Part 1. Neural Networks using NumPy

1.1 Helper Functions

1. ReLU():

def relu(x):

2. Softmax():

return x*(x>0)

```
def softmax(x):
    return np.exp(x)/np.sum(np.exp(x),axis=0)
```

3. compute():

```
def computeLayer(X, W, b):
    S = np.dot(np.tranpose(W),X) + b
    return S
```

4. averageCE():

```
def CE(target, prediction):
    return -np.sum(np.sum(np.transpose(target)*np.log(prediction),axis=0))/len(target)
```

5. gradCE():

aveage CE =
$$-\frac{1}{N} \sum_{n=1}^{N} \sum_{k=1}^{K} t_k^n \log s_k^n$$

compute gradient of Cross Entropy loss E with respect to activation function: $\frac{\partial E}{\partial a_j}$ where E is the average CE, a_i is the activation function input.

For simplicity set N = 1, then E =
$$-\sum_{k=1}^{K} t_k \log s_k$$

Then softmax function output is $s_k = \frac{e^{a_k}}{\sum_{k=1}^{k} e^{a_k}}$
 $\frac{\partial E}{\partial a_j} = \frac{\partial E}{\partial s_k} \frac{\partial s_k}{\partial a_j} = -\sum_{k=1}^{k} \frac{t_k}{s_k} \frac{\partial s_k}{\partial a_j} \quad j = 1, \dots, K$
For $j = k$, $\frac{\partial s_k}{\partial a_j} = \frac{e^{a_j}(\sum_{k=1}^{k} e^{a_k} - e^{a_j})}{(\sum_{k=1}^{k} e^{a_k})^2} = s_k(1 - s_j)$

For
$$j \neq k$$
, $\frac{\partial s_k}{\partial a_j} = \frac{-e^{a_j}e^{a_k}}{\left(\sum_{k=1}^k e^{a_k}\right)^2} = -s_j s_k$

Combine all the equations above,

$$\frac{\partial E}{\partial a_j} = -t_j (1 - s_j) + \sum_{k \neq j} t_k s_j = s_j - t_j \quad j = 1, \dots K$$

def gradCE(target, prediction):

gradientCE = np.transpose(prediction - np.transpose(target))

return gradientCE

1.2 Backward Propagation

1. The gradient of the loss with respect to the outer layer weights

$$\frac{\partial L}{\partial w_0} = \frac{\partial L}{\partial a_i} \frac{\partial a_j}{\partial w_0} = \bar{x} \cdot (\bar{s} - \bar{t})^T$$

where:

x is the output data from the first layer

t is the data label

s is the output from softmax

2. The gradient of the loss with respect to the outer layer biases:

$$\frac{\partial L}{\partial b_0} = \frac{\partial L}{\partial a_i} \frac{\partial a_j}{\partial b_0} = (\bar{s} - \bar{t})^T$$

where:

t is the data label

s is the output from softmax

3. The gradient of the loss with respect to the hidden layer weights:

$$\frac{\partial L}{\partial w_h} = \mathbf{x}^{(0)} \cdot (\mathbf{w}^{(2)} \cdot \delta^{(2)} \otimes \theta'(s^{(1)}))^T$$

$$\theta'(s^{(1)}) = \text{derivative of ReLu} = 0 \text{ if } s^{(1)} < 0, \qquad 1 \text{ if } s^{(1)} > 0$$

where:

x⁽⁰⁾ is the input data

w⁽²⁾ is the weight matrices for the outer layer

 $\delta^{(2)}$ is the derivative of loss with respect to softmax input

 θ ' is the derivative of the ReLu

4. The gradient of the loss with respect to the hidden layer biases:

$$\frac{\partial \mathbf{L}}{\partial \mathbf{b_h}} = (\mathbf{w}^{(2)} \cdot \delta^{(2)} \otimes \theta'(s^{(1)}))^T$$

where:

w⁽²⁾ is the weight matrices for the outer layer

 $\delta^{\ ^{(2)}}$ is the derivative of loss with respect to softmax input

 θ ' is the derivative of the ReLu

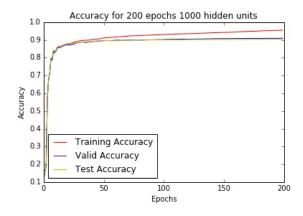
For neural network update implementation, the gradients are the averages of all sample data gradients.

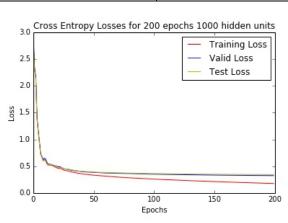
```
1. def grad_weight2(X,Y,S):
2. delta = gradCE(Y,S)
   return np.dot(X,delta)/len(Y)
4.
   def grad_bias2(Y,S):
5.
6. b = np.sum((S-np.transpose(Y)),axis=1)
7. return np.transpose(np.reshape(b,(len(b),1)))/len(Y)
8.
9. def d relu(x):
10. x[x<=0] = 0
11. x[x>0] = 1
12. return x
13.
14. def grad_weight1(X,W,delta,dtheta):
15. delta0 = np.transpose(np.dot(W,np.transpose(delta))*dtheta)
16. return np.dot(X,delta0)/len(X[1,:])
17.
18. def grad_bias1(W,delta,dtheta):
19. b = np.sum(np.transpose(np.dot(W,np.transpose(delta))*dtheta),axis=0)
20. return np.transpose(np.reshape(b,(len(W),1)))/len(delta)
```

1.3 Learning

For implementation of the model, epoch is set to 200 with 1000 hidden units. The learning rate is set to 0.05 with with a momentum parameter 0.9. The weights and biases are initialized via Xavier initialization scheme.

| | Train | Validation | Test |
|----------|--------|------------|--------|
| Loss | 0.1787 | 0.3255 | 0.3451 |
| Accuracy | 0.9547 | 0.9095 | 0.9035 |



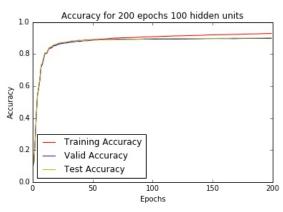


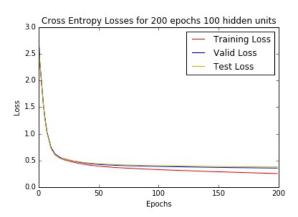
1.4 Hyperparameter Investigation

1. Number of Hidden Units

1. Hidden units = 100

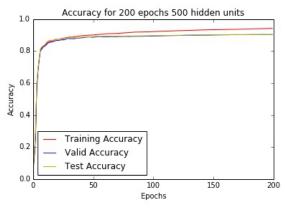
| | Train | Validation | Test |
|----------|--------|------------|--------|
| Loss | 0.2562 | 0.3584 | 0.3784 |
| Accuracy | 0.9298 | 0.8990 | 0.9023 |

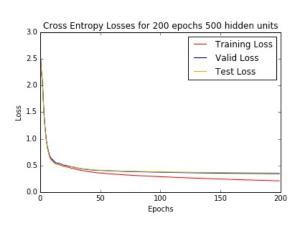




2. Hidden units = 500

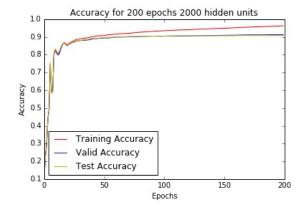
| | Train | Validation | Test |
|----------|--------|------------|--------|
| Loss | 0.2123 | 0.3456 | 0.3614 |
| Accuracy | 0.9422 | 0.9042 | 0.9031 |

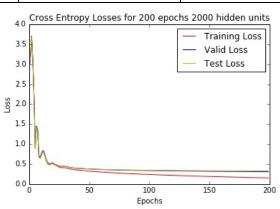




3. Hidden units = 2000

| | Train | Validation | Test |
|----------|--------|------------|--------|
| Loss | 0.1566 | 0.3126 | 0.3309 |
| Accuracy | 0.9628 | 0.9123 | 0.9075 |

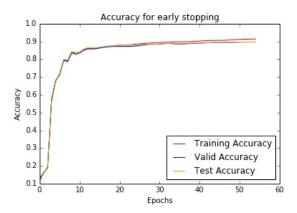


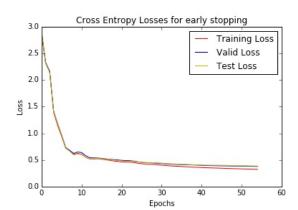


2. Early Stopping

If the accuracy for validation set starts to decrease, then it means that there is overfitting in the training process. In order to implement early stopping in the model, a condition is added to the model. As the training error becomes steady (ie. after 50 epochs), if the validation accuracy starts decreasing, then stop the training process. In this case, for a hidden units of 1000, learning rate of 0.05, the training stops at 55 epochs.

| | Train | Validation | Test |
|----------|--------|------------|--------|
| Loss | 0.3253 | 0.3804 | 0.3877 |
| Accuracy | 0.9137 | 0.8962 | 0.8965 |





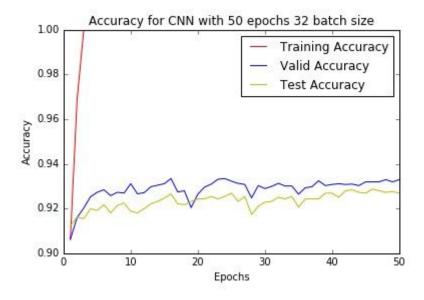
Part 2. Neural Network in Tensorflow

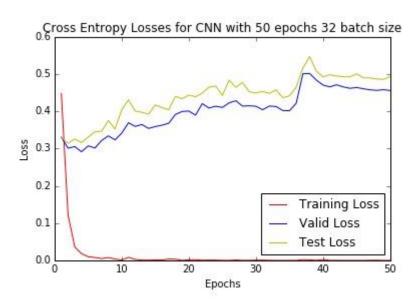
2.1 Model Implementation

```
3. # Define convolutional layer
  def conv_layer(X,W,b,stride=1):
       X = tf.nn.conv2d(X,W,strides=[1,stride,stride,1],padding = 'SAME')
5.
6.
       X = tf.nn.bias_add(X,b)
       return tf.nn.relu(X)
   # Define max pooling layer
8.
  def max pooling(X,K=2):
       return tf.nn.max_pool(X,ksize = [1,K,K,1], strides = [1,K,K,1], padding = 'SAME')
10.
11. # Define batch normalization and flatten layer
12. def batch_norm_flatten(X):
       mean,variance = tf.nn.moments(X,axes=[0,1,2])
13.
14.
       X = tf.nn.batch_normalization(X,mean,variance,offset=None,scale=None,variance_epsilon=1e-3)
15.
       size = X.get_shape().as_list()
       X = tf.reshape(X,[-1,size[1]*size[2]*size[3]])
16.
       return X
17.
   # Define fully connected layer
19. def fully_c(X,W,b):
       return tf.add(tf.matmul(X,W),b)
20.
21. # Combine all the layers together
22. def con_net(X,Y,W,b):
```

```
23.
       conv = conv_layer(X,W['wc1'],b['bc1'],stride=1)
24.
       pool = max_pooling(conv,K=2)
       flatpool = batch_norm_flatten(pool)
25.
       fc1=tf.nn.relu(fully_c(flatpool,W['wfc1'],b['bfc1']))
26.
       fc2=fully c(fc1,W['wfc2'],b['bfc2'])
27.
       return fc2
28.
29.
30. def reshape_data(X):
    return X.reshape(-1,28,28,1)
32.
33. trainData = trainData.reshape(-1,28,28,1)
34. validData = validData.reshape(-1,28,28,1)
35. testData = testData.reshape(-1,28,28,1)
37. epoch = 50
38. batch size = 32
39. learning rate = 1e-4
40. reg=0.5
41. p= 0.25
42.
43. tf.reset_default_graph()
44. weights = {
               'wc1': tf.get_variable('W0', shape=(3,3,1,32), initializer=tf.contrib.layers.xavier_ini
45.
   tializer()),
               'wfc1': tf.get_variable('W1', shape=(14*14*32,784), initializer=tf.contrib.layers.xavie
46.
   r initializer()),
47.
               'wfc2': tf.get_variable('W2', shape=(784,10), initializer=tf.contrib.layers.xavier_init
   ializer())
48.}
49.
50. biases = {
             'bc1': tf.get_variable('B0', shape=(32), initializer=tf.contrib.layers.xavier_initialize
   r()),
             'bfc1': tf.get_variable('B1', shape=(784), initializer=tf.contrib.layers.xavier_initiali
52.
   zer()),
            'bfc2': tf.get_variable('B2', shape=(10), initializer=tf.contrib.layers.xavier_initializ
53.
   er()),
54. }
55. X = tf.placeholder("float",[None, 28,28,1])
56. Y = tf.placeholder("float",[None, 10])
57. keep prob = tf.placeholder("float")
58. pred = con_net(X,Y,weights,biases,keep_prob)
59. last layer = tf.nn.softmax(pred)
60. # Compute the cost through softmax cross entropy function
61. cost = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits_v2(logits=pred,labels=Y))
62. optimizer = tf.train.AdamOptimizer(learning_rate).minimize(cost)
63. correct_prediction = tf.equal(tf.argmax(last_layer, 1), tf.argmax(Y, 1))
64. accuracy = tf.reduce mean(tf.cast(correct prediction, tf.float32))
65.
```

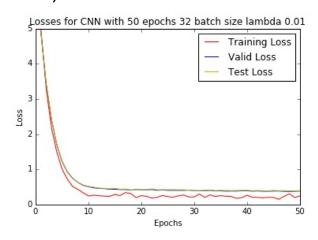
```
66. init = tf.global variables initializer()
67.
68. with tf.Session() as sess:
       sess.run(init)
69.
70.
        train loss = []
71.
       valid_loss = []
72.
       test loss = []
73.
       train_accuracy = []
74.
       valid_accuracy = []
75.
       test_accuracy = []
76.
        iterations = []
       curr itr = 0
77.
78.
        summary_writer = tf.summary.FileWriter('./Output', sess.graph)
79.
        for i in range(epoch):
            trainData, newtrain = shuffle(trainData, newtrain)
80.
            for batch in range(len(trainData)//batch_size):
81.
82.
83.
                batch_x = trainData[batch*batch_size:(batch+1)*batch_size]
                batch_y = newtrain[batch*batch_size:(batch+1)*batch_size]
84.
85.
                opt = sess.run(optimizer, feed_dict={X: batch_x,
86.
                                                                    Y: batch_y, keep_prob:p})
87.
88.
            loss, acc = sess.run([cost, accuracy], feed_dict={X: batch_x,
                                                                    Y: batch_y, keep_prob:p})
89.
            print("Iter " + str(i) + ", Loss= " + \
90.
                          "{:.6f}".format(loss) + ", Training Accuracy= " + \
91.
92.
                          "{:.5f}".format(acc))
93.
            print("Optimization Finished!")
94.
95.
            # Calculate accuracy
            test_acc,test_cost = sess.run([accuracy,cost], feed_dict={X: testData,Y : newtest, keep_pr
96.
   ob:p})
97.
            valid_acc,valid_cost = sess.run([accuracy,cost], feed_dict={X: validData,Y : newvalid, kee
   p_prob:p})
98.
           train_loss.append(loss)
99.
            test_loss.append(test_cost)
100.
             valid_loss.append(valid_cost)
             train_accuracy.append(acc)
101.
102.
             test_accuracy.append(test_acc)
             valid_accuracy.append(valid_acc)
103.
104.
             curr itr+=1
             iterations.append(curr_itr)
105.
             print("Validation Accuracy:","{:.5f}".format(valid_acc))
106.
             print("Testing Accuracy:","{:.5f}".format(test_acc))
107.
108.
        summary_writer.close()
```

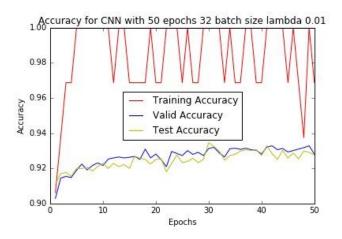


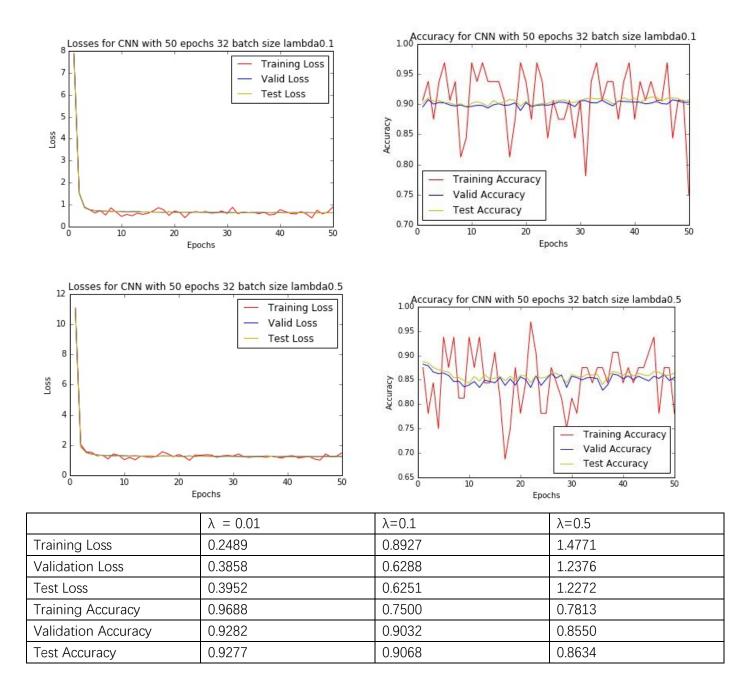


2.3 Hyperparameter Investigation

a) L2 Normalization







Without L2 normalization, there is overfitting in the CNN model implemented above. In section 2.2, the plots have shown that there is a huge gap between the training losses and validation losses. As the training loss gets increasingly smaller, the validation and test losses are getting larger. These are the signals of overfitting of the data. While using L2 regularization parameter of 0.01, the model works well. The are only small differences between the training loss and validation loss, and the validation and test accuracies are improving. The final accuracies are higher, and the losses are smaller when using L2 regularization of 0.01. Therefore, the overfitting is reduced. However, the model is underfitted when using parameter of 0.1 and 0.5 where the losses for validation and training data are almost the same and the training accuracies are highly fluctuated. The final accuracies are worse for parameter of 0.1 and 0.5.

b) Dropout

