CHEM277B Homework 9

Trevor Oldham

(A)

Process the MNIST data set into a training and test set, with one channel of 32x32 images.

```
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)

normalized_train_set_x = gray_img_train / 255
normalized_train_set_x = normalized_train_set_x.reshape((-1, 1, 32, 32))

print(normalized_train_set_x.shape)


gray_img_test = np.array(validation_set[0]).astype('uint8')
gray_img_test = gray_img_test.reshape(10000, 32, 32)

normalized_test_set_x = gray_img_test / 255
normalized_test_set_x = normalized_test_set_x.reshape((-1, 1, 32, 32))

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, 1, 32, 32)
```

Create a pytorch model based on the specifications in the homework problem.

```
import torch
from torch import nn
class CNN(nn.Module):
    def __init__(self):
        super(CNN, self).__init__()
        self.conv = nn.ModuleList([nn.Conv2d(1, 6, kernel_size=6, padding=2), # be
                                   nn.Conv2d(6, 12, kernel_size=5, padding=2)]) # (E
        self.pooling = nn.ModuleList([nn.MaxPool2d(kernel_size=3), nn.MaxPool2d(ke
        self.fc = nn.ModuleList([nn.Linear(300,300),nn.Linear(300,10)])
        self.activation = nn.ReLU()
        self.bn = [nn.BatchNorm2d(6), nn.BatchNorm2d(12)]

    def forward(self, inp):
        x = self.bn[0](self.conv[0](inp))
        x = self.pooling[0](self.activation(x))
        x = self.pooling[1](self.activation(self.bn[1](self.conv[1](x))))
        x = nn.Flatten()(x)
        residual = x
        y = self.fc[0](x)
        y = y + residual
        y = self.activation(y)
        y = nn.Softmax(dim = -1)(self.fc[1](y))
        return y
```

```
from torchsummary import summary
model = CNN()
summary(model, (1, 32, 32))
```

```
----------------------------------------------------------------
        Layer (type)               Output Shape         Param #
================================================================
            Conv2d-1            [-1, 6, 31, 31]             222
              ReLU-2            [-1, 6, 31, 31]               0
         MaxPool2d-3            [-1, 6, 10, 10]               0
            Conv2d-4           [-1, 12, 10, 10]           1,812
              ReLU-5           [-1, 12, 10, 10]               0
         MaxPool2d-6             [-1, 12, 5, 5]               0
            Linear-7                  [-1, 300]          90,300
              ReLU-8                  [-1, 300]               0
            Linear-9                   [-1, 10]           3,010
================================================================
Total params: 95,344
Trainable params: 95,344
Non-trainable params: 0
----------------------------------------------------------------
Input size (MB): 0.00
```

```
Forward/backward pass size (MB): 0.12
Params size (MB): 0.36
Estimated Total Size (MB): 0.49
----------------------------------------------------------------
```

Create a trainer class to train the model.

```
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
```

```
        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()
        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)
```

```
        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
```

Run the model with and without batch normalization. Which give you better test accuracy?

```
import matplotlib.pyplot as plt

def train_and_validate(model, inputs, outputs):

  total_num=len(inputs)

  model = model
  t = Trainer(model, optimizer_type='adam', learning_rate=1e-3, epoch=30, batch_siz
  train_in,val_in,train_real,val_real=train_test_split(inputs,outputs, train_size =

  dictionary = t.train(train_in, train_real, val_in, val_real,early_stop=True,l2=Fa

  return dictionary, model
```

Running the model with batch normalization:

```
model = CNN()
dictionary_1, model_1 = train_and_validate(model, normalized_train_set_x[0:10000],
```

```
  0%|          | 0/30 [00:00<?, ?it/s]<ipython-input-23-5a654197e45b>:125: Us
  inputs = torch.tensor(inputs, dtype=torch.float32)
<ipython-input-23-5a654197e45b>:126: UserWarning: To copy construct from a te
  outputs = torch.tensor(outputs, dtype=torch.long)
  3%|▍         | 1/30 [00:03<01:44,  3.61s/it]Epoch 1/30 - Loss: 1.684 - Acc:
               Val_loss: 1.695 - Val_acc: 0.794
 37%|███▋      | 11/30 [00:43<01:14,  3.94s/it]Epoch 11/30 - Loss: 1.478 - Ac
               Val_loss: 1.494 - Val_acc: 0.971
 70%|███████   | 21/30 [01:23<00:37,  4.13s/it]Epoch 21/30 - Loss: 1.469 - Ac
               Val_loss: 1.487 - Val_acc: 0.976
                                       func:'train'  took: 121.5386 s
```

Create a new CNN model without batch normalization.

```
class CNN_2(nn.Module):
    def __init__(self):
        super(CNN_2, self).__init__()
        self.conv = nn.ModuleList([nn.Conv2d(1, 6, kernel_size=6, padding=2), # be1
                                   nn.Conv2d(6, 12, kernel_size=5, padding=2)]) # (E
        self.pooling = nn.ModuleList([nn.MaxPool2d(kernel_size=3), nn.MaxPool2d(ke1
        self.fc = nn.ModuleList([nn.Linear(300,300),nn.Linear(300,10)])
        self.activation = nn.ReLU()


    def forward(self, inp):
        x = self.conv[0](inp)
        x = self.pooling[0](self.activation(x))
        x = self.pooling[1](self.activation(self.conv[1](x)))
        x = nn.Flatten()(x)
        residual = x
        y = self.fc[0](x)
        y = y + residual
        y = self.activation(y)
        y = nn.Softmax(dim = -1)(self.fc[1](y))
        return y


model = CNN_2()
summary(model, (1, 32, 32))
```

```
----------------------------------------------------------------
        Layer (type)               Output Shape         Param #
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            Conv2d-1            [-1, 6, 31, 31]             222
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              ReLU-5           [-1, 12, 10, 10]               0
         MaxPool2d-6             [-1, 12, 5, 5]               0
            Linear-7                  [-1, 300]          90,300
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Total params: 95,344
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Non-trainable params: 0
----------------------------------------------------------------
Input size (MB): 0.00
Forward/backward pass size (MB): 0.12
Params size (MB): 0.36
Estimated Total Size (MB): 0.49
----------------------------------------------------------------
```
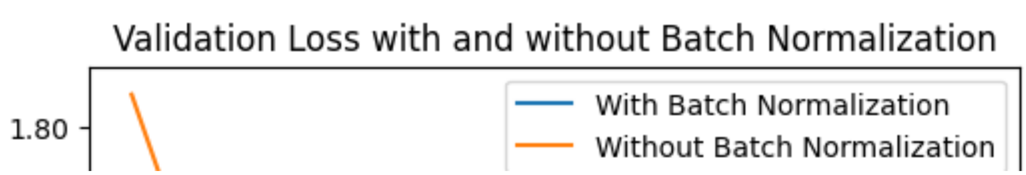

```
model = CNN_2()
```

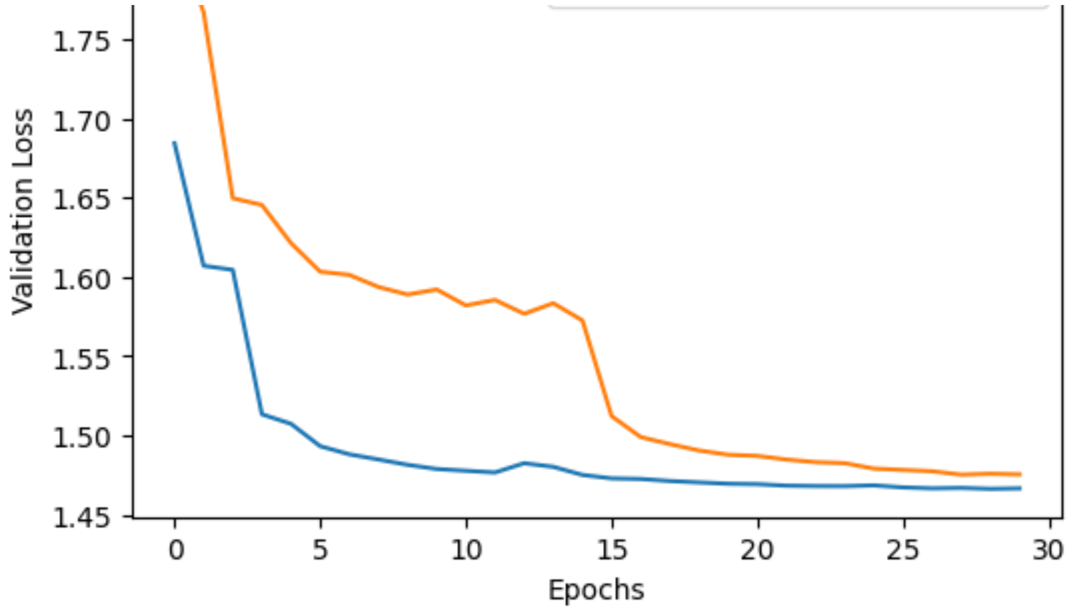
```
model = CNN_2()
dictionary_2, model_2 = train_and_validate(model, normalized_train_set_x[0:10000],
```

```
  0%|          | 0/30 [00:00<?, ?it/s]<ipython-input-23-5a654197e45b>:125: Us
  inputs = torch.tensor(inputs, dtype=torch.float32)
<ipython-input-23-5a654197e45b>:126: UserWarning: To copy construct from a te
  outputs = torch.tensor(outputs, dtype=torch.long)
  3%|▎         | 1/30 [00:03<01:51,  3.84s/it]Epoch 1/30 - Loss: 1.820 - Acc:
            Val_loss: 1.807 - Val_acc: 0.693
 37%|███▋      | 11/30 [00:34<00:58,  3.08s/it]Epoch 11/30 - Loss: 1.582 - Ac
            Val_loss: 1.592 - Val_acc: 0.873
 70%|███████   | 21/30 [01:07<00:28,  3.18s/it]Epoch 21/30 - Loss: 1.487 - Ac
            Val_loss: 1.500 - Val_acc: 0.964
                          func:'train'  took: 95.7824 se
```

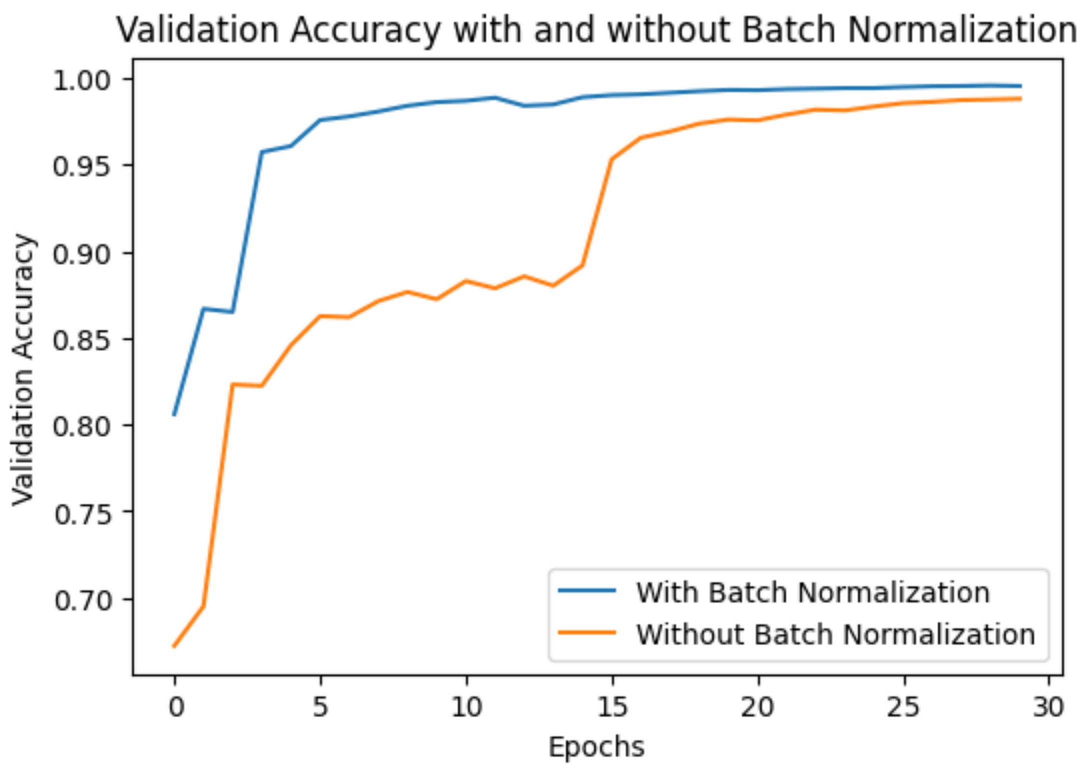
Plot the resulting Training Error and Training Accuracy

```
fig, ax = plt.subplots(1, 1, figsize=[6, 4])
losses_1 = dictionary_1['losses']
losses_1 = np.asarray(losses_1)
losses_2 = dictionary_2['losses']
losses_2 = np.asarray(losses_2)

plt.plot(np.arange(len(losses_1)),losses_1,label='With Batch Normalization')
plt.plot(np.arange(len(losses_2)), losses_2, label = 'Without Batch Normalization')
plt.xlabel('Epochs')
plt.ylabel('Validation Loss')
plt.title("Validation Loss with and without Batch Normalization")
plt.legend()
plt.show()

########################

fig, ax = plt.subplots(1, 1, figsize=[6, 4])
acc_1 = dictionary_1['accuracies']
acc_1 = np.asarray(acc_1)
acc_2 = dictionary_2['accuracies']
acc_2 = np.asarray(acc_2)

plt.plot(np.arange(len(acc_1)),acc_1,label='With Batch Normalization')
plt.plot(np.arange(len(acc_2)), acc_2, label = 'Without Batch Normalization')
plt.xlabel('Epochs')
plt.ylabel('Validation Accuracy')
plt.title("Validation Accuracy with and without Batch Normalization")
plt.legend()
```






```
<matplotlib.legend.Legend at 0x7f21c82079a0>
```



The testing accuracy is best when the model is run with batch normalization enabled, and the loss is minimized faster over fewer training epochs. Both models approach a similar value for validation accuracy but the first model trains faster.

(B)

Run the model with and without the skip connection at learning rate of 5e-3 for 10 epochs. Do you see faster training and/or better test accuracy with the skip connection?

```
### define a model with no skip connection
class CNN_3(nn.Module):
    def __init__(self):
        super(CNN_3, self).__init__()
        self.conv = nn.ModuleList([nn.Conv2d(1, 6, kernel_size=6, padding=2), # bef
                                  nn.Conv2d(6, 12, kernel_size=5, padding=2)]) # (E
        self.pooling = nn.ModuleList([nn.MaxPool2d(kernel_size=3), nn.MaxPool2d(ker
        self.fc = nn.ModuleList([nn.Linear(300,300),nn.Linear(300,10)])
        self.activation = nn.ReLU()
        self.bn = [nn.BatchNorm2d(6), nn.BatchNorm2d(12)]

    def forward(self, inp):
        x = self.bn[0](self.conv[0](inp))
        x = self.pooling[0](self.activation(x))
        x = self.pooling[1](self.activation(self.bn[1](self.conv[1](x))))
        x = nn.Flatten()(x)

        x = self.fc[0](x)

        x = self.activation(x)
        x = nn.Softmax(dim = -1)(self.fc[1](x))
        return x
```

Define a new train and validation function with a learning rate of 5e-3 and 10 epochs.

```
def train_and_validate_2(model, inputs, outputs):

  total_num=len(inputs)

  model = model
  t = Trainer(model, optimizer_type='adam', learning_rate=5e-3, epoch=10, batch_siz
  train_in,val_in,train_real,val_real=train_test_split(inputs,outputs, train_size =

  dictionary = t.train(train_in, train_real, val_in, val_real,early_stop=True,l2=Fa

  return dictionary, model
```

Run the model without the skip connection and record the validation loss and accuracy over 10 epochs.

```
model = CNN_3()
dictionary_3, model_3 = train_and_validate_2(model, normalized_train_set_x[0:10000]
```

```
    0%|          | 0/10 [00:00<?, ?it/s]<ipython-input-23-5a654197e45b>:125: Use
    inputs = torch.tensor(inputs, dtype=torch.float32)
  <ipython-input-23-5a654197e45b>:126: UserWarning: To copy construct from a ter
```

```
  outputs = torch.tensor(outputs, dtype=torch.long)
 10%|█          | 1/10 [00:04<00:37,  4.14s/it]Epoch 1/10 - Loss: 1.599 - Acc:
             Val_loss: 1.610 - Val_acc: 0.854
                                                   func:'train'  took: 40.2127 se
```

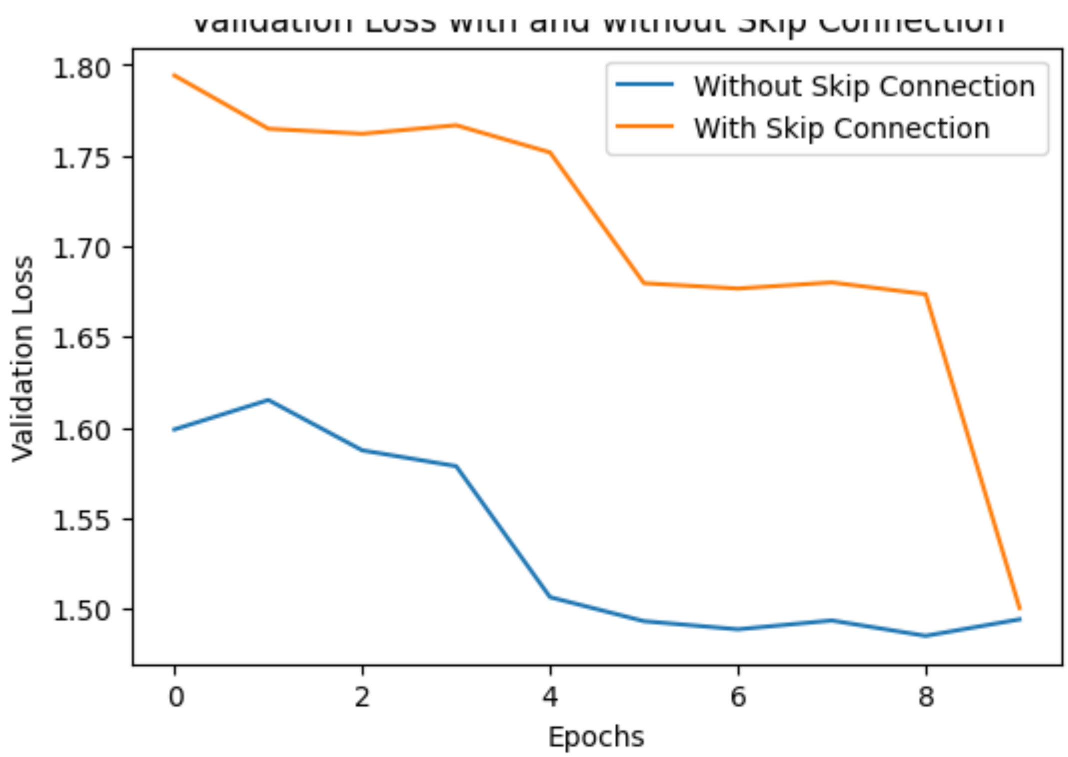
Run the model with the skip connection and record the validation loss and accuracy over 10 epochs.

```
model = CNN()
dictionary_4, model_4 = train_and_validate_2(model, normalized_train_set_x[0:10000]
```

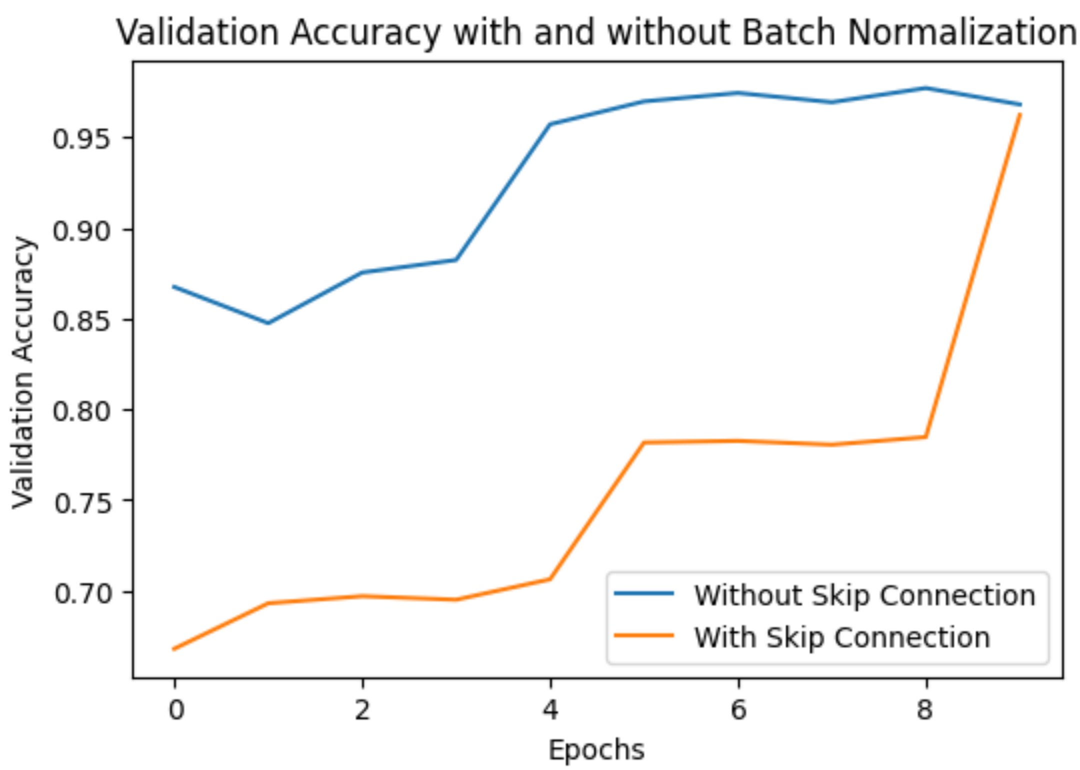
```
  0%|          | 0/10 [00:00<?, ?it/s]<ipython-input-23-5a654197e45b>:125: Us
  inputs = torch.tensor(inputs, dtype=torch.float32)
<ipython-input-23-5a654197e45b>:126: UserWarning: To copy construct from a te
  outputs = torch.tensor(outputs, dtype=torch.long)
 10%|█          | 1/10 [00:03<00:35,  3.99s/it]Epoch 1/10 - Loss: 1.794 - Acc:
             Val_loss: 1.809 - Val_acc: 0.653
                                                   func:'train'  took: 40.2632 se
```

```
fig, ax = plt.subplots(1, 1, figsize=[6, 4])
losses_3 = dictionary_3['losses']
losses_3 = np.asarray(losses_3)
losses_4 = dictionary_4['losses']
losses_4 = np.asarray(losses_4)

plt.plot(np.arange(len(losses_3)),losses_3,label='Without Skip Connection')
plt.plot(np.arange(len(losses_4)), losses_4, label = 'With Skip Connection')
plt.xlabel('Epochs')
plt.ylabel('Validation Loss')
plt.title("Validation Loss with and without Skip Connection")
plt.legend()
plt.show()

########################

fig, ax = plt.subplots(1, 1, figsize=[6, 4])
acc_3 = dictionary_3['accuracies']
acc_3 = np.asarray(acc_3)
acc_4 = dictionary_4['accuracies']
acc_4 = np.asarray(acc_4)

plt.plot(np.arange(len(acc_3)),acc_3,label='Without Skip Connection')
plt.plot(np.arange(len(acc_4)), acc_4, label = 'With Skip Connection')
plt.xlabel('Epochs')
plt.ylabel('Validation Accuracy')
plt.title("Validation Accuracy with and without Batch Normalization")
plt.legend()
```

Validation Loss with and without Skip Connection




```
<matplotlib.legend.Legend at 0x7f21c87753a0>
```



It seems counterintuitive but the results show that the model without a skip connection will start out with higher accuracy and lower loss, but at the point of epoch 10 the two models approach the same value. I imagine that the model with the recurrence layer will begin to perform better than the other model as the epochs increase past ten, and eventually improve to a higher accuracy as the training progresses further. We could run the model again with 30 epochs to observe if this is true observe if this is true.