Backpropagation Overview In this exercise we will use backpropagation to train a multi-layer perceptron (with a single hidden layer). We will experiment with different patterns and see how quickly or slowly the weights converge. We will see the imparant interplay of different parameters such as learning rate, number of iterations, and number of data points.
and interplay of different parameters such as learning rate, number of iterations, and number of data points. In [1]: #Setup import numpy as np import matplotlib.pyplot as plt In this exercise, we will prepare code to create a multi-layer perceptron with a single hidden layer (with 4 nodes) and train it via back-propagation. We will take the following steps: 1. Initialize the weights to random values between -1 and 1 2. Perform the food forward computation.
 2. Perform the feed-forward computation 3. Compute the loss function 4. Calculate the gradients for all the weights via back-propagation 5. Update the weight matrices (using a learning_rate parameter) 6. Execute steps 2-5 for a fixed number of iterations 7. Plot the accuracies and log loss and observe how they change over time Once the code is running, we can address the following questions:
 Which patterns was the neural network able to learn quickly and which took longer? What learning rates and numbers of iterations worked well? ## This code below generates two x values and a y value according to different patterns ## It also creates a "bias" term (a vector of 1s) ## The goal is then to learn the mapping from x to y using a neural network via back-propagation num_obs = 500
<pre>x_mat_1 = np.random.uniform(-1,1,size = (num_obs,2)) x_mat_bias = np.ones((num_obs,1)) x_mat_full = np.concatenate((x_mat_1,x_mat_bias), axis=1) # # Diamond Pattern y = ((np.abs(x_mat_full[:,0]) + np.abs(x_mat_full[:,1]))<1).astype(int) print('shape of x_mat_full is {}'.format(x_mat_full.shape)) print('shape of y is {}'.format(y.shape))</pre>
<pre>fig, ax = plt.subplots(figsize=(5, 5)) ax.plot(x_mat_full[y==1, 0], x_mat_full[y==1, 1], 'ro', label='class 1', color='darkslateblue') ax.plot(x_mat_full[y==0, 0], x_mat_full[y==0, 1], 'bx', label='class 0', color='chocolate') # ax.grid(True) ax.legend(loc='best') ax.axis('equal'); shape of x_mat_full is (500, 3) shape of y is (500,)</pre>
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<pre>checking other with other patterns In [5]: num_obs = 500 x_mat_1 = np.random.uniform(-1,1,size = (num_obs,2)) x_mat_bias = np.ones((num_obs,1)) x_mat_full = np.concatenate((x_mat_1,x_mat_bias), axis=1) ## Circle pattern y = (np.sqrt(x_mat_full[:,0]**2 + x_mat_full[:,1]**2)<.75).astype(int)</pre>
<pre>print('shape of x_mat_full is {}'.format(x_mat_full.shape)) print('shape of y is {}'.format(y.shape)) fig, ax = plt.subplots(figsize=(5, 5)) ax.plot(x_mat_full[y==1, 0], x_mat_full[y==1, 1], 'ro', label='class 1', color='darkslateblue') ax.plot(x_mat_full[y==0, 0], x_mat_full[y==0, 1], 'bx', label='class 0', color='chocolate') # ax.grid(True) ax.legend(loc='best') ax.axis('equal');</pre>
shape of x_mat_full is (500, 3) shape of y is (500,) 100
0.00
In [7]: num_obs = 500 x_mat_1 = np.random.uniform(-1,1,size = (num_obs,2)) x_mat_bias = np.ones((num_obs,1)) x_mat_full = np.concatenate((x_mat_1,x_mat_bias), axis=1) ## Centered square y = ((np.maximum(np.abs(x_mat_full[:,0]), np.abs(x_mat_full[:,1])))<.5).astype(int)
<pre>print('shape of x_mat_full is {}'.format(x_mat_full.shape)) print('shape of y is {}'.format(y.shape)) fig, ax = plt.subplots(figsize=(5, 5)) ax.plot(x_mat_full[y==1, 0], x_mat_full[y==1, 1], 'ro', label='class 1', color='darkslateblue') ax.plot(x_mat_full[y==0, 0], x_mat_full[y==0, 1], 'bx', label='class 0', color='chocolate') # ax.grid(True) ax.legend(loc='best')</pre>
ax.axis('equal'); shape of x_mat_full is (500, 3) shape of y is (500,) 100 0.75 0.50 Class 1 x class 0
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-1.00 -0.75 -0.50 -0.25 0.00 0.25 0.50 0.75 100 In [8]: num_obs = 500
<pre>y = (((np.maximum((x_mat_full[:,0]), (x_mat_full[:,1])))<.5) & ((np.maximum((x_mat_full[:,0]), (x_mat_full[:,1])))>5)).astype(int) print('shape of x_mat_full is {}'.format(x_mat_full.shape)) print('shape of y is {}'.format(y.shape)) fig, ax = plt.subplots(figsize=(5, 5)) ax.plot(x_mat_full[y==1, 0], x_mat_full[y==1, 1], 'ro', label='class 1', color='darkslateblue') ax.plot(x_mat_full[y==0, 0], x_mat_full[y==0, 1], 'bx', label='class 0', color='chocolate') # ax.grid(True) ax.legend(loc='best') ax.ayis('logual');</pre>
ax.axis('equal'); shape of x_mat_full is (500, 3) shape of y is (500,) 100 0.75
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-1.00 -0.75 -0.50 -0.25 0.00 0.25 0.50 0.75 100 In [9]: num_obs = 500
<pre>y = (((np.maximum((x_mat_full[:,0]), (x_mat_full[:,1])))<.5) & ((np.maximum((x_mat_full[:,0]), (x_mat_full[:,1])))>0)).astype(int) print('shape of x_mat_full is {}'.format(x_mat_full.shape)) print('shape of y is {}'.format(y.shape)) fig, ax = plt.subplots(figsize=(5, 5)) ax.plot(x_mat_full[y==1, 0], x_mat_full[y==1, 1], 'ro', label='class 1', color='darkslateblue') ax.plot(x_mat_full[y==0, 0], x_mat_full[y==0, 1], 'bx', label='class 0', color='chocolate') # ax.grid(True)</pre>
ax.legend(loc='best') ax.axis('equal'); shape of x_mat_full is (500, 3) shape of y is (500,) 100 0.75 0.50 0.75 0.50
0.25 - 0.00 - 0.25 - 0.05 - 0.
-1.00 -0.75 -0.50 -0.25 0.00 0.25 0.50 0.75 100 In [10]: ## This code below generates two x values and a y value according to different patterns ## It also creates a "bias" term (a vector of 1s) ## The goal is then to learn the mapping from x to y using a neural network via back-propagation num_obs = 500 x_mat_1 = np.random.uniform(-1,1,size = (num_obs,2))
<pre>x_mat_bias = np.ones((num_obs,1)) x_mat_full = np.concatenate((x_mat_1,x_mat_bias), axis=1) # PICK ONE PATTERN BELOW and comment out the rest. # Circle pattern # y = (np.sqrt(x_mat_full[:,0]**2 + x_mat_full[:,1]**2)<.75).astype(int) # Diamond Pattern y = ((np.abs(x_mat_full[:,0]) + np.abs(x_mat_full[:,1]))<1).astype(int)</pre>
<pre># # Centered square # y = ((np.maximum(np.abs(x_mat_full[:,0]), np.abs(x_mat_full[:,1])))<.5).astype(int) # # Thick Right Angle pattern # y = (((np.maximum((x_mat_full[:,0]), (x_mat_full[:,1])))<.5) & ((np.maximum((x_mat_full[:,0]), (x_mat_full[:,1])))>5)).astype(int) # # Thin right angle pattern # y = (((np.maximum((x_mat_full[:,0]), (x_mat_full[:,1])))<.5) & ((np.maximum((x_mat_full[:,0]), (x_mat_full[:,1])))>0)).astype(int)</pre>
<pre>print('shape of x_mat_full is {}'.format(x_mat_full.shape)) print('shape of y is {}'.format(y.shape)) fig, ax = plt.subplots(figsize=(5, 5)) ax.plot(x_mat_full[y==1, 0], x_mat_full[y==1, 1], 'ro', label='class 1', color='darkslateblue') ax.plot(x_mat_full[y==0, 0], x_mat_full[y==0, 1], 'bx', label='class 0', color='chocolate') # ax.grid(True) ax.legend(loc='best')</pre>
ax.axis('equal'); shape of x_mat_full is (500, 3) shape of y is (500,) 100 0.75 0.50 x x x x x x x x x x x x x x x x x x x
0.25 - 0.00 - 0.25 - 0.00 - 0.
-1.00 -0.75 -0.50 -0.25 0.00 0.25 0.50 0.75 1.00 Here are some helper functions In [22]: def sigmoid(x): """ Sigmoid function """
<pre>return 1.0 / (1.0 + np.exp(-x)) def loss_fn(y_true, y_pred, eps=1e-16): """ Loss function we would like to optimize (minimize) We are using Logarithmic Loss http://scikit-learn.org/stable/modules/model_evaluation.html#log-loss """ y_pred = np.maximum(y_pred,eps)</pre>
y_pred = np.minimum(y_pred,(1-eps)) return -(np.sum(y_true * np.log(y_pred)) + np.sum((1-y_true)*np.log(1-y_pred)))/len(y_true) def forward_pass(W1, W2): """ Does a forward computation of the neural network Takes the input `x_mat` (global variable) and produces the output `y_pred` Also produces the gradient of the log loss function """
<pre>global x_mat global y global num_ # First, compute the new predictions `y_pred` z_2 = np.dot(x_mat, W_1) a_2 = sigmoid(z_2) z_3 = np.dot(a_2, W_2) y_pred = sigmoid(z_3).reshape((len(x_mat),)) # Now compute the gradient</pre>
<pre>J_z_3_grad = -y + y_pred J_W_2_grad = np.dot(J_z_3_grad, a_2) a_2_z_2_grad = sigmoid(z_2)*(1-sigmoid(z_2)) J_W_1_grad = (np.dot((J_z_3_grad).reshape(-1,1), W_2.reshape(-1,1).T)*a_2_z_2_grad).T.dot(x_mat).T gradient = (J_W_1_grad, J_W_2_grad) # return return y_pred, gradient</pre>
<pre>def plot_loss_accuracy(loss_vals, accuracies): fig = plt.figure(figsize=(16, 8)) fig.suptitle('Log Loss and Accuracy over iterations') ax = fig.add_subplot(1, 2, 1) ax.plot(loss_vals) ax.grid(True) ax.set(xlabel='iterations', title='Log Loss') ax = fig.add_subplot(1, 2, 2)</pre>
<pre>ax.plot(accuracies) ax.grid(True) ax.set(xlabel='iterations', title='Accuracy'); n [26]: #### Initialize the network parameters np.random.seed(1241) W_1 = np.random.uniform(-1,1,size=(3,4)) # (3,4) 3 dimensions as x1,x2 and bias term with 4 nodes</pre>
<pre>W_2 = np.random.uniform(-1,1,size=(4)) num_iter = 5000 learning_rate = .001 x_mat = x_mat_full loss_vals, accuracies = [], [] for i in range(num_iter): ### Do a forward computation, and get the gradient y_pred, (J_W_1_grad, J_W_2_grad) = forward_pass(W_1, W_2)</pre>
<pre>## Update the weight matrices W_1 = W_1 - learning_rate*J_W_1_grad W_2 = W_2 - learning_rate*J_W_2_grad ### Compute the loss and accuracy curr_loss = loss_fn(y,y_pred) loss_vals.append(curr_loss) acc = np.sum((y_pred>=.5) == y)/num_obs accuracies.append(acc)</pre>
<pre>## Print the loss and accuracy for every 200th iteration if((i%200) == 0): print('iteration {}, log loss is {:.4f}, accuracy is {}'.format(</pre>
iteration 400, log loss is 0.6489, accuracy is 0.59 iteration 600, log loss is 0.5871, accuracy is 0.748 iteration 800, log loss is 0.5196, accuracy is 0.77 iteration 1000, log loss is 0.4933, accuracy is 0.774 iteration 1200, log loss is 0.4559, accuracy is 0.792 iteration 1400, log loss is 0.3832, accuracy is 0.864 iteration 1600, log loss is 0.3248, accuracy is 0.898 iteration 1800, log loss is 0.2847, accuracy is 0.916 iteration 2000, log loss is 0.2549, accuracy is 0.92 iteration 2200, log loss is 0.2329, accuracy is 0.934 iteration 2400, log loss is 0.2329, accuracy is 0.934 iteration 2400, log loss is 0.2167, accuracy is 0.942
iteration 2600, log loss is 0.2045, accuracy is 0.946 iteration 2800, log loss is 0.1949, accuracy is 0.948 iteration 3000, log loss is 0.1873, accuracy is 0.95 iteration 3200, log loss is 0.1809, accuracy is 0.952 iteration 3400, log loss is 0.1708, accuracy is 0.952 iteration 3600, log loss is 0.1708, accuracy is 0.952 iteration 3800, log loss is 0.1667, accuracy is 0.952 iteration 4000, log loss is 0.1630, accuracy is 0.954 iteration 4200, log loss is 0.1597, accuracy is 0.954 iteration 4400, log loss is 0.1562, accuracy is 0.954 iteration 4600, log loss is 0.1562, accuracy is 0.954 iteration 4600, log loss is 0.15642, accuracy is 0.954
iteration 4600, log loss is 0.1542, accuracy is 0.954 iteration 4800, log loss is 0.1517, accuracy is 0.954 Log Loss and Accuracy over iterations Accuracy 0.8 0.9
0.5
0.4
Plot the predicted answers, with mistakes in yellow [30]: pred1 = (y_pred>=.5)
<pre>pred0 = (y_pred<.5) fig, ax = plt.subplots(figsize=(8, 8)) # true predictions ax.plot(x_mat[pred1 & (y==1),0],x_mat[pred1 & (y==1),1], 'ro', label='true positives') ax.plot(x_mat[pred0 & (y==0),0],x_mat[pred0 & (y==0),1], 'bx', label='true negatives') # false predictions ax.plot(x_mat[pred1 & (y==0),0],x_mat[pred1 & (y==0),1], 'yx', label='false positives', markersize=15) ax.plot(x_mat[pred0 & (y==1),0],x_mat[pred0 & (y==1),1], 'yo', label='false negatives', markersize=15, alpha=.6) ax.set(title='Truth vs Prediction')</pre>
ax.legend(bbox_to_anchor=(1, 0.8), fancybox=True, shadow=True, fontsize='x-large'); Truth vs Prediction 100
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-1.00 -0.75 -0.50 -0.25 0.00 0.25 0.50 0.75 1.00