CS189–Fall 2015 — Homework 6 Solutions

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1. A. Stochastic Gradient Descent Updates, Square Loss

Derivation for Square Loss

For the stochastic forward pass using square loss, the necessary values to calculate the output layer were
$z^2 = x.W^1$ where x is an input training example appended by a bias column.
$a^2 = tanh(z^2)$, which calculates the activation of the hidden layer. In this implementation, we append a bias column of ones to a^2 here.
$z^3 = a^2.W^2$, the input to the output layer.
And, finally, $h_k(x) = sigmoid(z^3)$, where the loss function is defined as $J = 0.5 * \sum_{k=1}^{n_{out}} (y_k - h_k(x))^2$
Using this, we can compute the gradients $\frac{\partial J}{\partial W^2}$ and $\frac{\partial J}{\partial W^1}$ by repeated application of the chain rule.
First, we calculate $\frac{\partial J}{\partial W^2} = \frac{\partial J}{\partial h_k(x)} * \frac{\partial h_k(x)}{\partial W^2}$
The derivative of the loss function with respect to the output is $\frac{\partial J}{\partial h_k(x)} = -(y - h(x))$.
Now, $\frac{\partial h_k(x)}{\partial W^2} = \frac{\partial h_k(x)}{\partial z^3} * \frac{\partial z^3}{\partial W^2}$.
For the first part, $\frac{\partial h_k(x)}{\partial z^3} = sigmoid'(z^3) = (1 - sigmoid(z^3)) * sigmoid(z^3)$ and as $z^3 = a^2.W^2$, the second part is computed as $\frac{\partial z^3}{\partial W^2} = a^2.T$
Putting this together, $\frac{\partial J}{\partial W^2} = (a^2.T).[(1 - sigmoid(z^3) * sigmoid(z^3).*(-(y - h(x)))]$
Now we can compute $\frac{\partial J}{\partial W^1}$ as $\frac{\partial J}{\partial W^1} = \frac{\partial J}{\partial h_k(x)} * \frac{\partial h_k(x)}{\partial z^3} * \frac{\partial z^3}{\partial W^1}$.
The first two terms in this multiplication we have already computed, and will define as $delta3 = \frac{\partial J}{\partial h_k(x)} * \frac{\partial h_k(x)}{\partial z^3}$.
The final term can be broken into $\frac{\partial z^3}{\partial W^1} = \frac{\partial z^3}{\partial a^2} * \frac{\partial a^2}{\partial z^2} * \frac{\partial z^2}{\partial W^1}$.
Now, again, since $z^3 = a^2.W^2$, $\frac{\partial z^3}{\partial a^2} = a^2.T$.
As $a^2 = tanh(z^2)$, $\frac{\partial a^2}{\partial z^2} = 1 - tanh(z^2)^2$.
Finally, since $z^2 = x.W^1$, the final term is $\frac{\partial z^2}{\partial W^1} = x.T$.
Putting this all together, $\frac{\partial z^3}{\partial W^1} = (x.T).[(delta3.(W2.T)).*(1 - tanh(z^2)^2]$
These two partial derivatives are sufficient to compute the update during stochastic gradient descent, $W1 = W1 - \frac{\partial J}{\partial W^1}$ and $W2 = W2 - \frac{\partial J}{\partial W^2}$

1. B. Stochastic Gradient Descent Updates, Entropy Loss

Derivation for Entropy Loss

The derivation for the gradient descent update using entropy loss is very similar to that for square loss, but the full details are shown here.

For the stochastic forward pass using square loss, the necessary values to calculate the output layer were

$z^2 = x.W^1$ where x is an input training example appended by a bias column.

$a^2 = tanh(z^2)$, which calculates the activation of the hidden layer. In this implementation, we append a bias column of ones to a^2 here.

$z^3 = a^2.W^2$, the input to the output layer.

And, finally, $h_k(x) = sigmoid(z^3)$, where the loss function is defined as $J = -\sum_{k=1}^{n_{out}}[y_k * ln(h_k(x)) + (1 - y_k) * ln(1 - h_k(x))]$

Using this, we can compute the gradients $\frac{\partial J}{\partial W^2}$ and $\frac{\partial J}{\partial W^1}$ by repeated application of the chain rule.

First, we calculate $\frac{\partial J}{\partial W^2} = \frac{\partial J}{\partial h_k(x)} * \frac{\partial h_k(x)}{\partial W^2}$

The derivative of the loss function with respect to the output is $\frac{\partial J}{\partial h_k(x)} = -[\frac{y_k}{h_k(x)} - \frac{1-y_k}{1-h_k(x)}]$.

Now, $\frac{\partial h_k(x)}{\partial W^2} = \frac{\partial h_k(x)}{\partial z^3} * \frac{\partial z^3}{\partial W^2}$.

For the first part, $\frac{\partial h_k(x)}{\partial z^3} = sigmoid'(z^3) = (1 - sigmoid(z^3)) * sigmoid(z^3)$ and as $z^3 = a^2.W^2$, the second part is computed as $\frac{\partial z^3}{\partial W^2} = a^2.T$

Putting this together, $\frac{\partial J}{\partial W^2} = (a^2.T).[(1 - sigmoid(z^3) * sigmoid(z^3). * (\frac{y_k}{h_k(x)} - \frac{1-y_k}{1-h_k(x)})]$

Now we can compute $\frac{\partial J}{\partial W^1}$ as $\frac{\partial J}{\partial W^1} = \frac{\partial J}{\partial h_k(x)} * \frac{\partial h_k(x)}{\partial z^3} * \frac{\partial z^3}{\partial W^1}$.

The first two terms in this multiplication we have already computed, and will define as $delta3 = \frac{\partial J}{\partial h_k(x)} * \frac{\partial h_k(x)}{\partial z^3}$.

The final term can be broken into $\frac{\partial z^3}{\partial W^1} = \frac{\partial z^3}{\partial a^2} * \frac{\partial a^2}{\partial z^2} * \frac{\partial z^2}{\partial W^1}$.

Now, again, since $z^3 = a^2.W^2$, $\frac{\partial z^3}{\partial a^2} = a^2.T$.

As $a^2 = tanh(z^2)$, $\frac{\partial a^2}{\partial z^2} = 1 - tanh(z^2)^2$.

Finally, since $z^2 = x.W^1$, the final term is $\frac{\partial z^2}{\partial W^1} = x.T$.

Putting this all together, $\frac{\partial z^3}{\partial W^1} = (x.T).[(delta3.(W2.T)). * (1 - tanh(z^2)^2]$

These two partial derivatives are sufficient to compute the update during stochastic gradient descent, $W1 = W1 - \frac{\partial J}{\partial W^1}$ and $W2 = W2 - \frac{\partial J}{\partial W^2}$

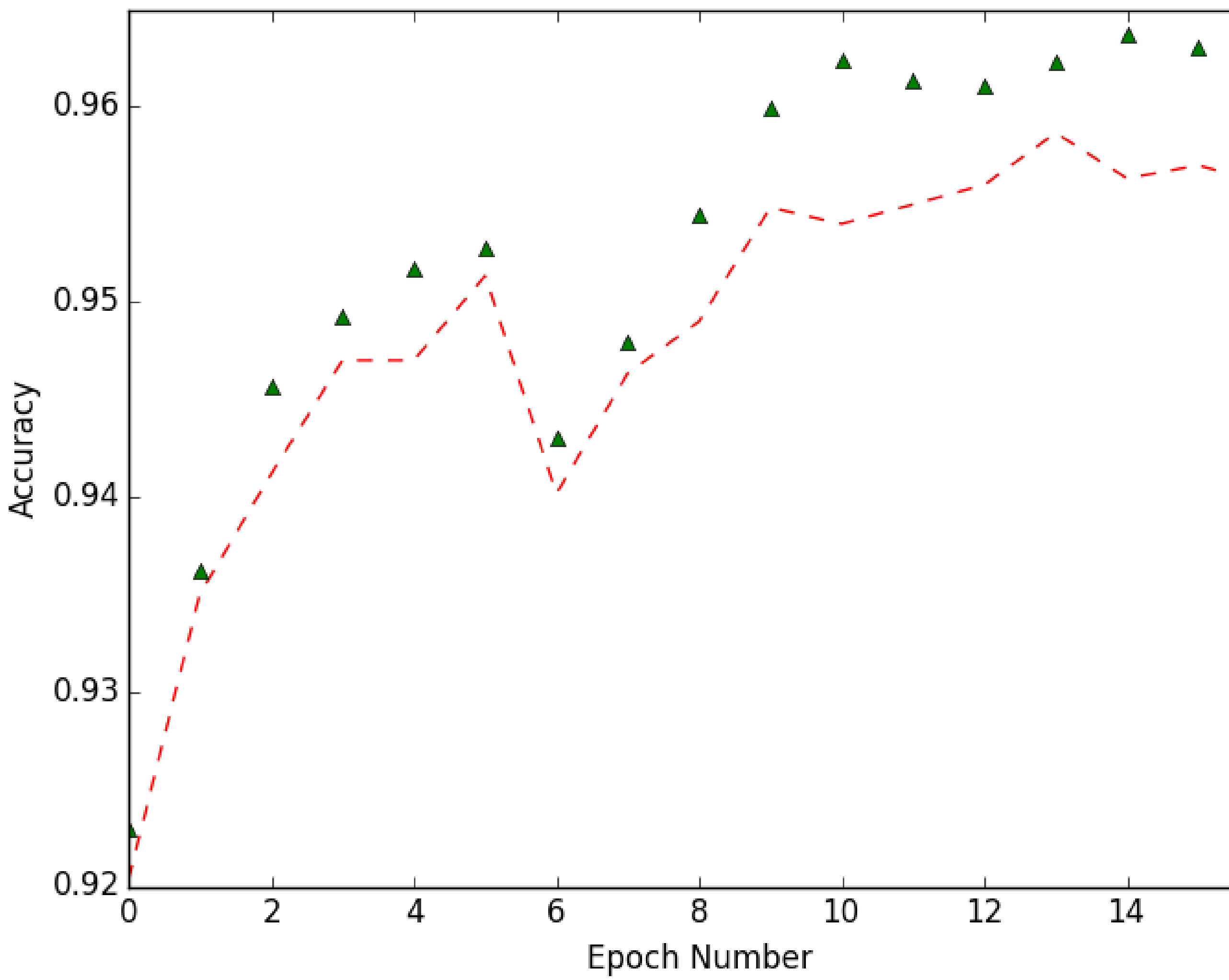
2.Neural Net Implementation

(a) **Hyperparameter tuning**. The learning rate, alpha, and the standard deviation for the weight initialization given mean zero, init scale were both tuned. A good value for alpha was found to be 0.003125 using grid search on a smaller training size, and this proved suitable for the full training set. A good value for init scale was found to be 0.01, and small alterations from this value were not seen to influence the final result significantly.

(b) Final training accuracy on 16 passes through the full training set was found to be 0.95550, with a validation accuracy of 0.96205.

(c) Total running time for 16 epochs was 37 minutes and 16 seconds.

(d) Plots for training error and classification error are given below. Validation error is plotted by red dashes, training accuracy is shown by green triangles.



(e) Interestingly, I found square error to work better (train faster) than entropy loss. This may have been an error with my implementation of entropy loss backpropogation (or a failure to find properly tuned values of alpha), as square error places too much emphasis on incorrect outputs and entropy loss should train faster than square error in this case.

3. Implementation Notes and Kaggle Score

Using a 'smoothed rectifier unit' as the choice of nonlinearity instead of tanh did speed up training, but did not improve overall results and so is not included here.
My final Kaggle Score was 0.95560.

4. Code

```
import random
import csv
import numpy as np
from scipy.io import loadmat
import time
import matplotlib.pyplot as plt

######    Establish some Data Constants    ######
######    for easy access                                ######

image_size = 28*28
image_count = 60000
test_image_count = 10000

######    Load Train Data                  ######

train_data = loadmat("./dataset/train.mat")

train_images = train_data["train_images"]
train_labels = train_data["train_labels"]

train_images = np.swapaxes(train_images, 0, 2)
train_images = np.reshape(train_images, (image_count, image_size))

train_temp = np.zeros((train_images.shape[0], 10))

# Adjust labels for 10 categories
for i in range(train_labels.shape[0]):
        k = train_labels[i]
        train_temp[i][k] = 1

train_labels = train_temp

# Randomly shuffle training data
data = zip(train_images, train_labels)
np.random.shuffle(data)
(X, y) = zip(*data)
train_images = np.array(X)
train_labels = np.array(y)


###### Load Test Data                                      ######

test_data = loadmat("./dataset/test.mat")

test_images = test_data["test_images"]
test_images = np.swapaxes(test_images, 0, 2)
test_images = np.reshape(test_images, (test_image_count, image_size))


######### CLASS DEFINITION ##########
```

```
class Neural_Network(object):
        def __init__(self, alpha=0.0001, init_scale=0.01):
                # Hyperparamters
                self.inputLayerSize = 784
                self.hiddenLayerSize = 200
                self.outputLayerSize = 10
                self.alpha = alpha
                self.init_scale = init_scale
                self.W1 = np.array(self.init_scale*np.random.randn(self.inputLayerS
                self.W2 = np.array(self.init_scale*np.random.randn(self.hiddenLayer

        def forward(self, X):
                # Forward propogate inputs through the network
                # W1 is (785x200)
                # W2 is (201x10)
                N = X.shape[0]
                bias_col = np.ones((N,1))

                # Append bias and multiply to get hidden layer z2

                self.X_bias = np.concatenate((X, bias_col), axis=1)

                # 1x784 x 784x200 = 1x200
                self.z2 = np.dot(self.X_bias, self.W1)
                # append bias

                # Tanh for hidden layer activation
                # 1x200
                self.a2 = self.smooth_rectifier(self.z2)
                self.a2_bias = np.concatenate((self.a2, bias_col), axis=1)

                # Multiply to get output layer
                # 1x200 * 200*10 = 1x10
                self.z3 = np.dot(self.a2_bias, self.W2)

                # Sigmoid and return self.outputLayerSize predictions
                # 1x10
                yHat = self.sigmoid(self.z3)

                # Return prediction
                return yHat

        def sigmoid(self, z):
                # Apply Numerically stable sigmoid activation function
                z_new = np.zeros(z.shape)
                for i in range(z.shape[0]):
                        for j in range(z.shape[1]):
                                x = z[i][j]
                                if x >= 0:
                                        l = np.exp(-x)
                                        l = 1.0 / (1.0 + l)
                                else:
                                        l = np.exp(x)
                                        l = l / (1.0 + l)
```

```
                    z_new[i][j] = 1

        return z_new
        # return 1/(1+np.exp(-z))

    def sigmoid_prime(self, z):
        # Apply derivative of sigmoid function
        return self.sigmoid(z)*(1-self.sigmoid(z))

    def tanh(self, z):
        # Apply tanh activation function
        return (np.exp(2*z) - 1.0)/(np.exp(2*z) + 1.0)


    def tanh_prime(self, z):
        # Apply derivative of tanh function
        return 1 - np.multiply(self.tanh(z), self.tanh(z))

    def smooth_rectifier(self, z):
        # Numerically stable smooth rectifier
        z_new = np.ones(z.shape)
        for i in range(z.shape[0]):
            for j in range(z.shape[1]):
                x = z[i][j]
                if x >= 15:
                    x = 15
                z_new[i][j] = x

        return np.log(1.0 + np.exp(z_new))

    def smooth_rectifier_prime(self, z):
        # Numerically unstable smooth rectifier prime
        return self.sigmoid(z)

    def coarse_rectifier(self, z):
        # Numerically stable coarse rectifier
        z_new = np.zeros(z.shape)
        for i in range(z.shape[0]):
            for j in range(z.shape[1]):
                x = z[i][j]
                z_new[i][j] = max(0,x)

        return z_new

    def coarse_rectifier_prime(self, z):
        # Numerically stable coarse rectifier derivative
        z_new = np.zeros(z.shape)
        for i in range(z.shape[0]):
            for j in range(z.shape[1]):
                x = z[i][j]
                if (x <= 0):
                    x = 0
                else:
                    x = 1
```

```
                    z_new[i][j] = x

            return z_new

    def square_error_cost(self, X, y):
            self.yHat = self.forward(X)
            J = 0.5*(sum((y-self.yHat)**2))
            return J

    def square_error_prop(self, X, y):
            # Compute derivatives with respect to W1 and W2

            # 1x10
            self.yHat = self.forward(X)

            # Compute dj/dw1
            # delta3 is backprop error at third layer
            # nx10 = nx10 .* nx10
            delta3 = np.multiply((-(y-self.yHat)), self.sigmoid_prime(self.z3))
            # 201x10 = 201xn * nx10
            dJdW2 = np.dot(self.a2_bias.T, delta3)


            # Compute dj/dw2
            # delta2 is backprop error at second layer
            # (nx10 * 10x201) .* nx200
            delta2 = np.multiply(np.dot(delta3, self.W2[0:self.hiddenLayerSize]

            dJdW1 = np.dot(self.X_bias.T, delta2)

            return (dJdW1, dJdW2)

    def entropy_error_prop(self, X, y):
            # Compute derivatives with respect to W1 and W2

            self.yHat = self.forward(X)

            # Compute dj/dw1
            # delta3 is backprop error at third layer
            # 1x10 by 1x10 = 1x10
            cost_grad = np.add(np.divide(y+0.0, self.yHat+0.0), -1*np.divide(1.0
            delta3 = np.multiply(cost_grad, self.sigmoid_prime(self.z3))
            #  200x1 * 1x10 = 200x10
            dJdW2 = np.dot(self.a2_bias.T, delta3)


            # Compute dj/dw2
            # delta2 is backprop error at second layer
            # 1x10 * 10x200 * 1x200
            delta2 = np.multiply(np.dot(delta3, self.W2[0:self.hiddenLayerSize]

            dJdW1 = np.dot(self.X_bias.T, delta2)

            return (dJdW1, dJdW2)
```

```
    def stochastic_train(self, X, y, error="square"):
        for k in range(X.shape[0]):
            if ((k % 20000) == 0):
                print ""
            elif ((k % 1000 ) == 0):
                print ".",

            i = random.choice(range(X.shape[0]))

            ############# Prop ############
            # Compute values for each layer
            # Backprop to find Gradient
            Xin = np.reshape(X[i], (1,X[i].shape[0]))
            Yin = np.reshape(y[i], (1,y[i].shape[0]))
            if (error == "square"):
                dJdW1, dJdW2 = self.square_error_prop(Xin, Yin)
            else:
                dJdW1, dJdW2 = self.entropy_error_prop(Xin, Yin)

            ######## Gradient Descent #####
            # Update weights

            self.W1 = self.W1 - self.alpha*dJdW1
            self.W2 = self.W2 - self.alpha*dJdW2

        return

    def predict(self, X):
        return self.forward(X)

    def score(self, X, y):
        yHat = np.argmax(self.predict(X), axis=1)

        yVal = np.argmax(y, axis=1)
        score = 0
        for i in range(len(yHat)):

            if (yHat[i] == yVal[i]):
                score += 1.0

        print((score+ 0.0) / X.shape[0])
        print ""
        return (score +0.0) / X.shape[0]

    def cv_score(self, X, y, num_folds=10, error="square"):
        print "CV Training Stochastic Model"
        np.random.seed(1)

        data = zip(X,y)
        np.random.shuffle(data)
        (X, y) = zip(*data)
        X = np.array(X)
```

```
        y = np.array(y)
        N = X.shape[0]
        score = 0

        # Train on new cuts
        for i in range(num_folds):

                # Clear weights for training
                self.clear_weights()

                # Establish cuts
                cut0 = int(i*(N/num_folds))
                cut1 = int((i+1)*(N/num_folds))

                # Slice Validation data
                X_val = X[cut0:cut1]
                y_val = y[cut0:cut1]

                # Slice Training data
                X_train = np.concatenate((X[0:cut0],X[cut1:]), axis=0)
                y_train = np.concatenate((y[0:cut0],y[cut1:]), axis=0)

                # Train model
                for i in range(1):
                        self.stochastic_train(X_train, y_train, error)

                # Adjust sum scores across each model
                score += self.score(X_val, y_val)

        return (score +0.0) / num_folds

def cv_plot_score(self, X, y, num_iter=10, error="square"):
        print "CV Training Stochastic Model"
        t = time.clock()
        np.random.seed(1)

        data = zip(X,y)
        np.random.shuffle(data)
        (X, y) = zip(*data)
        X = np.array(X)
        y = np.array(y)
        N = X.shape[0]
        score = 0


        # Clear weights for training
        self.clear_weights()

        # Establish cuts
        cut0 = 0
        cut1 = int(N/10)

        # Slice Validation data
        X_val = X[cut0:cut1]
```

```
                y_val = y[cut0:cut1]

                # Slice Training data
                X_train = np.concatenate((X[0:cut0],X[cut1:]), axis=0)
                y_train = np.concatenate((y[0:cut0],y[cut1:]), axis=0)

                # Train model
                val_scores = []
                train_scores = []
                for i in range(num_iter):
                        # overfit like crazy?
                        self.stochastic_train(X_train, y_train, error)
                        val_score = self.score(X_val, y_val)
                        train_score = self.score(X_train, y_train)
                        val_scores.append(val_score)
                        train_scores.append(train_score)
                        print("Current run-time for " + str(i+1) + " epochs is " +
t))

                        if (i%2 == 0):
                                x = range(len(val_scores))
                                plt.plot(x, val_scores, 'r--', x, train_scores, 'g^
                                plt.xlabel("Epoch Number")
                                plt.ylabel("Accuracy")
                                plt.show()

                                # Learning rate decay
                                self.alpha = self.alpha*0.75

                                # Update predictions .csv
                                self.write_prediction(test_images)

                # Adjust sum scores across each model
                score += self.score(X_val, y_val)
                plt.show()

                return score

        def clear_weights(self):
                self.W1 = np.array(self.init_scale*np.random.randn(self.inputLayerS
                self.W2 = np.array(self.init_scale*np.random.randn(self.hiddenLayer

        def write_prediction(self, X):
                yHat = np.argmax(self.predict(X), axis=1)
                output = enumerate(yHat, start=1)
                with open('test_digit.csv', 'wb') as fp:
                        a = csv.writer(fp, delimiter=',')
                        data = output
                        a.writerow(["Id", "Category"])
                        a.writerows(data)

############ Training ##############
# Train a 1-hidden layer neural net
# 784 input features
```

```
# 200 features in Hidden Layer
# 10 output classes

# W1 is an (nin +1) x (nhid) matrix, the additional row is a bias.
# (i,j) entry is the weight connecting the i-th unit in the input layer
# to the j-th unit in the hidden layer

# W2 is a (nhid +1) x (nout) matrix where the (i,j) entry
# represents the weight connecting the i-th unit in the hidden layer
# to the j-th unit in the output layer. Additional row for bias.

# Use tanh activation function as the choice o non-linear
# function and output units should use the sigmoid function.

# Use stochastic gradient Descent

######### Testing #########

# Build num_folds classifiers with slices of data
# Evaluate each classifier, average accuracies

# Try both mean-squared error and cross-entropy error


iteration_large = [0.01, 0.1, 1.0, 10.0, 100.0]
iteration_small = [0.50, 0.625, 0.75, 0.875, 1.0, 1.25, 1.5, 1.75, 2.0]
best_alpha = 0.003125
granularity = 1.0


NN = Neural_Network(alpha=best_alpha, init_scale=0.01)
print(NN.cv_plot_score(train_images[0:60000], train_labels[0:60000], 1000, "square"
```