CHEM277B Homework 8

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(A)

Importing the MNIST Data and printing out relevant dimensions

```
import pandas as pd
import numpy as np
import cv2
import matplotlib.pyplot as plt

training_set, validation_set = pd.read_pickle('mnist.pkl')

#examine the shape of the training set
print(len(training_set[0]))
print(len(training_set[0][0]))
print(len(training_set[0][0][0]))
print(len(validation_set[0]))

#normalized the training data and reshape to shape (ndata, nfeatures)
gray_img_train = np.array(training_set[0]).astype('uint8')
gray_img_train = gray_img_train.reshape(60000, 32, 32)
rgb_img_train = np.zeros((60000, 32, 32, 3))
for i in range(len(gray_img_train[0])):
  rgb_img_train[i] = cv2.cvtColor(gray_img_train[i],  cv2.COLOR_GRAY2RGB)
print(gray_img_train.shape)
print(rgb_img_train.shape)
rgb_img_train = np.transpose(rgb_img_train, (0, 3, 1, 2))  # (60000, 3, 32, 32)
normalized_train_set_x = rgb_img_train / 255
print(normalized_train_set_x.shape)

plt.show()

gray_img_test = np.array(validation_set[0]).astype('uint8')
gray_img_test = gray_img_test.reshape(10000, 32, 32)
rgb_img_test = np.zeros((10000, 32, 32, 3))
for i in range(len(gray_img_test[0])):
  rgb_img_test[i] = cv2.cvtColor(gray_img_test[i],  cv2.COLOR_GRAY2RGB)
print(gray_img_test.shape)
print(rgb_img_test.shape)
rgb_img_test = np.transpose(rgb_img_test, (0, 3, 1, 2))  # (10000, 3, 32, 32)
normalized_test_set_x = rgb_img_test / 255
print(normalized_test_set_x.shape)
```

```
train_set_y = np.array(training_set[1])
test_set_y = np.array(validation_set[1])
```

```
60000
32
32
10000
(60000, 32, 32)
(60000, 32, 32, 3)
(60000, 3, 32, 32)
(10000, 32, 32)
(10000, 32, 32, 3)
(10000, 3, 32, 32)
```

Calculate the size of the output after each convolution sequentially applied to the black and white 32x32 image.

(i). Convolution Filter size of 2x2, number of filters 33, stride of 2, padding of 0

(ii). Convolution Filter size of 3x3, number of filters 55, stride of 1, padding of 1

(iii). Convolution Filter size of 3x3, number of filters 77, stride of 1, padding of 1. Followed by a Max Pooling with filter size of 2x2 and stride 2

Using the equation below:

$$\frac{I - K + 2P}{S} + 1$$

where I is the input dimension (32), K is the size of the filter, P is the size of the padding, and S is the stride.

(i)

$$\frac{32 - 2 + 2(0)}{2} + 1 = 16$$

So in this case we get a 16x16 image for each of the 33 feature maps.

(ii)

$$\frac{16 - 3 + 2(1)}{1} + 1 = 16$$

This case returns a 16x16 image for each of the 55 feature maps.

(iii)

$$\frac{16 - 3 + 2(1)}{1} + 1 = 16$$

Then we apply the max pooling operation with 2x2 filter and stride 2:

$$\frac{16 - 2 + 2(0)}{2} + 1 = 8$$

Which yields an 8x8 image for each of the 77 feature maps.

(B)

The MNIST data set was, in fact, in color (RGB). This means the depth of the input image would be 3. Calculate the dimensionality of the output for the following convolutions sequentially applied to a RGB MNIST input:

(i). Convolution Filter size of 2x2, number of filters 33, stride of 2, padding of 0

(ii). Convolution Filter size of 3x3, number of filters 55, stride of 1, padding of 1. Followed by a max pooling layer of kernel size 3x3, stride of 1, padding of 0

(iii). Convolution Filter size of 3x3, number of filters 77, stride of 1, padding of 1. Followed by a Max Pooling with filter size of 2x2 and stride 2.

(i)

$$\frac{32 - 2 + 2(0)}{2} + 1 = 16$$

This convolution yields a 16x16x3 image for each 33 filters.

(ii)

$$\frac{16 - 3 + 2(1)}{1} + 1 = 16$$

Followed by a max pooling layer with F=3, S = 1, we use the equation below:

$$H2 = \frac{H1 - F}{S} + 1$$
$$H2 = \frac{16 - 3}{1} + 1 = 14$$

The calculation for the width is the same and thus we have a 14x14x3 image for each of the 55 filters.

(iii)

$$14 - 3 + 2(1)$$

$$\frac{14 - 3 + 2(1)}{1} + 1 = 14$$

Followed by a max pooling layer with F=2, S = 2, we use the equation below:

$$H2 = \frac{H1 - F}{S} + 1$$
$$H2 = \frac{14 - 2}{2} + 1 = 7$$

So this layer yields an image of 7x7x3 for each of the 77 filters.

(C)

```
from functools import wraps
from time import time

def timing(f):
    @wraps(f)
    def wrap(*args, **kw):
        ts = time()
        result = f(*args, **kw)
        te = time()
        print('func:%r  took: %2.4f sec' % (f.__name__,  te-ts))
        return result
    return wrap


from torch.optim import SGD, Adam
import torch.nn.functional as F
import random
from tqdm import tqdm
import math
from sklearn.model_selection import train_test_split, KFold

def create_chunks(complete_list, chunk_size=None, num_chunks=None):
    '''
    Cut a list into multiple chunks, each having chunk_size (the last chunk might b
    '''
    chunks = []
    if num_chunks is None:
        num_chunks = math.ceil(len(complete_list) / chunk_size)
    elif chunk_size is None:
        chunk_size = math.ceil(len(complete_list) / num_chunks)
    for i in range(num_chunks):
        chunks.append(complete_list[i * chunk_size: (i + 1) * chunk_size])
```

```
        return chunks

class Trainer():
    def __init__(self, model, optimizer_type, learning_rate, epoch, batch_size, inp
        """ The class for training the model
        model: nn.Module
            A pytorch model
        optimizer_type: 'adam' or 'sgd'
        learning_rate: float
        epoch: int
        batch_size: int
        input_transform: func
            transforming input. Can do reshape here
        """
        self.model = model
        if optimizer_type == "sgd":
            self.optimizer = SGD(model.parameters(), learning_rate,momentum=0.9)
        elif optimizer_type == "adam":
            self.optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)

        self.epoch = epoch
        self.batch_size = batch_size
        self.input_transform = input_transform
        self.learning_rate = learning_rate


    @timing
    def train(self, inputs, outputs, val_inputs, val_outputs,early_stop=False,l2=Fa
        """ train self.model with specified arguments
        inputs: np.array, The shape of input_transform(input) should be (ndata,nfea
        outputs: np.array shape (ndata,)
        val_nputs: np.array, The shape of input_transform(val_input) should be (nda
        val_outputs: np.array shape (ndata,)
        early_stop: bool
        l2: bool
        silent: bool. Controls whether or not to print the train and val error duri

        @return
        a dictionary of arrays with train and val losses and accuracies
        """
        ### convert data to tensor of correct shape and type here ###
        inputs = torch.tensor(inputs, dtype=torch.float32)
        outputs = torch.tensor(outputs, dtype=torch.long)
        val_inputs = torch.tensor(val_inputs, dtype=torch.float32)
        val_outputs = torch.tensor(val_outputs, dtype=torch.long)

        losses = []
        accuracies = []
        val_losses = []
        val_accuracies = []
        weights = self.model.state_dict()
```

```
        weights = self.model.state_dict()
        lowest_val_loss = np.inf

        for n_epoch in tqdm(range(self.epoch), leave=False):
            self.model.train()
            batch_indices = list(range(inputs.shape[0]))
            random.shuffle(batch_indices)
            batch_indices = create_chunks(batch_indices, chunk_size=self.batch_size
            epoch_loss = 0
            epoch_acc = 0
            for batch in batch_indices:
                batch_importance = len(batch) / len(outputs)
                batch_input = inputs[batch]
                batch_output = outputs[batch]
                ### make prediction and compute loss with loss function of your cho
                batch_predictions = self.model.forward(batch_input)
                loss_func = nn.CrossEntropyLoss()
                loss = loss_func(batch_predictions, batch_output)
                if l2:
                    ### Compute the loss with L2 regularization ###
                    self.optimizer = torch.optim.Adam(model.parameters(), lr = self
                    loss = loss_func(batch_predictions, batch_output)
                self.optimizer.zero_grad()
                loss.backward()
                self.optimizer.step()
                ### Compute epoch_loss and epoch_acc
            epoch_loss, epoch_acc = self.evaluate(inputs, outputs)
            val_loss, val_acc = self.evaluate(val_inputs, val_outputs, print_acc=Fa
            if n_epoch % 10 ==0 and not silent:
                print("Epoch %d/%d - Loss: %.3f - Acc: %.3f" % (n_epoch + 1, self.e
                print("              Val_loss: %.3f - Val_acc: %.3f" % (val_loss, v
            losses.append(epoch_loss.detach().numpy())
            accuracies.append(epoch_acc)
            val_losses.append(val_loss.detach().numpy())
            val_accuracies.append(val_acc)
            if early_stop:
                if val_loss < lowest_val_loss:
                    lowest_val_loss = val_loss
                    weights = self.model.state_dict()

        if early_stop:
            self.model.load_state_dict(weights)

        return {"losses": losses, "accuracies": accuracies, "val_losses": val_losse

    def evaluate(self, inputs, outputs, print_acc=False):
        """ evaluate model on provided input and output
        inputs: np.array, The shape of input_transform(input) should be (ndata,nfea
        outputs: np.array shape (ndata,)
        print_acc: bool
```

```
        @return
        losses: float
        acc: float
        """

        inputs = torch.tensor(inputs, dtype=torch.float32)
        outputs = torch.tensor(outputs, dtype=torch.long)

        loss_func = nn.CrossEntropyLoss()

        pred = self.model.forward(inputs)

        losses = loss_func(pred, outputs)
        #print("pred = ", pred)
        #print("truth = " ,outputs)

        sum = 0
        for i in range(len(outputs)):
          if outputs[i] == torch.argmax(pred[i]):
            sum += 1
        acc = sum / len(outputs)
        if print_acc:
            print("Accuracy: %.3f" % acc)
        return losses, acc
```

```
from torch import nn
import torch
class ConvMLP(nn.Module):
    def __init__(self):
        super(ConvMLP, self).__init__()
        self.conv = nn.Conv2d(3, 3, kernel_size = 5, stride=1, padding = 2)
        self.fc = nn.Linear(3*32*32, 10)
        self.activation = nn.ReLU()

    def forward(self, x):
        x = self.activation(self.conv(x))
        x = nn.Flatten()(x)
        x = self.activation(self.fc(x))
        return x
```

```
from torchsummary import summary
model = ConvMLP()
summary(model, (3, 32, 32))
```

```
----------------------------------------------------------------
        Layer (type)               Output Shape         Param #
================================================================
            Conv2d-1            [-1, 3, 32, 32]             228
              ReLU-2            [-1, 3, 32, 32]               0
            Linear-3                   [-1, 10]          30,730
```

```
              ReLU-4                    [-1, 10]               0
================================================================
Total params: 30,958
Trainable params: 30,958
Non-trainable params: 0
----------------------------------------------------------------
Input size (MB): 0.01
Forward/backward pass size (MB): 0.05
Params size (MB): 0.12
Estimated Total Size (MB): 0.18
----------------------------------------------------------------
```

```
import matplotlib.pyplot as plt
from sklearn.model_selection import KFold
def Kfold_validation(n, inputs, outputs):

    total_num=len(inputs)
    kf=KFold(n_splits=n,shuffle=True)



    for train_selector,test_selector in kf.split(range(total_num)):
        ### Decide training examples and testing examples for this fold ###
        train_Xs= inputs[train_selector]
        test_Xs=  inputs[test_selector]
        train_ys= outputs[train_selector]
        test_ys= outputs[test_selector]

        model = ConvMLP()
        t = Trainer(model, optimizer_type='adam', learning_rate=1e-3, epoch=30, bat
        train_in,val_in,train_real,val_real=train_test_split(train_Xs,train_ys, tra

        dictionary = t.train(train_in, train_real, val_in, val_real,early_stop=True

    return dictionary, model


dictionary, model = Kfold_validation(3, normalized_train_set_x[0:1000], train_set_y
```

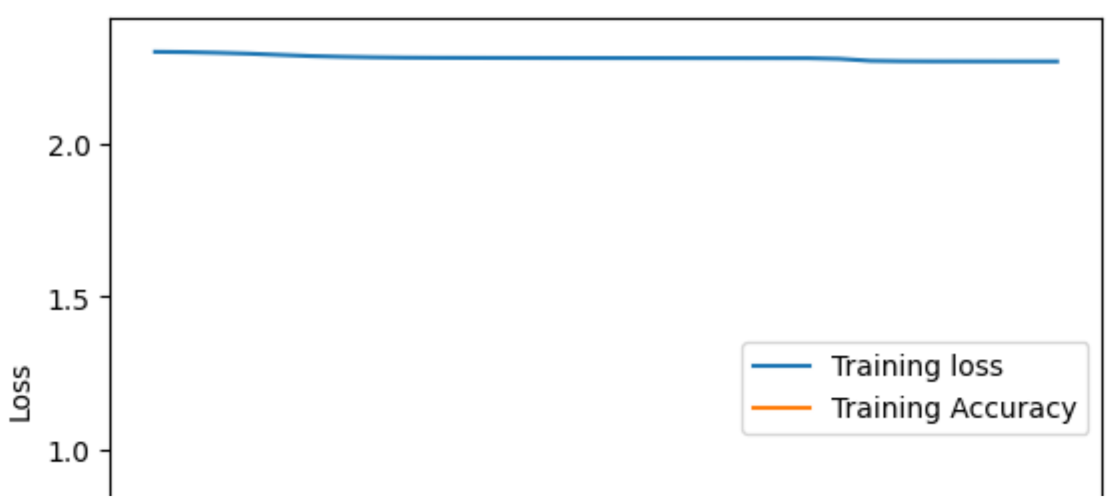
```
  0%|          | 0/30 [00:00<?, ?it/s]<ipython-input-141-5a654197e45b>:125: U
  inputs = torch.tensor(inputs, dtype=torch.float32)
<ipython-input-141-5a654197e45b>:126: UserWarning: To copy construct from a te
  outputs = torch.tensor(outputs, dtype=torch.long)
  7%|▋         | 2/30 [00:00<00:03,  7.84it/s]Epoch 1/30 - Loss: 2.299 - Acc:
              Val_loss: 2.301 - Val_acc: 0.103
 40%|████      | 12/30 [00:01<00:02,  7.90it/s]Epoch 11/30 - Loss: 2.282 - Acc
              Val_loss: 2.295 - Val_acc: 0.126
 73%|███████▎  | 22/30 [00:02<00:00,  8.01it/s]Epoch 21/30 - Loss: 2.281 - Acc
              Val_loss: 2.292 - Val_acc: 0.126
func:'train'  took: 3.8070 sec
  3%|▎         | 1/30 [00:00<00:03,  8.41it/s]Epoch 1/30 - Loss: 2.301 - Acc:
              Val_loss: 2.305 - Val_acc: 0.090
```

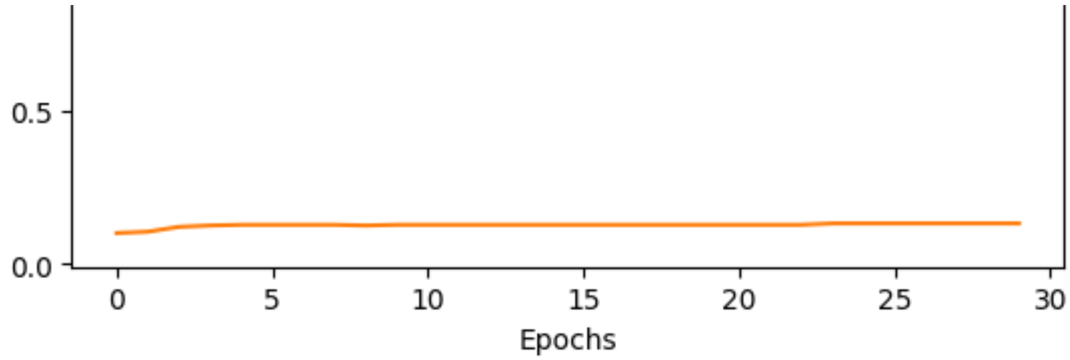
```
 40%|████      | 12/30 [00:01<00:02,  6.09it/s]Epoch 11/30 - Loss: 2.272 - Ac
               Val_loss: 2.314 - Val_acc: 0.094
 73%|███████   | 22/30 [00:03<00:01,  6.72it/s]Epoch 21/30 - Loss: 2.271 - Ac
               Val_loss: 2.318 - Val_acc: 0.099
func:'train'  took: 4.5425 sec
  3%|▎         | 1/30 [00:00<00:03,  7.63it/s]Epoch 1/30 - Loss: 2.301 - Acc:
               Val_loss: 2.303 - Val_acc: 0.090
 40%|████      | 12/30 [00:01<00:02,  7.92it/s]Epoch 11/30 - Loss: 2.281 - Ac
               Val_loss: 2.301 - Val_acc: 0.135
 73%|███████   | 22/30 [00:02<00:00,  8.18it/s]Epoch 21/30 - Loss: 2.280 - Ac
               Val_loss: 2.304 - Val_acc: 0.135
                                 func:'train'  took: 3.7226 sec
```

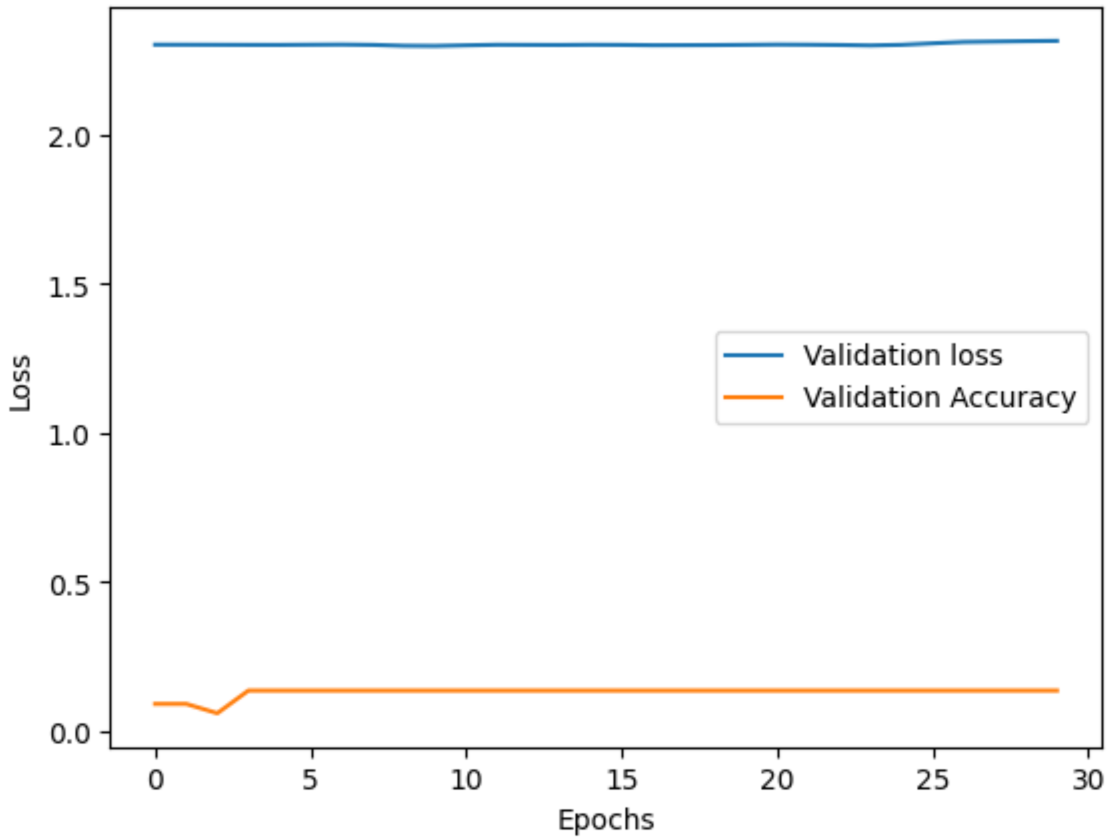
```
losses = dictionary['losses']
accuracies = dictionary['accuracies']
accuracies = np.asarray(accuracies)
losses = np.asarray(losses)
plt.figure()
plt.plot(np.arange(len(losses)),losses,label='Training loss')
plt.plot(np.arange(len(accuracies)),accuracies,label='Training Accuracy')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.legend()

val_losses = dictionary['val_losses']
val_accuracies = dictionary['val_accuracies']
val_accuracies = np.asarray(val_accuracies)
val_losses = np.asarray(val_losses)
plt.figure()
plt.plot(np.arange(len(val_losses)),val_losses,label='Validation loss')
plt.plot(np.arange(len(val_accuracies)),val_accuracies,label='Validation Accuracy')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.legend()
```

```
<matplotlib.legend.Legend at 0x7f716c277d00>
```








```
#feed forward into the model with the test data from MNIST and compare the results
output = model.forward(torch.tensor(normalized_test_set_x, dtype = torch.float32))
sum = 0
for i in range(len(output)):
  if (test_set_y[i] == torch.argmax(output[i])):
    sum += 1
print(sum/len(output))
```

```
0.1034
```

(D)

```
class ConvMLP2(nn.Module):
    def __init__(self):
        super(ConvMLP2, self).__init__()
        self.conv = nn.ModuleList([nn.Conv2d(3, 16, kernel_size=3, stride=1, paddir
                                   nn.Conv2d(16, 16, kernel_size=3, stride=1, paddir
        self.pool = nn.MaxPool2d(kernel_size=2, stride=2)
        self.fc = nn.ModuleList([nn.Linear(16 * 8 * 8, 128), nn.Linear(128, 10)])
        self.activation = nn.ReLU()

    def forward(self, x):
        x = self.pool(self.activation(self.conv[0](x)))
        x = self.pool(self.activation(self.conv[1](x)))
        x = nn.Flatten()(x)
        x = self.activation(self.fc[0](x))
        x = self.activation(self.fc[1](x))
        return x


model = ConvMLP2()
summary(model, (3, 32, 32))
```

```
----------------------------------------------------------------
        Layer (type)               Output Shape         Param #
================================================================
            Conv2d-1           [-1, 16, 32, 32]             448
              ReLU-2           [-1, 16, 32, 32]               0
         MaxPool2d-3           [-1, 16, 16, 16]               0
            Conv2d-4           [-1, 16, 16, 16]           2,320
              ReLU-5           [-1, 16, 16, 16]               0
         MaxPool2d-6             [-1, 16, 8, 8]               0
            Linear-7                  [-1, 128]         131,200
              ReLU-8                  [-1, 128]               0
            Linear-9                   [-1, 10]           1,290
             ReLU-10                   [-1, 10]               0
================================================================
Total params: 135,258
Trainable params: 135,258
Non-trainable params: 0
----------------------------------------------------------------
Input size (MB): 0.01
Forward/backward pass size (MB): 0.35
Params size (MB): 0.52
Estimated Total Size (MB): 0.88
----------------------------------------------------------------
```

```
def Kfold_validation_2(n, inputs, outputs):

    total_num=len(inputs)
    kf=KFold(n_splits=n,shuffle=True)
```

```
    for train_selector,test_selector in kf.split(range(total_num)):
        ### Decide training examples and testing examples for this fold ###
        train_Xs= inputs[train_selector]
        test_Xs=  inputs[test_selector]
        train_ys= outputs[train_selector]
        test_ys= outputs[test_selector]

        model = ConvMLP2()
        t = Trainer(model, optimizer_type='adam', learning_rate=1e-3, epoch=30, bat
        train_in,val_in,train_real,val_real=train_test_split(train_Xs,train_ys, tra

        dictionary = t.train(train_in, train_real, val_in, val_real,early_stop=Fals

    return dictionary, model


dictionary, model = Kfold_validation_2(3, normalized_train_set_x[0:1000], train_set
```

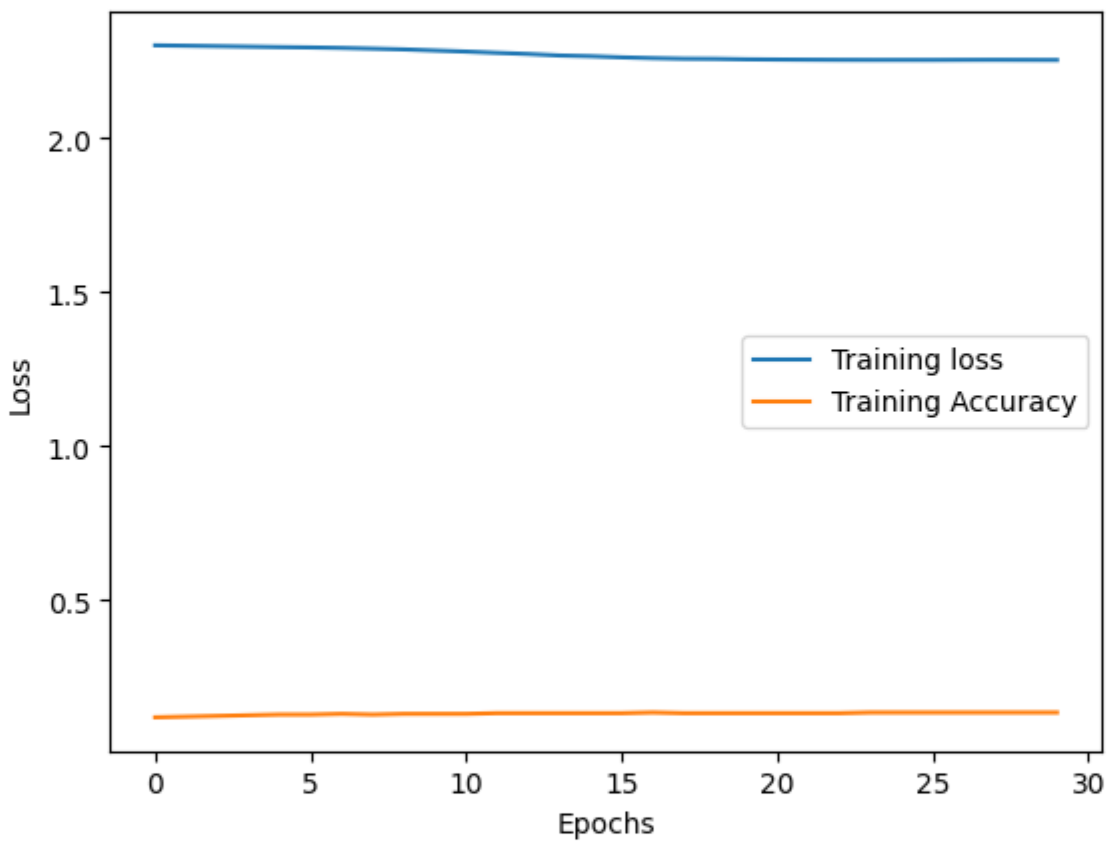
```
  0%|          | 0/30 [00:00<?, ?it/s]<ipython-input-141-5a654197e45b>:125: Us
  inputs = torch.tensor(inputs, dtype=torch.float32)
<ipython-input-141-5a654197e45b>:126: UserWarning: To copy construct from a te
  outputs = torch.tensor(outputs, dtype=torch.long)
  3%|▎         | 1/30 [00:00<00:08,  3.36it/s]Epoch 1/30 - Loss: 2.301 - Acc:
             Val_loss: 2.300 - Val_acc: 0.130
 37%|███▋      | 11/30 [00:02<00:04,  4.58it/s]Epoch 11/30 - Loss: 2.300 - Acc
             Val_loss: 2.301 - Val_acc: 0.112
 70%|███████   | 21/30 [00:05<00:02,  3.24it/s]Epoch 21/30 - Loss: 2.300 - Acc
             Val_loss: 2.301 - Val_acc: 0.112
func:'train'  took: 7.7381 sec
  3%|▎         | 1/30 [00:00<00:06,  4.73it/s]Epoch 1/30 - Loss: 2.298 - Acc:
             Val_loss: 2.301 - Val_acc: 0.099
 37%|███▋      | 11/30 [00:02<00:04,  4.64it/s]Epoch 11/30 - Loss: 2.271 - Acc
             Val_loss: 2.306 - Val_acc: 0.126
 70%|███████   | 21/30 [00:04<00:01,  4.64it/s]Epoch 21/30 - Loss: 2.253 - Acc
             Val_loss: 2.300 - Val_acc: 0.126
func:'train'  took: 6.4801 sec
  3%|▎         | 1/30 [00:00<00:06,  4.75it/s]Epoch 1/30 - Loss: 2.301 - Acc:
             Val_loss: 2.304 - Val_acc: 0.090
 37%|███▋      | 11/30 [00:02<00:04,  3.83it/s]Epoch 11/30 - Loss: 2.281 - Acc
             Val_loss: 2.308 - Val_acc: 0.117
 70%|███████   | 21/30 [00:05<00:02,  3.87it/s]Epoch 21/30 - Loss: 2.255 - Acc
             Val_loss: 2.304 - Val_acc: 0.117
                              func:'train'  took: 7.4687 sec
```

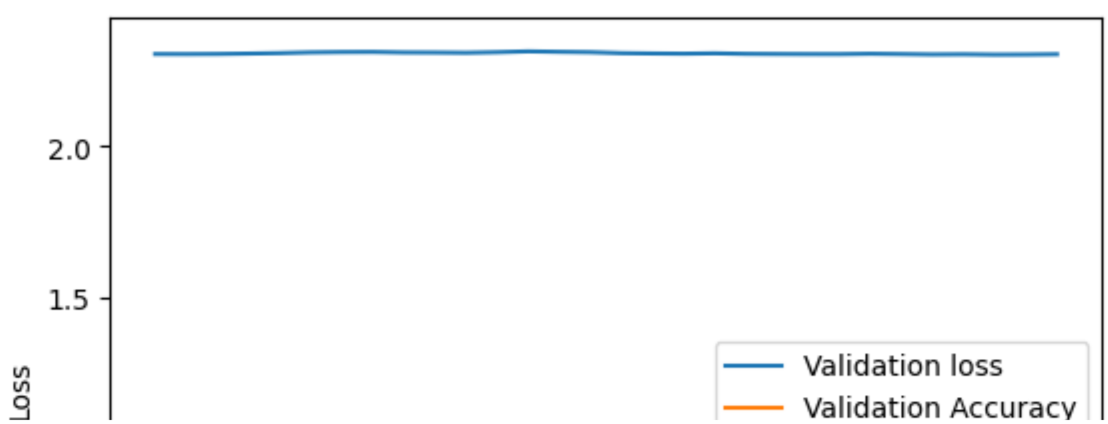
```
losses = dictionary['losses']
accuracies = dictionary['accuracies']
accuracies = np.asarray(accuracies)
losses = np.asarray(losses)
plt.figure()
plt.plot(np.arange(len(losses)),losses,label='Training loss')
```

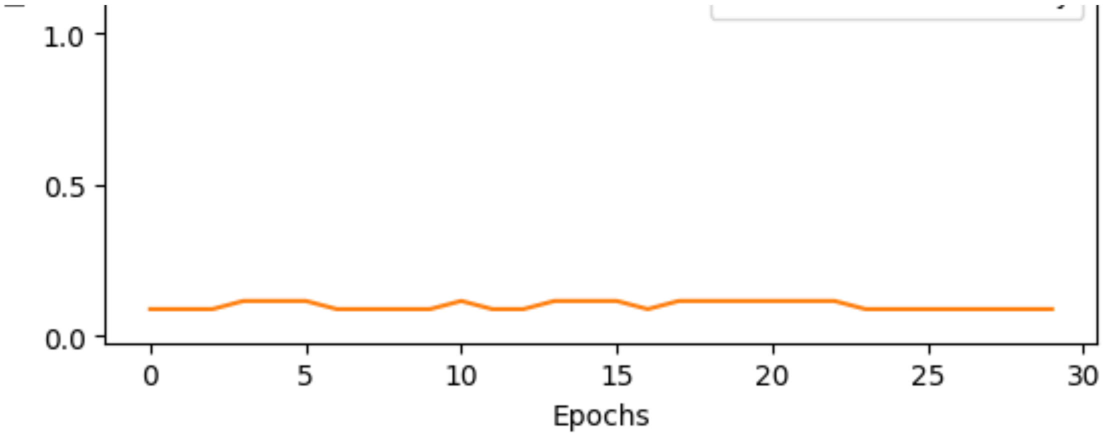
```
plt.plot(np.arange(len(accuracies)),accuracies,label='Training Accuracy')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.legend()

val_losses = dictionary['val_losses']
val_accuracies = dictionary['val_accuracies']
val_accuracies = np.asarray(val_accuracies)
val_losses = np.asarray(val_losses)
plt.figure()
plt.plot(np.arange(len(val_losses)),val_losses,label='Validation loss')
plt.plot(np.arange(len(val_accuracies)),val_accuracies,label='Validation Accuracy')
plt.xlabel('Epochs')
plt.ylabel('Loss')
plt.legend()
```

```
<matplotlib.legend.Legend at 0x7f7199390d60>
```






1.0
0.5
0.0
0
5
10
15
20
25
30
Epochs