## CS480/680, Spring 2023, Assignment 2

## Designer: Yimu Wang; Instructor: Hongyang Zhang

Released: June 5; Due: \*\*Extended: June 29, noon\*\*

#### Link of the Assignment

#### Tips:

- Please save a copy of this notebook to avoid losing your changes.
- Debug your code and ensure that it can run.
- Save the output of each cell. Failure to do so may result in your coding questions not being graded.
- To accelerate the training time, you can choose 'Runtime' -> 'Change runtime type' -> 'Hardware accelerator' and set 'Hardware accelerator' to 'GPU'. With T4, all the experiments can be done in 5 minutes. In total, this notebook can be run in 20 minutes. (You can either use or not use GPU to accelearte. It is your choice and it does not affect your grades.)
- Your grade is independent of the test accuracy (unless it is 10%, as 10% is the accuracy of random guess).

### Tips for sumbission:

- Do not change the order of the problems.
- Select 'Runtime' -> 'Run all' to run all cells and generate a final "gradable" version
  of your notebook and save your ipynb file.
- We recommend using Chrome to generate the PDF.
- Also use 'File' -> 'Print' and then print your report from your browser into a PDF file.
- Submit both the .pdf and .ipynb files.
- We do not accept any hand-written report.

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Question 0. [Important] Please name your submission as {Last-name}\_{First-name}\_assignment2.ipynb and {Last-name}\_{First-name}\_assignment2.pdf. If you do not follow this rule, your grade of assignment 2 will be 0.

Question 1. Basics of MLP, CNN, and Transformers (40 points)

1.1 Given an MLP with an input layer of size 100, two hidden layers of size 50 and 25, and an output layer of size 10, calculate the total number of parameters in the network. (10 points)

This MLP network is a standard MLP with bias terms. The activation function is ReLU. But you do not need to consider the parameters of the activation function.

Solution: [Your answer here, You should give the full calculation process.]

Number of parameters = 
$$(100+1) imes 50 + (50+1) imes 25 + (25+1) imes 10 = 6585$$

1.2 Given the loss functions of mean squared error (MSE) and CE (cross-entropy) loss (between logits and target), and the predicted logit of a data example (before softmax) is [0.5, 0.3, 0.8], while the target of a data example is [0.3, 0.6, 0.1], calculate the value of the loss (MSE and CE). (10 points)

The loss functions of MSE and CE are as follows,

$$egin{aligned} \ell_{MSE}(\hat{y},y) &= \sum_{i \in C} (\hat{y}_c - y_c)^2, \ \ \ell_{ ext{CE}}(\hat{y},y) &= -\sum_{i = 1}^C y_i \log \Bigg(rac{\exp(\hat{y}_i)}{\sum_{j \in [C]} \exp(\hat{y}_j)}\Bigg)\,, \end{aligned}$$

where  $\hat{y}_i$  is the i-th element of predict logit (before softmax), y is the i-th element of target, and C is the number of classes.

Solution: [Your answer here, You should give the full calculation process.]

$$\begin{split} l_{MSE} &= (0.5-0.3)^2 + (0.3-0.6)^2 + (0.8-0.1)^2 = 0.62 \\ l_{CE} &= - (0.3 \times \log \left(\frac{exp(0.5)}{exp(0.5) + exp(0.3) + exp(0.8)}\right) + 0.6 \times \log \left(\frac{exp(0.3)}{exp(0.5) + exp(0.3) + exp(0.8)}\right) + 0. \end{split}$$

# 1.3 Given a convolutional layer in a CNN with an input feature map of size 32x32, a filter size of 3x3, a stride of 1, and no padding, calculate the size of the output feature map. (10 points)

You can refer to PyTorch Convolutional Layer for the definition of the convolutional layer.

Solution: [Your answer here, You should give the full calculation process.]

Output size = 
$$\lfloor 1 + rac{32+0-3}{1} 
floor imes \lfloor 1 + rac{32+0-3}{1} 
floor = 30 imes 30$$

# 1.4 Given a Transformer encoder with 1 layer, the input and output dimensions of attention of 256, and 8 attention heads, calculate the total number of parameters in the **self-attention mechanism**. (10 points)

You can refer to Attention is all you need (Transformer paper) for reference.

Solution: [Your answer here, You should give the full calculation process.]

$$\frac{256}{8} = 32$$

Number of parameters =  $3 \times 256 \times 32 \times 8 + 256 \times 256 = 262144$ 

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## Question 2. Implementation of Multi-Layer Perceptron and understanding Gradients (60 points)

In this question, you will learn how to implment a Multi-Layer Perceptron (MLP) PyTorch, test the performance on CIFAR10, and learn what is gradient. Please refer to CIFAR10 and PyTorch for details.

Assuming the MLP follows the following construction

$$\hat{y} = \operatorname{softmax}(W_2 \operatorname{sigmoid}(W_1 x + c_1) + c_2),$$

where  $\hat{y}$  is the prediction (probability) of the input x by the MLP and  $W_1$ ,  $W_2$ ,  $c_1$ , and  $c_2$  are four learnable parameters of the MLP. softmax and sigmoid are the softmax and sigmoid function.

Please note that the label is one-hot vectors, i.e.,  $y_i$  are either 0 or 1. And the sum of prediction is equal to 1, i.e.,  $\sum_{i \in [C]} \hat{y}_i = 1$ . However, usually in PyTorch, the labels are integers. You may need to transfer integers into one-hot vectors.

Tips: The process of using SGD to train a model is as follows:

- 1. Initialize the model parameters.
- 2. Calculate the gradients of the model parameters.
- 3. Update the model parameters using the gradients.
- 4. Test the model.
- 5. Repeat 2 4 until the model converges or for a given epochs.

You do not need to implement the training procedure. Please follow the instruction of each question. This is just set to help you understanding the training procedure.

You can also refer to SGD and PyTorch Tutorial for inspiration.

Please note that you are allowed to use any PyTorch api and any public code to complete the following coding questions. This assignment is help you to learn PyTorch.

## 2.0 Get CIFAR10 data (0 points)

We will show you how to get the data using PyTorch. You are not allowed to edit the following code. Please see Dataset and DataLoaders for details.

```
In [1]: ### YOU ARE NOT ALLOWED TO EDIT THE FOLLOWING CODE. ###
        import torch
        import torchvision.datasets as datasets
        import torchvision.transforms as transforms
        from torch.utils.data import DataLoader
        def get_CIFAR10():
            # Set the random seed for reproducibility
            torch.manual seed(480)
            # Load the CIFAR10 dataset and apply transformations
            train dataset = datasets.CIFAR10(root='./data', train=True,
                                              transform=transforms.ToTensor(),
                                              download=True)
            test dataset = datasets.CIFAR10(root='./data', train=False,
                                             transform=transforms.ToTensor())
            # Define the data loaders
            batch size = 100
            train_loader = DataLoader(train_dataset, batch_size=batch_size, shuffle=
            test loader = DataLoader(test dataset, batch size=batch size, shuffle=Fa
            return train_dataset, test_dataset, train_loader, test_loader
```

### 2.1 Implement the MLP with PyTorch (15 points)

The shape of  $W_1$  and  $W_2$  should be  $256 \times 3072$  and  $10 \times 256$ .

You can refer to Define a NN for inspiration.

```
In [2]: import torch.nn as nn
        import torchvision.models as models
        import torch.nn.functional as F
        ##### COMPLETE THE FOLLOWING CODE, YOU ARE ALLOWED TO CHANGE THE SKLETON COL
        # Define the MLP model in PyTorch
        class MLPinPyTorch(nn.Module):
            def init (self, input dim=3072, hidden dim=256, output dim=10):
                super(MLPinPyTorch, self).__init__()
                # TODO: Your code here: init with parameters
                        you are allowed to use any initialization method
                # Define layers
                self.fc1 = nn.Linear(input_dim, hidden_dim)
                self.fc2 = nn.Linear(hidden dim, output dim)
                # Initialize parameters
                nn.init.xavier uniform (self.fcl.weight)
                nn.init.xavier uniform (self.fc2.weight)
                nn.init.zeros_(self.fc1.bias)
                nn.init.zeros (self.fc2.bias)
            def forward(self, x):
                # TODO: Your code here: forward
                x = self.fcl(x)
                x = F.sigmoid(x)
                x = self.fc2(x)
                # Apply softmax to x
                output = F.softmax(x, dim=1)
                return output
```

## 2.2 Calculate the accuracy given true labels and predicted labels (5 points)

You should complete the following code, including the calculation of the accuracy.

## 2.3 Test your implementation on CIFAR10 and reports the accuracy on training and testing datasets (20 points)

```
In [4]: device = torch.device("cuda:0" if torch.cuda.is available() else "cpu")
        ##### COMPLETE THE FOLLOWING CODE, YOU ARE ALLOWED TO CHANGE THE SKLETON COL
        def test(model, train dataloader, test dataloader):
            # TODO: Your code here: calculate accuracy
            predict train = []
            predict test = []
            train labels = []
            test labels = []
            for inputs, labels in train dataloader:
                inputs = inputs.view(-1, 3072).to(device)
                train labels.extend(labels.tolist())
                # Forward pass
                output = model(inputs)
                ,predict = torch.max(output, 1)
                predict train.extend(predict.tolist())
            for inputs, labels in test_dataloader:
                inputs = inputs.view(-1, 3072).to(device)
                test labels.extend(labels.tolist())
                # Forward pass
                output = model(inputs)
                _,predict = torch.max(output, 1)
                predict test.extend(predict.tolist())
            train_acc = accuracy(train_labels, predict_train)
            test acc = accuracy(test labels, predict test)
            return train acc, test acc
        ##### the following is served for you to check the functions #####
        ##### you can change but ensure the following code can output the accuracies
        model = MLPinPyTorch()
        train dataset, test dataset, train loader, test loader = get CIFAR10()
        train_acc, test_acc = test(model, train_loader, test_loader)
        print("train acc: ", train acc)
        print("test_acc: ", test_acc)
        Files already downloaded and verified
        train acc: 0.10372
```

test\_acc: 0.103

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## 2.4 Calculate the gradients $\frac{\partial \ell}{\partial W_1}$ , $\frac{\partial \ell}{\partial c_1}$ , $\frac{\partial \ell}{\partial W_2}$ , and $\frac{\partial \ell}{\partial c_2}$ using algebra given a data example (x,y) (20 points)

The loss function we use for training the MLP is the log-loss, which is defined as follows:

$$\ell(\hat{y},y) = -\sum_{i=1}^C y_i \log(\hat{y}_i)\,,$$

where C is the number of classes,  $y_i$  and  $\hat{y}_i$  are the i-th index of y and  $\hat{y}$ .

Considering the MLP model in question 2, please use chainrule to calculate the gradients. You can directly write LaTex/Markdown in the following cell.

Solution: [Your answer here]

For softmax function:

Let 
$$s_i = softmax(x_i)$$

$$\frac{\partial}{\partial x_j} \log(s_i) = \frac{1}{s_i} \cdot \frac{\partial s_i}{\partial x_j}$$

Rearrange to get  $rac{\partial s_i}{\partial x_i} = s_i \cdot rac{\partial}{\partial x_i} \mathrm{log}(s_i)$ 

Note that 
$$\log(s_i) = \log\Bigl(rac{exp(x_i)}{\sum_k exp(x_k)}\Bigr) = x_i - \log\bigl(\sum_k exp(x_k)\bigr)$$

Thus, 
$$rac{\partial}{\partial x_i} \mathrm{log}(s_i) = rac{\partial x_i}{\partial x_j} - rac{\partial}{\partial x_j} \mathrm{log}ig(\sum_k exp(x_k)ig)$$

Note that when i=j,  $\frac{\partial x_i}{\partial x_j}=1$ , otherwise 0.

$$rac{\partial}{\partial x_j} \mathrm{log}ig( \sum_k exp(x_k) ig) = rac{1}{\sum_k exp(x_k)} \cdot \Big( rac{\partial}{\partial x_j} \sum_k exp(x_k) \Big) = rac{1}{\sum_k exp(x_k)} exp(x_j) = s_j$$

Therefore,  $rac{\partial}{\partial x_j} \log(s_i) = 1 - s_j$  when i = j, and  $-s_j$  otherwise.

Thus,  $softmax'(x) = softmax(x)(I - softmax(x))^T$ 

For sigmoid function:

$$sigmoid(x) = \frac{1}{1 + exp(-x)}$$

Applying chain rule to get: 
$$\frac{\partial}{\partial x} sigmoid(x) = \frac{exp(-x)}{(1+exp(-x))^2}$$
  $x = \text{input}$  
$$z = W_1 x + c_1$$
 
$$h = Sigmoid(z) = \frac{1}{1+exp(-z)}$$
 
$$\theta = W_2 h + c_2$$
 
$$\hat{y} = softmax(\theta)$$
 
$$l = -y \log(\hat{y})$$
 
$$\frac{\partial l}{\partial \hat{y}} = -\frac{y}{\hat{y}}$$
 
$$\frac{\partial l}{\partial \theta} = \frac{\partial l}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial \theta} = -\frac{y}{\hat{y}} \cdot softmax'(\theta) = -\frac{y}{\hat{y}} softmax(\theta)(I - softmax(\theta))^T$$
 
$$\frac{\partial l}{\partial W_2} = \frac{\partial l}{\partial \theta} \frac{\partial \theta}{\partial W_2} = -\frac{y}{\hat{y}} softmax(\theta)(I - softmax(\theta))^T$$
 
$$\frac{\partial l}{\partial c_2} = \frac{\partial l}{\partial \theta} \frac{\partial \theta}{\partial h} \frac{\partial e}{\partial c_2} = -\frac{y}{\hat{y}} softmax(\theta)(I - softmax(\theta))^T$$
 
$$\frac{\partial l}{\partial h} = \frac{\partial l}{\partial \theta} \frac{\partial \theta}{\partial h} = -W_2^T \frac{y}{\hat{y}} softmax(\theta)(I - softmax(\theta))^T$$

 $rac{\partial l}{\partial W_1} = rac{\partial l}{\partial z}rac{\partial z}{\partial W_1} = -W_2^Trac{y}{\hat{y}}softmax( heta)(I-softmax( heta))^Trac{exp(-z)}{(1+exp(-z))^2}x^T$ 

$$rac{\partial l}{\partial c_1} = rac{\partial l}{\partial z}rac{\partial z}{\partial c_1} = -W_2^Trac{y}{\hat{y}}softmax( heta)(I-softmax( heta))^Trac{exp(-z)}{(1+exp(-z))^2}$$

 $rac{\partial l}{\partial z} = rac{\partial l}{\partial h}rac{\partial h}{\partial z} = -W_2^Trac{y}{\hat{y}}softmax( heta)(I-softmax( heta))^Trac{exp(-z)}{(1+exp(-z))^2}$ 

In [ ]: