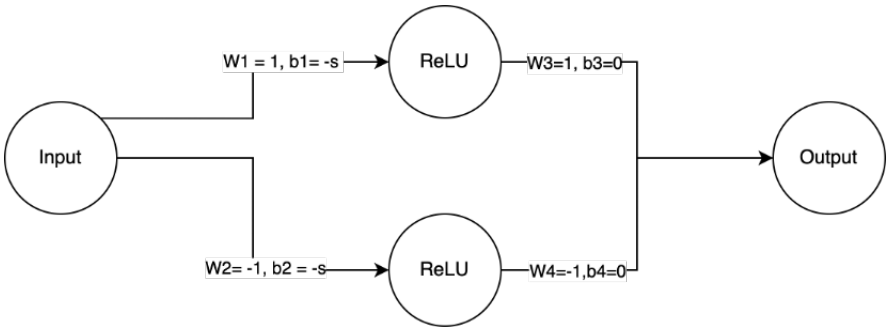
When $x > 1$, $-ReLU(2x-1)$ will a negative number < -1, so $1 - ReLU(2x+1) < 0$, , and the whole equation yield 0 after the final ReLU.

Exercise 9. $f(x) = max(|x| - s, 0) * sign(x)$

Solution. The function can be written as

$$\boxed{NN(x) = w_3 * ReLU\left(w_1 x - b_1\right) + b_3 + w_4 * ReLU\left(w_2 * x + b_2\right) + b_4}$$

which have parameters like the image below:



So essentially it becomes:

$$\boxed{ReLU\,(x-s) - ReLU\,(-x-s)}$$

The thinking process is based on the fact that two key points are $x = s$ and $x = -s$.

When $x < -s$, $-x-s$ is going to be positive so we have $f(x) = (-x-s)*-1 = x + s$

Contrary,When $x > s$, $x - s$ is going to be positive so we have $f(x) = (x - s - 0) * 1 = x - s$

Within $-s$ and s, then we simply have $f(x) = 0$, since $|x| - s \leq 0$

From the above three, since at most one of them will be positive and they are all linear for positive input, just applying ReLU to both should be sufficient. However, in order to convert $-x - s$ to $x + s$ after ReLU it has to be negated again, so we put a minus sign before it. This in the end gives:

$$\boxed{ReLU\,(x-s) - ReLU\,(-x-s)}$$

4 Problem 4

Exercise 10. *First create a nn.module with a variable that defines the number of feedforward layers,*

Solution. See the Jupyter notebook.Jump to Jupyter

Exercise 11. *Write a function to initialize your model and biases to 0.*

Solution. See the Jupyter notebook.Jump to Jupyter

Exercise 12. *Perform this for each of the 4 initializations to obtain 4 curves*

Solution. See the Jupyter notebook. Jump to Jupyter

Exercise 13. *Record the training accuracy and testing accuracy after each epoch and plot them versus epochs.*

Solution. See the Jupyter notebook. Jump to Jupyter

Exercise 14. *Briefly (max 1 paragraph) discuss your findings: how does depth and initialization affect the activations, gradients, and convergence*

Solution. The deeper the layer, the more likely the gradient is affected due to chain rule and hence leads to gradient vanishing or explosion. Poor initialization, with weight too small and too large, could also lead to the same result. This means the activation will become saturated and make the network impossible to learn. As for the convergence, if the network is too shallow then the complexity of the data could not be captured, but with deeper networks, gradient vanishing/explosion may cause it to not converge. Appropriate weight initialization is needed for efficient convergence. Generally, the should be a balance and Xavier's initialization seems to give a good result.

5 Problem 5

Exercise 15. *Find the expression of the gradient and minimizer of the loss*

Solution. We have $\frac{1}{2}\|Xw-y\|^2 = \frac{1}{2}(Xw-y)^T(Xw-y) = \frac{1}{2}(w^TX^T-y^T)(Xw-y) =$

$$\frac{w^TX^TXw - w^TX^Ty - y^TXw + y^Ty}{2}$$

Since X^TX is symmetric ($(X^TX)^T = X^T(X^T)^T$), therefore the gradient of above in respective to w is

$$\nabla w\mathcal{L}(X,w,y) = \frac{1}{2}(2X^TXw - X^Ty - (y^TX)^T - 0)$$

$$= \frac{1}{2}(2X^TXw - 2X^Ty)$$

$$= X^T(Xw-y)$$

If we take the second derivative we have X^TX which is positive definite, therefore this function is convex. To minimize this, we need to set the gradient to 0, hence:

$$X^TXw - X^Ty = 0$$

where we have

$$argmin_w\mathcal{L}(X,w,y) = (X^TX)^{-1}X^Ty$$

Exercise 16. *Take w_0 as the initialization for gradient descent with step size α and show an expression for the first and second iterates w_1 and w_2 only in terms of α, w_0, X, y*

Solution.

$$w_1 = w_0 - \alpha X^T(Xw_0 - y)$$

$$w_2 = w_0 - \alpha X^T(Xw_0 - y) - \alpha X^T(X(w_0 - \alpha X^T(Xw_0 - y)) - y)$$

In the context of matrix, the identity matrix I is the equivalent of 1 in scalar.

So we have

$$w_1 = (I - \alpha X^T X)w_0 + \alpha X^T y$$

$$w_2 = w_0 - \alpha X^T X w_0 + \alpha X^T y - \alpha X^T X w_0 + (\alpha X^T X)^2 w_0 - \alpha X^T X \alpha X^T y + \alpha X^T y$$

$$= w_0 - 2\alpha X^T X w_0 + (\alpha X^T X)^2 w_0 + (I - \alpha X^T X)\alpha X^T y + \alpha X^T y$$

$$= (I - \alpha X^T X)^2 w_0 + (I - \alpha X^T X)\alpha X^T y + \alpha X^T y$$

Exercise 17. *Generalize this to show an expression for w_k*

Solution. Using the same steps as in (b) we have

$$w_3 = (I - \alpha X^T X)^3 w_0 + (I - \alpha X^T X)^2 \alpha X^T y + (I - \alpha X^T X)\alpha X^T y + \alpha X^T y$$

Obviously, we have a pattern here. The idea is to prove it using mathematical induction. The base case k=1 is already proved in (b). I will assume that the equation is true for some k. That is,

$$w_k = (I - \alpha X^T X)^k w_0 + \alpha \sum_{i=0}^{k-1} (I - \alpha X^T X)^i X^T y$$

We want to show that the equation is also true for k+1, i.e.,

$$w_{k+1} = (I - \alpha X^T X)^{k+1} w_0 + \alpha \sum_{i=0}^{k} (I - \alpha X^T X)^i X^T y$$

To derive w_{k+1}, we can use the same update rule as before, but with w_k instead of w_0. That is,

$$w_{k+1} = w_k - \alpha \nabla J(w_k)$$

$$w_{k+1} = (I - \alpha X^T X)w_k + \alpha X^T y$$

Substituting w_k using the assumption, we get

$$w_{k+1} = (I - \alpha X^T X)((I - \alpha X^T X)^k w_0 + \alpha \sum_{i=0}^{k-1} (I - \alpha X^T X)^i X^T y) + \alpha X^T y$$

$$w_{k+1} = (I - \alpha X^T X)^{k+1} w_0 + \alpha \sum_{i=0}^{k} (I - \alpha X^T X)^i X^T y$$

Therefore, the equation is true for k+1.

By the principle of mathematical induction, the equation is true for all iterations k.

So the generalized expression is :

$$w_k = (I - \alpha X^T X)^k w_0 + \alpha \sum_{i=0}^{k-1} (I - \alpha X^T X)^i X^T y$$

Exercise 18. *Using the above show that gradient descent converges to the minimum in (a).*

Solution. We already have a few assumptions in (a), namely,

Assumptions on $X^T X$:

$X^T X$ is positive definite, which implies that all its eigenvalues are positive. X has full column rank, which implies that the columns of X are linearly independent. This ensures that $X^T X$ is invertible.

We will make some assumptions for the step size,

Assumptions on α:

$0 < \alpha < \frac{2}{\lambda_{\max}}$, where $\lambda_{\max}$ is the maximum eigenvalue of $X^T X$. This will make the eigenvalues of $I - \alpha X^T X$ are less than 1 in magnitude.

Now we can evaluate w_k, since the magnitude is always less than 1, it implies that $(I - \alpha X^T X)^k$ approaches the zero matrix as k approaches infinity.

Therefore, the first term:

$$(I - \alpha X^T X)^{\infty} w_0 = 0 * w_0 = 0$$

For the second term, we can write:

$$\begin{aligned}
\lim_{k\to\infty} \alpha \sum_{i=0}^{k-1} (I - \alpha X^T X)^i X^T y &= \alpha \sum_{i=0}^{\infty} (I - \alpha X^T X)^i X^T y \\
&= \alpha (I - (I - \alpha X^T X))^{-1} X^T y \\
&= \alpha (\alpha X^T X)^{-1} X^T y \\
&= (X^T X)^{-1} X^T y,
\end{aligned}$$

where we have used the formula for the sum of an infinite geometric series and the fact that $(I - \alpha X^T X)$ is invertible since $I - \alpha X^T X$ is positive definite.

Thus, the iterative update rule converges to:

$$w_{\infty} = 0 + (X^T X)^{-1} X^T y = (X^T X)^{-1} X^T y$$

But from (a) we already have :

$$argmin_w \mathcal{L}(X, w, y) = (X^T X)^{-1} X^T y$$

Therefore, w_{∞} is the solution of w for $argmin_w \mathcal{L}$, and we have proved gradient descent converges to the minimum in (a).

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1 Question 1

1.0.1 Exercise 1.(b)

[ ]:
```
#1-hidden layer neural network y=w2^T*tanh(w1*x+b1)+b2
#W1: 20 *10
#W2: 1 * 20

import numpy as np
import matplotlib.pyplot as plt
import math
import random
import time
import torch

#generate data
device = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")

h_1 = 20
h_2 = 1
param_dict = {"W1": torch.randn(h_1,10,device=device,requires_grad=True),
              "b1":torch.randn(h_1,1,device=device,requires_grad=True),
              "W2":torch.randn(h_1,h_2,device=device,requires_grad=True),
              "b2":torch.randn(1, device=device,requires_grad=True)}

#generate data
x = torch.randn(100,10,1,device=device)
y = torch.randn(100,1,1,device=device)


def my_nn(x,param_dict):

    x = x.clone().detach().requires_grad_(True)
    x = torch.tanh(param_dict["W1"]@x+param_dict["b1"])
    x = param_dict["W2"].T@x+param_dict["b2"]
    return x

def my_MAE(y_hat,y):
```

```
    # abs value
    return torch.mean(torch.abs(y_hat-y))

def my_loss_grad(y_hat,y):
    return torch.sign(y_hat-y)

def my_nn_grad(x,y_hat,y,param_dict):

    x = x.clone().detach().requires_grad_(True)
    y_hat = y_hat.clone().detach().requires_grad_(True)
    y = y.clone().detach().requires_grad_(True)

    grad_dict = {}
    mlg = my_loss_grad(y_hat,y)
    grad_dict["b2"] = torch.mean(mlg)
    # my_loss_grad(y_hat,y) is 100*1*1
    # torch.tanh(param_dict["W1"]@x+param_dict["b1"]) is 100*20*1
    pre_w2 = mlg * torch.tanh(param_dict["W1"]@x+param_dict["b1"])
    grad_dict["W2"] = torch.mean(pre_w2,dim=0)
    pre_b1 = mlg * param_dict["W2"] * (1-torch.
 ↪tanh(param_dict["W1"]@x+param_dict["b1"])**2)
    grad_dict["b1"] = torch.mean(pre_b1,dim=0)
    pre_w1 = pre_b1 @ x.permute(0,2,1)
    grad_dict["W1"] = torch.mean(pre_w1,dim=0)

    return grad_dict

def torch_grad_check(x,y,param_dict,eps=1e-6):
    # check my_nn_grad and torch.autograd.grad
    print("Floating point error tolerance is: ", eps)
    y_hat = my_nn(x,param_dict)
    #backwards
    loss = my_MAE(y_hat,y)
    loss.backward()
    grad_dict = my_nn_grad(x,y_hat,y,param_dict)
    for key in param_dict.keys():
        #use torch.linalg.norm to compare if smaller than eps
        print ("Key is: ", key)
        #print ("My grad is: ", grad_dict[key])
        #print ("Torch grad is: ", param_dict[key].grad)
        diff = torch.linalg.norm(grad_dict[key]-param_dict[key].grad)
        print ("Difference is: ", diff)
        #assert diff < eps, print error message if failed, print success␣
 ↪message if passed
        assert diff < eps, "error in "+key
        print("Success in "+key)
```

```
#check my_nn_grad and torch.autograd
torch_grad_check(x,y,param_dict)
```

```
Floating point error tolerance is:  1e-06
Key is:  W1
Difference is:  tensor(1.0802e-07, device='cuda:0',
grad_fn=<LinalgVectorNormBackward0>)
Success in W1
Key is:  b1
Difference is:  tensor(2.3591e-08, device='cuda:0',
grad_fn=<LinalgVectorNormBackward0>)
Success in b1
Key is:  W2
Difference is:  tensor(9.8421e-08, device='cuda:0',
grad_fn=<LinalgVectorNormBackward0>)
Success in W2
Key is:  b2
Difference is:  tensor(0., device='cuda:0', grad_fn=<LinalgVectorNormBackward0>)
Success in b2
```

1.0.2 Exercise 1.(c)

[ ]:
```
# Train this model on the sklearn California Housing Prices datasets
# https://scikit-learn.org/stable/modules/generated/sklearn.datasets.
  ↪fetch_california_housing.html#sklearn.datasets.fetch_california_housing

import scipy
import sklearn
import sklearn.datasets
import sklearn.linear_model
from torch.utils import data


# Generate a random California housing dataset
# half of the data is used for training, the other half for testing
# the data is normalized to have zero mean and unit variance
scaler = sklearn.preprocessing.StandardScaler()
X_train, X_test, y_train, y_test = sklearn.model_selection.train_test_split(
    scaler.fit_transform(sklearn.datasets.fetch_california_housing().data),
    sklearn.datasets.fetch_california_housing().target,
    test_size=0.5,
    random_state=42)
```

```
train_batch_size = 64
test_batch_size = 64

# dataloader to gpu
train_dataset = data.TensorDataset(torch.tensor(X_train,device=device,␣
 ↪dtype=torch.float32), torch.tensor(y_train,device=device, dtype=torch.
 ↪float32))
train_loader = data.DataLoader(train_dataset, batch_size=train_batch_size,␣
 ↪shuffle=True)
test_dataset = data.TensorDataset(torch.tensor(X_test,device=device,␣
 ↪dtype=torch.float32), torch.tensor(y_test,device=device, dtype=torch.
 ↪float32))
test_loader = data.DataLoader(test_dataset, batch_size=test_batch_size,␣
 ↪shuffle=True)

#validation set from training set
train_dataset, val_dataset = torch.utils.data.random_split(train_dataset,␣
 ↪[int(0.8*len(train_dataset)), int(0.2*len(train_dataset))])
val_loader = data.DataLoader(val_dataset, batch_size=test_batch_size,␣
 ↪shuffle=True)



# convenient xavier initialization, taking an existing dictionary of parameters

def xavier_init(param_dict):
    for key in param_dict.keys():
        if "W" in key:
            torch.nn.init.xavier_uniform_(param_dict[key])
        else:
            torch.nn.init.zeros_(param_dict[key])
        param_dict[key].requires_grad_(True)
    return param_dict

num_epochs = 40
optimizer = torch.optim.Adam(param_dict.values(), lr=0.001)
lr_scehudler = torch.optim.lr_scheduler.ReduceLROnPlateau(optimizer,␣
 ↪mode='min', factor=0.5, patience=5, verbose=True)
loss_fn = torch.nn.MSELoss()


#change w1 to 20*8 instead of 20*10
param_dict["W1"] = torch.randn(h_1,8,device=device,requires_grad=True)
param_dict = xavier_init(param_dict)
```

```
train_loss_per_epoch = []
val_loss_per_epoch = []
test_loss_per_epoch = []

for epoch in range(num_epochs):
    train_loss = 0
    for batch_idx, (x, y) in enumerate(train_loader):
        y_hat = my_nn(x.T,param_dict)
        y_hat = y_hat.squeeze()
        loss = loss_fn(y_hat,y)
        train_loss += loss.item()
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
    train_loss_per_epoch.append(train_loss/len(train_loader))

    #validation
    val_loss = 0
    for batch_idx, (x, y) in enumerate(val_loader):
        y_hat = my_nn(x.T,param_dict)
        y_hat = y_hat.squeeze()
        loss = loss_fn(y_hat,y)
        val_loss += loss.item()
    val_loss_per_epoch.append(val_loss/len(val_loader))

    #test
    test_loss = 0
    for batch_idx, (x, y) in enumerate(test_loader):
        y_hat = my_nn(x.T,param_dict)
        y_hat = y_hat.squeeze()
        loss = loss_fn(y_hat,y)
        test_loss += loss.item()
    test_loss_per_epoch.append(test_loss/len(test_loader))

    lr_scehudler.step(val_loss_per_epoch[-1])

    print("Epoch: ", epoch+1, "Train loss: ", train_loss_per_epoch[-1], "Val␣
 ↪loss: ", val_loss_per_epoch[-1], "Test loss: ", test_loss_per_epoch[-1])
```

```
Epoch:  1 Train loss:  5.044032322035895 Val loss:  3.3316544691721597 Test
loss:  3.393525270768154
Epoch:  2 Train loss:  2.5859341290262012 Val loss:  1.9377626036152695 Test
loss:  1.9524018433358934
Epoch:  3 Train loss:  1.721601414091793 Val loss:  1.5419075886408489 Test
loss:  1.4871438531963914
Epoch:  4 Train loss:  1.3943074684084198 Val loss:  1.2730701330936316 Test
loss:  1.2506829032927385
Epoch:  5 Train loss:  1.197239801471616 Val loss:  1.115936729041013 Test loss:
```

```
1.09769755307539
Epoch:  6 Train loss:  1.0572793358637962 Val loss:  0.9786306204217853 Test
loss:  0.9740997012014743
Epoch:  7 Train loss:  0.9532213448374359 Val loss:  0.8838369701847886 Test
loss:  0.8931483902313091
Epoch:  8 Train loss:  0.879164864803538 Val loss:  0.8152112274458914 Test
loss:  0.8267838559400889
Epoch:  9 Train loss:  0.8241120387374619 Val loss:  0.7637008609193744 Test
loss:  0.7833703031510483
Epoch:  10 Train loss:  0.7845521986852457 Val loss:  0.7297153779954622 Test
loss:  0.7470582377763442
Epoch:  11 Train loss:  0.7528036900876481 Val loss:  0.7253795257120421 Test
loss:  0.7179016147130801
Epoch:  12 Train loss:  0.7261243872804406 Val loss:  0.6736350890361902 Test
loss:  0.7003690690538029
Epoch:  13 Train loss:  0.7043016736890063 Val loss:  0.6553660956296053 Test
loss:  0.6786355808561231
Epoch:  14 Train loss:  0.6842405130097895 Val loss:  0.6433809038364526 Test
loss:  0.6633080869545172
Epoch:  15 Train loss:  0.6673020146511219 Val loss:  0.6208234637072592 Test
loss:  0.6473549278797927
Epoch:  16 Train loss:  0.6518398451584356 Val loss:  0.6257883617372224 Test
loss:  0.6334221640854706
Epoch:  17 Train loss:  0.6373407068075957 Val loss:  0.6025128427780035 Test
loss:  0.6211050255798999
Epoch:  18 Train loss:  0.6267520095463153 Val loss:  0.5792950581420552 Test
loss:  0.6134037903429549
Epoch:  19 Train loss:  0.6121738332289236 Val loss:  0.5672783535538297 Test
loss:  0.5998080964257688
Epoch:  20 Train loss:  0.6039698449549852 Val loss:  0.5628748201962673 Test
loss:  0.5916449381613437
Epoch:  21 Train loss:  0.5899881072986273 Val loss:  0.5591041689569299 Test
loss:  0.5856422231889066
Epoch:  22 Train loss:  0.5826923085583581 Val loss:  0.5524021495472301 Test
loss:  0.5753879381550683
Epoch:  23 Train loss:  0.5767295936375488 Val loss:  0.54508622397076 Test
loss:  0.5705345502974074
Epoch:  24 Train loss:  0.5666191531920138 Val loss:  0.5307529532548153 Test
loss:  0.5618704901433286
Epoch:  25 Train loss:  0.5597873111197977 Val loss:  0.5259086300026287 Test
loss:  0.5563819309075674
Epoch:  26 Train loss:  0.554042245870755 Val loss:  0.5206093580433817 Test
loss:  0.5521462962583259
Epoch:  27 Train loss:  0.5501569836963842 Val loss:  0.508394720879468 Test
loss:  0.5492178904421535
Epoch:  28 Train loss:  0.5428346321906572 Val loss:  0.5212305377830159 Test
loss:  0.5424251720125293
Epoch:  29 Train loss:  0.5377390726848885 Val loss:  0.5135678242553364 Test
```

```
loss:  0.537404578960972
Epoch:  30 Train loss:  0.5349510317599332 Val loss:  0.5021451169794257 Test
loss:  0.5358283481112233
Epoch:  31 Train loss:  0.5309245376675217 Val loss:  0.4959628970334024 Test
loss:  0.5323892357172789
Epoch:  32 Train loss:  0.5266576563870465 Val loss:  0.48921683882222033 Test
loss:  0.5283976944140446
Epoch:  33 Train loss:  0.5225555409251907 Val loss:  0.4931635901783452 Test
loss:  0.5227267550833431
Epoch:  34 Train loss:  0.5180010208745062 Val loss:  0.48791271538445447 Test
loss:  0.5207540957648077
Epoch:  35 Train loss:  0.5149259470679142 Val loss:  0.48354241251945496 Test
loss:  0.5174984735103301
Epoch:  36 Train loss:  0.5131255129789128 Val loss:  0.4836010418154977 Test
loss:  0.5138383341240295
Epoch:  37 Train loss:  0.5124582295064573 Val loss:  0.4761627876397335 Test
loss:  0.5123441249684051
Epoch:  38 Train loss:  0.5067326539644489 Val loss:  0.4771790450269526 Test
loss:  0.5125919190453895
Epoch:  39 Train loss:  0.5053969733876946 Val loss:  0.47334257851947437 Test
loss:  0.5084010419654258
Epoch:  40 Train loss:  0.503074386421545 Val loss:  0.4950639352653966 Test
loss:  0.5070931996092384
```

2 Question 2

2.0.1 Exercise 2.(a)

[ ]:
```python
def generate_dict(L,D,K,P):
    param_dict = {}
    param_dict["W1"] = torch.randn(K,D,device=device)
    for i in range(2,L+1):
        param_dict["W"+str(i)] = torch.randn(K,K,device=device)
    param_dict["WF"] = torch.randn(P,K,device=device)
    return param_dict

def my_nn_2a(x,L,param_dict):
    x = param_dict["W1"]@x
    for i in range(2,L+1):
        x = param_dict["W"+str(i)]@torch.tanh(x)
    x = param_dict["WF"]@torch.tanh(x)
    return x

# backward automatic differentiation from scratch
# using the chain rule

def my_backward_2a(x,L,param_dict):
```

```
    P = param_dict["WF"].shape[0]
    D = x.shape[0]
    #forward pass
    x = x.clone().detach().requires_grad_(True)
    x = param_dict["W1"]@x
    tanh_outputs =[x]
    for i in range(2,L+1):
        x = param_dict["W"+str(i)]@torch.tanh(x)
        tanh_outputs.append(x)
    x = param_dict["WF"]@torch.tanh(x)
    #backward pass for jacobian
    df_intermediate = torch.diag(1-torch.tanh(tanh_outputs[-1])**2)
    df_intermediate = param_dict["WF"]@df_intermediate
    for i in range(L,1,-1):
        df_intermediate = df_intermediate@ param_dict["W"+str(i)]@torch.
 ↪diag(1-torch.tanh(tanh_outputs[i-2])**2)
    df_intermediate = df_intermediate@param_dict["W1"]
    #copy df_intermediate to df_dx
    return df_intermediate




epsilon = 1e-2



D = 2
K= 30
P = 10
L = 10
param_dict = generate_dict(L,D,K,P)

start = time.time()
for i in range(1000):
    test = torch.randn(D,device=device,requires_grad=True)
    my_J = my_backward_2a(test,L,param_dict)
    J_autograd = torch.autograd.functional.jacobian(lambda x:␣
 ↪my_nn_2a(x,L,param_dict),test,create_graph=True,strategy="reverse-mode")
    #assert, print two jacobians if they are not equal
    assert torch.allclose(my_J,J_autograd,atol=epsilon), print(my_J,J_autograd)
    #Get time taken
end = time.time()
print("Time taken for 1000 iterations: ", end-start)
print ("Jacobian is correct")
```

```
Time taken for 1000 iterations:  9.11955213546753
Jacobian is correct
```

2.0.2 Exercise 2.(b)

[ ]:
```python
def my_forward_2b(x,L,param_dict):
    x = param_dict["W1"]@x
    df_dx = param_dict["W1"]
    for i in range(2,L+1):
        x = torch.tanh(x)
        #foward automatic differentiation
        df_intermediate = torch.diag(1-x**2)
        df_dx = param_dict["W"+str(i)]@df_intermediate@df_dx
        x = param_dict["W"+str(i)]@x
    x = torch.tanh(x)
    df_intermediate = torch.diag(1-x**2)
    df_dx = param_dict["WF"]@df_intermediate@df_dx
    x = param_dict["WF"]@x
    return df_dx

param_dict = generate_dict(L,D,K,P)

start = time.time()
for i in range(1000):
    test_2b = torch.randn(D,device=device,requires_grad=True)
    my_J_2b = my_forward_2b(test_2b,L,param_dict)
    J_autograd_2b = torch.autograd.functional.jacobian(lambda x:␣
 ↪my_nn_2a(x,L,param_dict),test_2b, strategy="forward-mode", vectorize=True)
    #assert, print two jacobians if they are not equal
    assert torch.allclose(my_J_2b,J_autograd_2b,atol=epsilon),␣
 ↪print(my_J_2b,J_autograd_2b)
end = time.time()
print("Time taken for 1000 iterations: ", end-start)
print ("Jacobian is correct")
```

```
Time taken for 1000 iterations:  4.200482368469238
Jacobian is correct
```

2.0.3 Exercise 2(c)

[ ]:
```
#Run on GPU
device = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")
print("Running on GPU: ", torch.cuda.is_available())

test_l = [3,5,10]

D= 1000
K = 1000
P =1

test = torch.randn(D,device=device,requires_grad=True)



print("""When D,K,P are large (1000,1000,1), the reverse mode is faster than␣
 ↪the forward mode.""")

for L in test_l:
    print("L = ", L)
    param_dict = generate_dict(L,D,K,P)

    start = time.time()
    for i in range(1000):
        my_J = my_backward_2a(test,L,param_dict)
    end = time.time()
    print ("Time taken for 1000 iterations of backward with L = ", L, " is ",␣
 ↪time.time()-start)
    start = time.time()
    for i in range(1000):
        my_J_2b = my_forward_2b(test,L,param_dict)
    end = time.time()
    print ("Time taken for 1000 iterations of forward with L =  ", L, " is ",␣
 ↪time.time()-start)
```

```
Running on GPU:  True
When D,K,P are large (1000,1000,1), the reverse mode is faster than the forward
mode.
L =  3
Time taken for 1000 iterations of backward with L =  3  is  0.5629339218139648
Time taken for 1000 iterations of forward with L =  3  is  0.7463889122009277
L =  5
Time taken for 1000 iterations of backward with L =  5  is  0.8709812164306641
Time taken for 1000 iterations of forward with L =  5  is  1.5786635875701904
L =  10
Time taken for 1000 iterations of backward with L =  10  is  1.6397125720977783
```

```
Time taken for 1000 iterations of forward with L =   10  is  3.675320863723755
```

[ ]:
```python
#Run on CPU
device = "cpu"
print("Running on CPU:")

test_l = [3,5,10]

D=1000
P=1
K=1000

test= torch.randn(D,device=device,requires_grad=True)


print("""When D,K,P are large (1000,1000,1), the reverse mode is faster than␣
 ↪the forward mode.""")



for L in test_l:
    print("L = ", L)
    param_dict = generate_dict(L,D,K,P)
    start = time.time()
    for i in range(1000):
        my_J = my_backward_2a(test,L,param_dict)
    end = time.time()
    print ("Time taken for 1000 iterations of backward with L = ", L, " is ",␣
 ↪(end-start))
    start = time.time()
    for i in range(1000):
        my_J_2b = my_forward_2b(test,L,param_dict)
    end = time.time()
    print ("Time taken for 1000 iterations of forward with L =  ", L, " is ",␣
 ↪(end-start))
```

```
Running on CPU:
When D,K,P are large (1000,1000,1), the reverse mode is faster than the forward
mode.
L =  3
Time taken for 1000 iterations of backward with L =  3  is  3.24117112159729
Time taken for 1000 iterations of forward with L =  3  is  21.133321046829224
L =  5
Time taken for 1000 iterations of backward with L =  5  is  5.777544736862183
Time taken for 1000 iterations of forward with L =  5  is  41.2066969871521
L =  10
Time taken for 1000 iterations of backward with L =  10  is  11.320931434631348
```

```
Time taken for 1000 iterations of forward with L =   10  is  91.34891438484192
```

3 Question 4

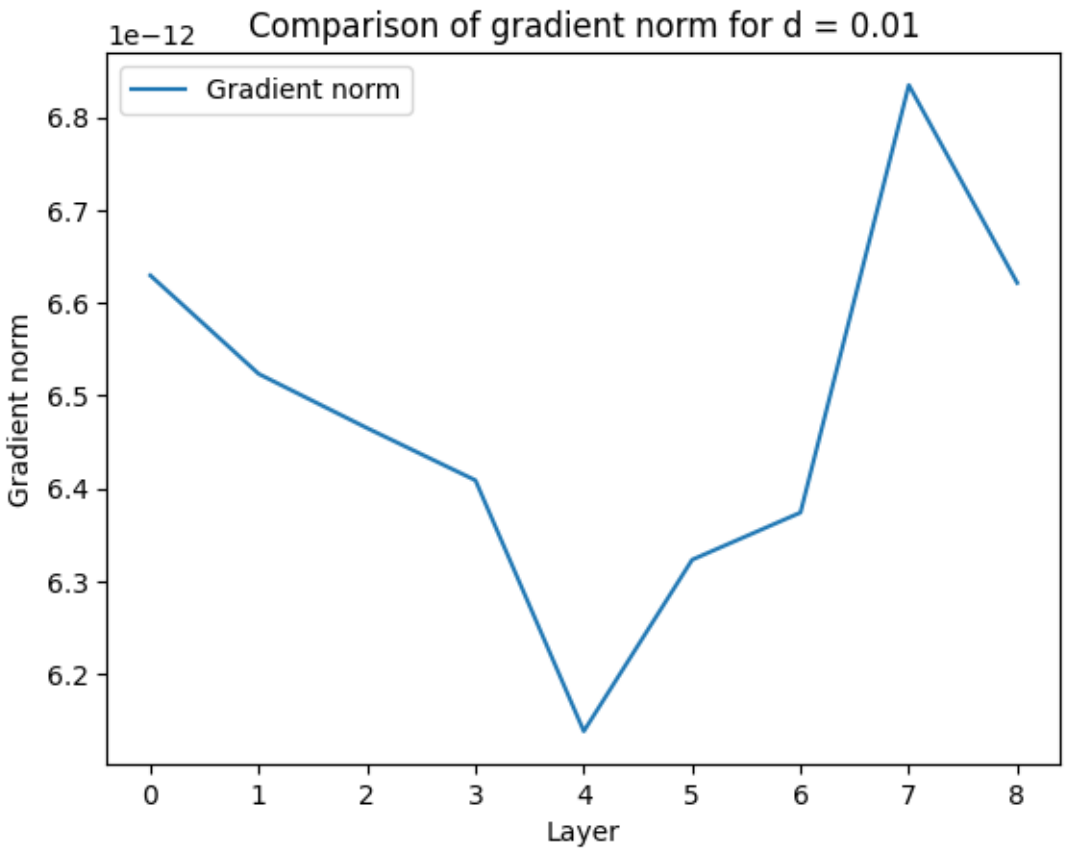
3.0.1 Exercise 4a) & 4b)

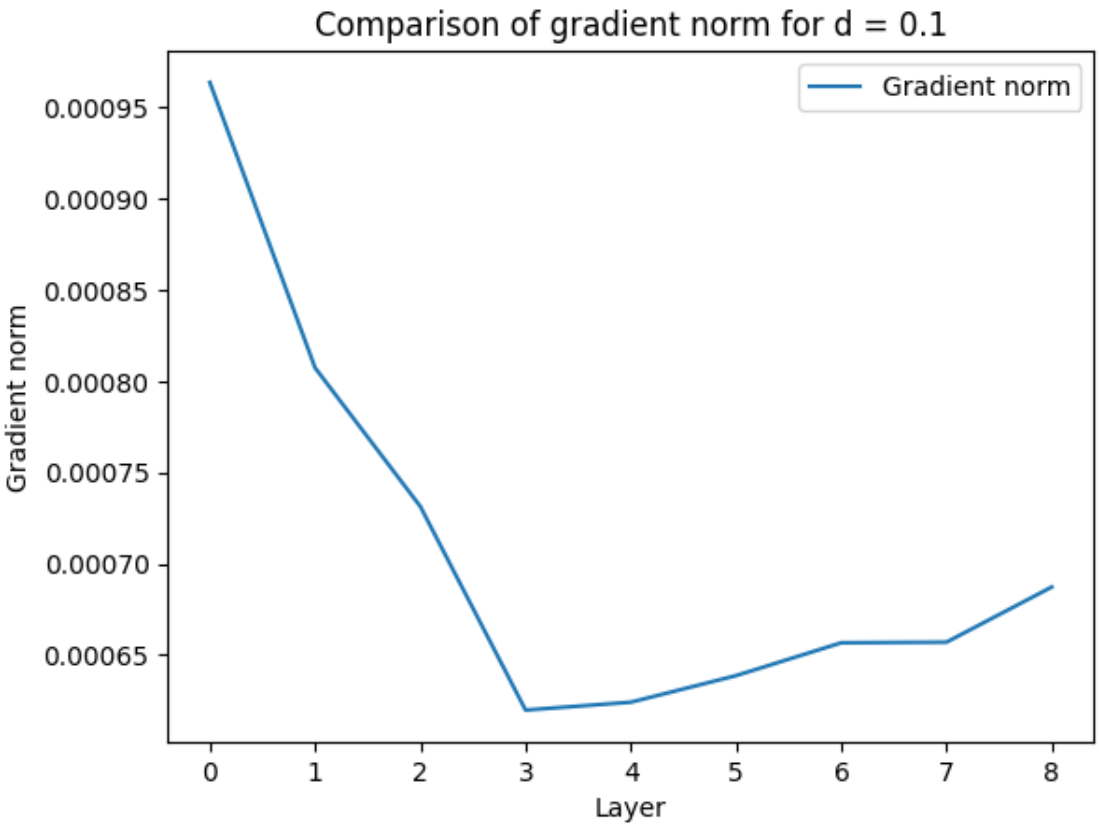
[ ]:
```python
device = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")

import torch.nn as nn

class My_nn_4a(nn.Module):
    def __init__(self,depth):
        super(My_nn_4a,self).__init__()
        self.depth = depth
        self.input_layer = nn.Linear(784,50)
        self.layers = nn.ModuleList([nn.Linear(50,50) for i in range(depth-1)])
        self.output_layer = nn.Linear(50,10)
        self.activation = nn.Tanh()

    def forward(self,x):
        x = x.view(-1,784)
        x= self.input_layer(x)
        x = self.activation(x)
        #x.retain_grad()
        for i in range(self.depth-1):
            x = self.layers[i](x)
            x = self.activation(x)
            #x.retain_grad()
        x = self.output_layer(x)
        return x

    def initialize_weights(self,d, xavier = False):
        #use torch.nn.init
        for m in self.modules():
            if isinstance(m, nn.Linear):
                if xavier:
                    d = np.sqrt(6/(m.in_features + m.out_features))
                    nn.init.uniform_(m.weight, -d, d)
                    nn.init.zeros_(m.bias)
                else:
                    nn.init.uniform_(m.weight, -d, d)
                    nn.init.zeros_(m.bias)

    # use cross entropy loss
    def loss(self, x, y):
        return nn.CrossEntropyLoss()(self.forward(x), y)
```

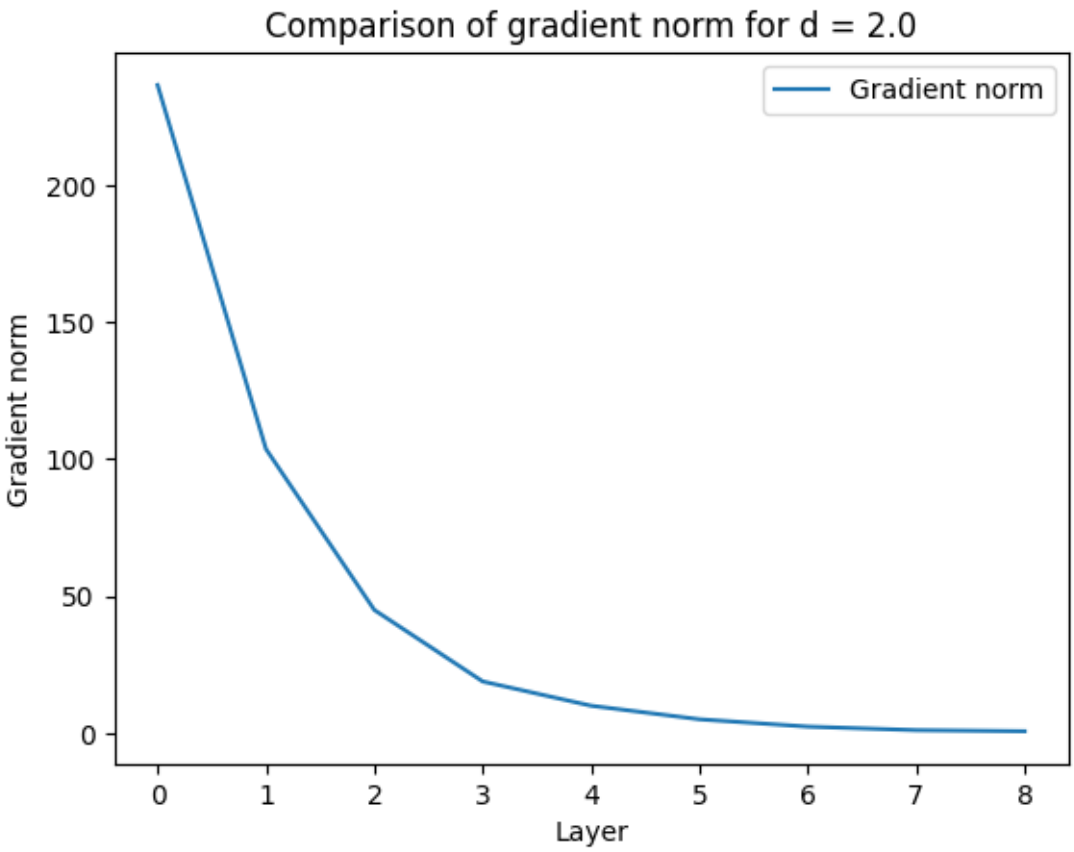
3.0.2 Exercise 4c)

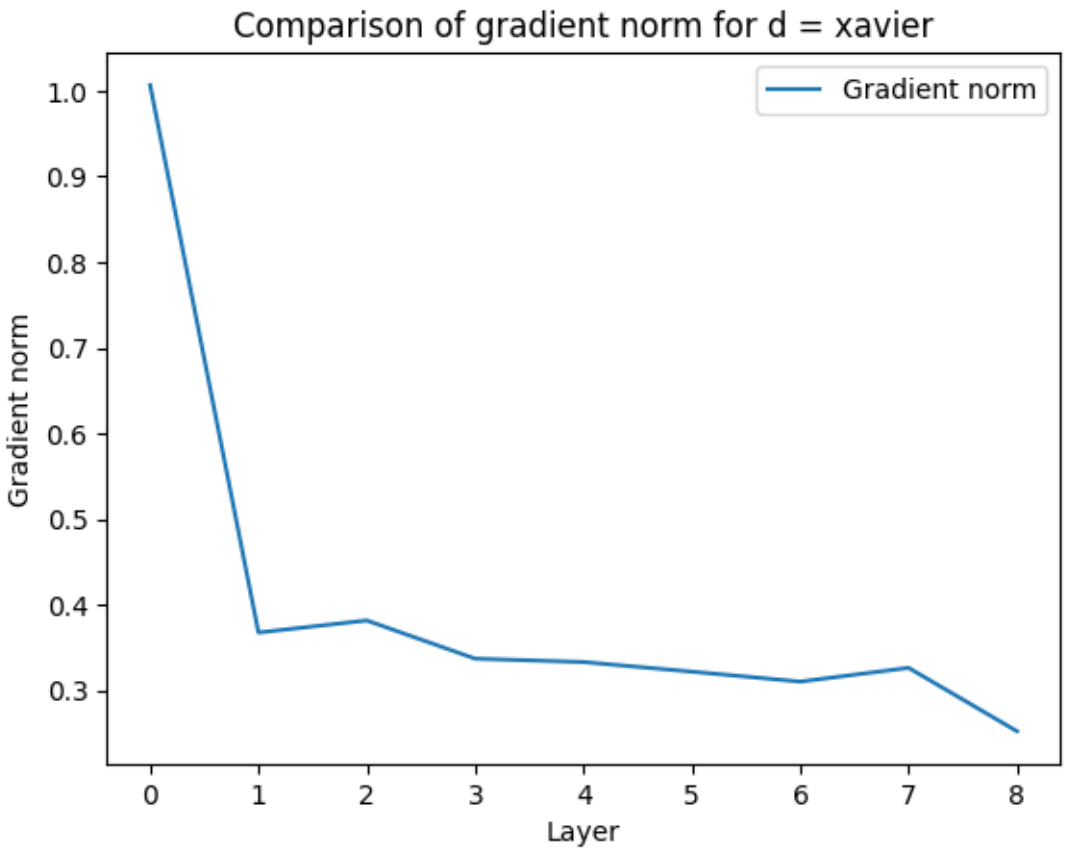
[ ]:
```
#forward and backward a minibatch of 256 MNIST digits through the network with␣
 ↪depth 8.


from torchvision import datasets, transforms
#load MNIST data
transform=transforms.Compose([
        transforms.ToTensor()
        ])

train_batch_size = 256
test_batch_size = 256

# load MNIST train and test sets
mnist_train = datasets.MNIST(root='.',
                             train=True,
                             download=True,
                              transform=transform)
mnist_test = datasets.MNIST(root='.',
                            train=False,
                            download=True,
                            transform=transform)

# initialize dataloaders for MNIST train and test sets
train_dataloader = data.
 ↪DataLoader(mnist_train,batch_size=train_batch_size,drop_last=True)
test_dataloader = data.
 ↪DataLoader(mnist_test,batch_size=test_batch_size,drop_last=True)

device = torch.device("cuda:0" if torch.cuda.is_available() else "cpu")

network = My_nn_4a(8).to(device)

#"""Just to check if the network is working"""
# def test(test_dataloader):
#     loss = 0
#     accuracy = 0
#     for x,y in test_dataloader:
#         x = x.to(device)
#         y = y.to(device)
#         output = network.forward(x)
#         prediciton = torch.argmax(output,dim=1)
#         accuracy += torch.sum(prediciton==y).item()/test_batch_size
```

```
#         loss += nn.functional.cross_entropy(output,y).item()
#     print(f'test loss: {loss/len(test_dataloader):4f}')
#     print(f'test accuracy: {accuracy/len(test_dataloader)*100:.2f}%')

# test(test_dataloader)

#Compute and visualize the gradient norm at each layer
def compute_grad_norm(network):
    grad_norm = []
    for m in network.modules():
        if isinstance(m, nn.Linear):
            grad_norm.append(torch.norm(m.weight.grad).item())
    return grad_norm

def visualize_grad_norm(grad_norm,title):
    plt.figure()
    plt.title(title)
    plt.plot(grad_norm, label="Gradient norm")
    plt.xlabel("Layer")
    plt.ylabel("Gradient norm")
    plt.legend()
    plt.show()

d_list = [0.01,0.1,2.0,"xavier"]



for d in d_list:
    if d == "xavier":
        network.initialize_weights(1,xavier=True)
    else:
        network.initialize_weights(d)

    title = "Comparison of gradient norm for d = " + str(d)

    for x,y in test_dataloader:
        x = x.to(device)
        y = y.to(device)
        loss = network.loss(x,y)
        loss.backward()
        grad_norm = compute_grad_norm(network)
        visualize_grad_norm(grad_norm,title)
        network.zero_grad()
        break
```


Comparison of gradient norm for d = 0.01
1e−12
Gradient norm
6.8
6.7
6.6
6.5
6.4
6.3
6.2
Gradient norm
0
1
2
3
4
5
6
7
8
Layer


Comparison of gradient norm for d = 0.1
Gradient norm
0.00095
0.00090
0.00085
0.00080
0.00075
0.00070
0.00065
Gradient norm
0
1
2
3
4
5
6
7
8
Layer


Comparison of gradient norm for d = 2.0
Gradient norm
Gradient norm
200
150
100
50
0
0
1
2
3
4
5
6
7
8
Layer



3.0.3 Exercise 4 d)

[ ]:
```
#Train the model for 5 epochs, minibatch size 128, and learning rate 0.01

import torch.optim as optim

train_batch_size = 128
test_batch_size = 128

train_dataloader = data.
 ↪DataLoader(mnist_train,batch_size=train_batch_size,drop_last=True)
test_dataloader = data.
 ↪DataLoader(mnist_test,batch_size=test_batch_size,drop_last=True)

def train(train_dataloader, test_dataloader, network, epochs, learning_rate):
    optimizer = optim.SGD(network.parameters(), lr=learning_rate)
    train_loss = []
    train_accuracy = []
    test_loss = []
```

```
    test_accuracy = []
    for epoch in range(epochs):
        # training
        network.train()
        for x,y in train_dataloader:
            optimizer.zero_grad()
            x = x.to(device)
            y = y.to(device)
            output = network.forward(x)
            loss = nn.functional.cross_entropy(output,y)
            loss.backward()
            optimizer.step()
            train_loss.append(loss.item())
            prediciton = output.argmax(dim=1)
            #print(prediciton)
            #print(network.layers[0].weight)
            train_accuracy.append(torch.sum(prediciton==y).item()/
 ↪train_batch_size)
        # testing
        network.eval()
        for x,y in test_dataloader:
            x = x.to(device)
            y = y.to(device)
            output = network.forward(x)
            prediciton = torch.argmax(output,dim=1)
            test_accuracy.append(torch.sum(prediciton==y).item()/
 ↪test_batch_size)
            test_loss.append(nn.functional.cross_entropy(output,y).item())
        print(f'epoch: {epoch+1}')
        print(f'train loss: {sum(train_loss)/ (len(train_dataloader) *␣
 ↪(epoch+1)):4f} - train accuracy: {sum(train_accuracy)/␣
 ↪(len(train_dataloader) * (epoch+1))*100:.2f}%')
        print(f'test loss: {sum(test_loss)/ (len(test_dataloader) * (epoch+1)):
 ↪4f} - test accuracy: {sum(test_accuracy)/ (len(test_dataloader) *␣
 ↪(epoch+1))*100:.2f}%')
for d in d_list:
    network = My_nn_4a(8).to(device)
    if d == "xavier":
        network.initialize_weights(1,xavier=True)
    else:
        network.initialize_weights(d)
    train(train_dataloader, test_dataloader, network, 5, 0.01)
```

```
epoch: 1
train loss: 2.302108 - train accuracy: 11.19%
test loss: 2.301665 - test accuracy: 11.35%
epoch: 2
```

```
train loss: 2.301826 - train accuracy: 11.21%
test loss: 2.301479 - test accuracy: 11.35%
epoch: 3
train loss: 2.301659 - train accuracy: 11.22%
test loss: 2.301366 - test accuracy: 11.35%
epoch: 4
train loss: 2.301553 - train accuracy: 11.23%
test loss: 2.301293 - test accuracy: 11.35%
epoch: 5
train loss: 2.301483 - train accuracy: 11.23%
test loss: 2.301243 - test accuracy: 11.35%
epoch: 1
train loss: 2.302034 - train accuracy: 11.36%
test loss: 2.301557 - test accuracy: 11.35%
epoch: 2
train loss: 2.301740 - train accuracy: 11.30%
test loss: 2.301373 - test accuracy: 11.35%
epoch: 3
train loss: 2.301572 - train accuracy: 11.28%
test loss: 2.301264 - test accuracy: 11.35%
epoch: 4
train loss: 2.301468 - train accuracy: 11.27%
test loss: 2.301193 - test accuracy: 11.35%
epoch: 5
train loss: 2.301397 - train accuracy: 11.26%
test loss: 2.301144 - test accuracy: 11.35%
epoch: 1
train loss: 6.039689 - train accuracy: 11.67%
test loss: 2.480055 - test accuracy: 12.66%
epoch: 2
train loss: 4.200424 - train accuracy: 12.47%
test loss: 2.397484 - test accuracy: 14.90%
epoch: 3
train loss: 3.554068 - train accuracy: 14.34%
test loss: 2.338540 - test accuracy: 16.49%
epoch: 4
train loss: 3.215720 - train accuracy: 15.50%
test loss: 2.286135 - test accuracy: 17.93%
epoch: 5
train loss: 3.001272 - train accuracy: 16.82%
test loss: 2.239740 - test accuracy: 19.48%
epoch: 1
train loss: 1.190881 - train accuracy: 70.15%
test loss: 0.639273 - test accuracy: 85.36%
epoch: 2
train loss: 0.856330 - train accuracy: 78.54%
test loss: 0.528139 - test accuracy: 87.41%
epoch: 3
```

```
train loss: 0.700018 - train accuracy: 82.28%
test loss: 0.464706 - test accuracy: 88.60%
epoch: 4
train loss: 0.606552 - train accuracy: 84.49%
test loss: 0.422158 - test accuracy: 89.43%
epoch: 5
train loss: 0.542731 - train accuracy: 86.02%
test loss: 0.390663 - test accuracy: 90.06%
```