Problem Set 4: Neural Networks

This assignment requires a working IPython Notebook installation, which you should already have. If not, please refer to the instructions in Problem Set 2.

The programming part is adapted from Stanford CS231n (http://cs231n.stanford.edu/).

In part 2 (programming) of this assignment, you DO NOT need to make any modification code in this IPython Notebook. Instead you will implement your own simple neural network in the mlp.py file. Please attach your written solutions for part 1 and part 3 in this IPython Notebook.

Total: 100 points.

[30pts] Problem 1: Backprop in a simple MLP

This problem asks you to derive all the steps of the backpropagation algorithm for a simple classification network. Consider a fully-connected neural network, also known as a multi-layer perceptron (MLP), with a single hidden layer and a one-node output layer. The hidden and output nodes use an elementwise sigmoid activation function and the loss layer uses cross-entropy loss:

$$f(z) = rac{1}{1 + exp(-z))} \ L(\hat{y},y) = -yln(\hat{y}) - (1-y)ln(1-\hat{y})$$

The computation graph for an example network is shown below. Note that it has an equal number of nodes in the input and hidden layer (3 each), but, in general, they need not be equal. Also, to make the application of backprop easier, we show the *computation graph* which shows the dot product and activation functions as their own nodes, rather than the usual graph showing a single node for both.



The forward and backward computation are given below. NOTE: We assume no regularization, so you can omit the terms involving Ω .

The forward step is:



and the backward step is:



Write down each step of the backward pass explicitly for all layers, i.e. for the loss and k=2,1, compute all gradients above, expressing them as a function of variables x,y,h,W,b. We start by giving an example. Note that we have replaced the superscript notation $u^{(i)}$ with u^i , and \odot stands for element-wise multiplication.

$$abla_{\hat{y}}L(\hat{y},y) =
abla_{\hat{y}}[-yln(\hat{y}) - (1-y)ln(1-\hat{y})] = rac{\hat{y}-y}{(1-\hat{y})\hat{y}} = rac{h^2-y}{(1-h^2)h^2}$$

Next, please derive the following.

Hint: you should substitute the updated values for the gradient g in each step and simplify as much as possible.

[5pts] Q1.1:
$$abla_{a^2}J$$

[5pts] Q1.2:
$$abla_{b^2}J$$

[5pts] Q1.3:
$$abla_{W^2} J$$

Hint: this should be a vector, since W^2 is a vector.

[5pts] Q1.4:
$$abla_{h^1}J$$

[5pts] Q1.5:
$$abla_{b^1}J$$
, $abla_{W^1}J$

$$\begin{array}{ll}
\boxed{11} \ \nabla_{A^{2}} J = \frac{dJ}{dh^{2}} \cdot \frac{dh^{2}}{da^{2}} = g \circ f'(a,^{*}) = \frac{h^{2} - y}{(1 + h^{2})^{2}} \cdot f(a,^{*})(1 - f(a,^{*})) = \frac{h^{2} - y}{(1 + h^{2})^{2}} \cdot \frac{1}{h^{2}} \cdot \frac{1}{h^{2}} \cdot \frac{1}{h^{2}} = \frac{dJ}{dh^{2}} \cdot \frac{1}{h^{2}} \cdot \frac{1}{h^{2}} = \frac{dJ}{dh^{2}} \cdot \frac{1}{h^{2}} \cdot \frac{1}{h^{2}} \cdot \frac{1}{h^{2}} \cdot \frac{1}{h^{2}} \cdot \frac{1}{h^{2}} = \frac{dJ}{dh^{2}} \cdot \frac{1}{h^{2}} \cdot \frac{1}{h^{2}} \cdot \frac{1}{h^{2}} = \frac{dJ}{dh^{2}} \cdot \frac{1}{h^{2}} \cdot \frac{1}{h^$$

[5pts] Q1.6 Briefly, explain how the computational speed of backpropagation would be affected if it did not include a forward pass

[double click here to add a solution]

[50pts] Problem 2 (Programming): Implementing a simple MLP

In this problem we will develop a neural network with fully-connected layers, or Multi-Layer Perceptron (MLP). We will use it in classification tasks.

In the current directory, you can find a file <code>mlp.py</code>, which contains the definition for class <code>TwoLayerMLP</code>. As the name suggests, it implements a 2-layer MLP, or MLP with 1 *hidden* layer. You will implement your code in the same file, and call the member functions in this notebook. Below is some initialization. The <code>autoreload</code> command makes sure that <code>mlp.py</code> is periodically reloaded.

```
In [21]: # setup
         import numpy as np
         import matplotlib.pyplot as plt
         from mlp import TwoLayerMLP
         %matplotlib inline
         plt.rcParams['figure.figsize'] = (10.0, 8.0) # set default size of plots
         plt.rcParams['image.interpolation'] = 'nearest'
         plt.rcParams['image.cmap'] = 'gray'
         # for auto-reloading external modules
         # see http://stackoverflow.com/questions/1907993/autoreload-of-modules-in-i
         python
         %load_ext autoreload
         %autoreload 2
         def rel_error(x, y):
              """ returns relative error """
             return np.max(np.abs(x - y) / (np.maximum(1e-8, np.abs(x) + np.abs(y)))
         ))))
```

The autoreload extension is already loaded. To reload it, use: %reload_ext autoreload

Next we initialize a toy model and some toy data, the task is to classify five 4-d vectors.

```
In [22]: # Create a small net and some toy data to check your implementations.
         # Note that we set the random seed for repeatable experiments.
         input size = 4
         hidden size = 10
         num classes = 3
         num inputs = 5
         def init toy model(actv, std=1e-1):
             np.random.seed(0)
             return TwoLayerMLP(input_size, hidden_size, num_classes, std=std, activ
         ation=actv)
         def init_toy_data():
             np.random.seed(1)
             X = 10 * np.random.randn(num inputs, input size)
             y = np.array([0, 1, 2, 2, 1])
             return X, y
         X, y = init_toy_data()
         print('X = ', X)
         print()
         print('y = ', y)
         X = [[16.24345364 -6.11756414 -5.28171752 -10.72968622]]
          [ 8.65407629 -23.01538697 17.44811764 -7.61206901]
          [ 3.19039096 -2.49370375 14.62107937 -20.60140709]
          [ -3.22417204 -3.84054355 11.33769442 -10.99891267]
          [ -1.72428208 -8.77858418
                                       0.42213747
                                                    5.82815214]]
         y = [0 1 2 2 1]
```

[5pts] Q2.1 Forward pass: Sigmoid

Our 2-layer MLP uses a softmax output layer (**note**: this means that you don't need to apply a sigmoid on the output) and the multiclass cross-entropy loss to perform classification. Both are defined in Problem Set 2.

Please take a look at method <code>TwoLayerMLP.loss</code> in the file <code>mlp.py</code>. This function takes in the data and weight parameters, and computes the class scores (aka logits), the loss L, and the gradients on the parameters.

• Complete the implementation of forward pass (up to the computation of scores) for the sigmoid activation: $\sigma(x)=rac{1}{1+exp(-x)}$.

Note 1: Softmax cross entropy loss involves the <u>log-sum-exp operation</u> (<u>https://en.wikipedia.org/wiki/LogSumExp</u>). This can result in numerical underflow/overflow. Read about the solution in the link, and try to understand the calculation of loss in the code.

Note 2: You're strongly encouraged to implement in a vectorized way and avoid using slower for loops. Note that most numpy functions support vector inputs.

Check the correctness of your forward pass below. The difference should be very small (<1e-6).

```
In [23]: net = init_toy_model('sigmoid')
    loss, _ = net.loss(X, y, reg=0.1)
    correct_loss = 1.182248
    print(loss)
    print('Difference between your loss and correct loss:')
    print(np.sum(np.abs(loss - correct_loss)))

1.1822479803941373
    Difference between your loss and correct loss:
    1.9605862711102873e-08
```

[10pts] Q2.2 Backward pass: Sigmoid

• For sigmoid activation, complete the computation of grads, which stores the gradient of the loss with respect to the variables W1, b1, W2, and b2.

Now debug your backward pass using a numeric gradient check. Again, the differences should be very small.

```
In [24]: # Use numeric gradient checking to check your implementation of the backwar
         d pass.
         # If your implementation is correct, the difference between the numeric and
         # analytic gradients should be less than 1e-8 for each of W1, W2, b1, and b
         2.
         from utils import eval_numerical_gradient
         loss, grads = net.loss(X, y, reg=0.1)
         # these should all be very small
         for param name in grads:
             f = lambda W: net.loss(X, y, reg=0.1)[0]
             param grad num = eval numerical gradient(f, net.params[param name], ver
         bose=False)
             print('%s max relative error: %e'%(param_name, rel_error(param_grad_num
         , grads[param_name])))
         W2 max relative error: 8.048892e-10
         b2 max relative error: 5.553999e-11
         W1 max relative error: 1.126755e-08
         b1 max relative error: 2.035406e-06
```

[5pts] Q2.3 Train the Sigmoid network

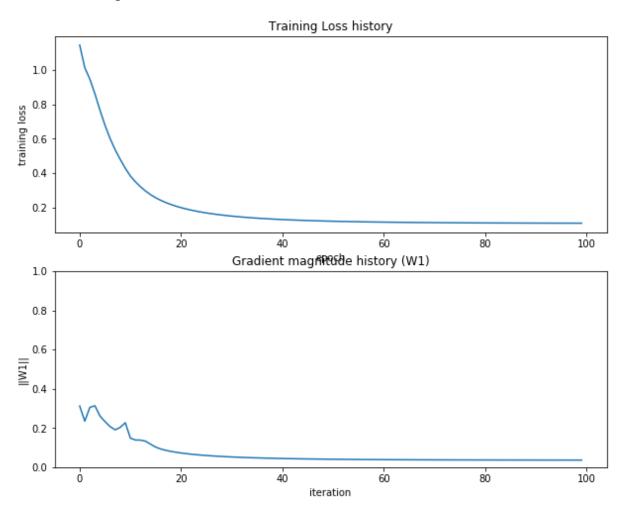
To train the network we will use stochastic gradient descent (SGD), implemented in TwoLayerNet.train. Then we train a two-layer network on toy data.

• Implement the prediction function TwoLayerNet.predict, which is called during training to keep track of training and validation accuracy.

You should get the final training loss around 0.1, which is good, but not too great for such a toy problem. One problem is that the gradient magnitude for W1 (the first layer weights) stays small all the time, and the neural net doesn't get much "learning signals". This has to do with the saturation problem of the sigmoid activation function.

```
In [25]:
         net = init_toy_model('sigmoid', std=1e-1)
         stats = net.train(X, y, X, y,
                            learning_rate=0.5, reg=1e-5,
                            num epochs=100, verbose=False)
         print('Final training loss: ', stats['loss_history'][-1])
         # plot the loss history and gradient magnitudes
         plt.subplot(2, 1, 1)
         plt.plot(stats['loss_history'])
         plt.xlabel('epoch')
         plt.ylabel('training loss')
         plt.title('Training Loss history')
         plt.subplot(2, 1, 2)
         plt.plot(stats['grad_magnitude_history'])
         plt.xlabel('iteration')
         plt.ylabel('||W1||')
         plt.ylim(0,1)
         plt.title('Gradient magnitude history (W1)')
         plt.show()
```

Final training loss: 0.10926794610680679



[5pts] Q2.4 Using ReLU activation

The Rectified Linear Unit (ReLU) activation is also widely used: ReLU(x) = max(0, x).

- Complete the implementation for the ReLU activation (forward and backward) in mlp.py.
- · Train the network with ReLU, and report your final training loss.

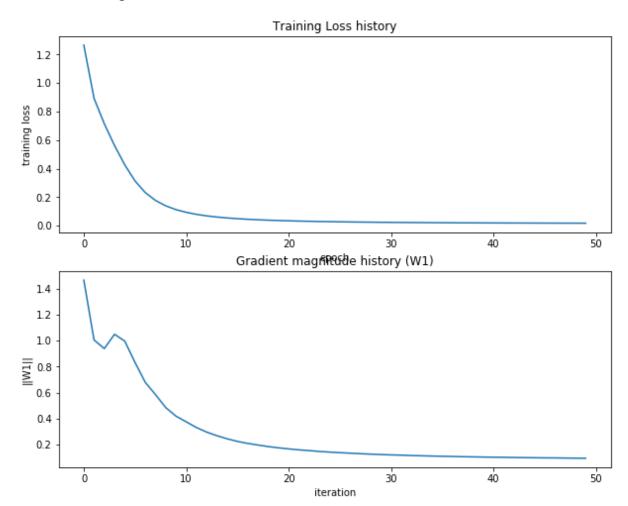
Make sure you first pass the numerical gradient check on toy data.

```
In [26]: net = init toy model('relu', std=1e-1)
         loss, grads = net.loss(X, y, reg=0.1)
         print('loss = ', loss) # correct loss = 1.320973
         # The differences should all be very small
         print('checking gradients')
         for param_name in grads:
             f = lambda W: net.loss(X, y, reg=0.1)[0]
             param_grad_num = eval_numerical_gradient(f, net.params[param_name], ver
         bose=False)
             print('%s max relative error: %e'%(param name, rel error(param grad num
         , grads[param_name])))
         loss = 1.3037878913298206
         checking gradients
         W2 max relative error: 3.440708e-09
         b2 max relative error: 3.865091e-11
         W1 max relative error: 3.561318e-09
         b1 max relative error: 8.994864e-10
```

Now that it's working, let's train the network. Does the net get stronger learning signals (i.e. gradients) this time? Report your final training loss.

```
In [27]: net = init_toy_model('relu', std=1e-1)
         stats = net.train(X, y, X, y,
                            learning_rate=0.1, reg=1e-5,
                            num epochs=50, verbose=False)
         print('Final training loss: ', stats['loss_history'][-1])
         # plot the loss history
         plt.subplot(2, 1, 1)
         plt.plot(stats['loss_history'])
         plt.xlabel('epoch')
         plt.ylabel('training loss')
         plt.title('Training Loss history')
         plt.subplot(2, 1, 2)
         plt.plot(stats['grad_magnitude_history'])
         plt.xlabel('iteration')
         plt.ylabel('||W1||')
         plt.title('Gradient magnitude history (W1)')
         plt.show()
```

Final training loss: 0.0178562204869839



Load MNIST data

Now that you have implemented a two-layer network that works on toy data, let's try some real data. The MNIST dataset is a standard machine learning benchmark. It consists of 70,000 grayscale handwritten digit images, which we split into 50,000 training, 10,000 validation and 10,000 testing. The images are of size 28x28, which are flattened into 784-d vectors.

Note 1: the function <code>get_MNIST_data</code> requires the <code>scikit-learn</code> package. If you previously did anaconda installation to set up your Python environment, you should already have it. Otherwise, you can install it following the instructions here: http://scikit-learn.org/stable/install.html (http://scikit-learn.org/stable/install.html)

Note 2: If you encounter a HTTP 500 error, that is likely temporary, just try again.

Note 3: Ensure that the downloaded MNIST file is 55.4MB (smaller file-sizes could indicate an incomplete download - which is possible)

```
In [28]: # Load MNIST
    from utils import get_MNIST_data
    X_train, y_train, X_val, y_val, X_test, y_test = get_MNIST_data()
    print('Train data shape: ', X_train.shape)
    print('Train labels shape: ', y_train.shape)
    print('Validation data shape: ', X_val.shape)
    print('Validation labels shape: ', y_val.shape)
    print('Test data shape: ', X_test.shape)
    print('Test labels shape: ', y_test.shape)
```

C:\Users\timpc\Anaconda3\lib\site-packages\sklearn\utils\deprecation.py:85: DeprecationWarning: Function fetch_mldata is deprecated; fetch_mldata was deprecated in version 0.20 and will be removed in version 0.22. Please use fetch openml.

warnings.warn(msg, category=DeprecationWarning)

C:\Users\timpc\Anaconda3\lib\site-packages\sklearn\utils\deprecation.py:85: DeprecationWarning: Function mldata_filename is deprecated; mldata_filename was deprecated in version 0.20 and will be removed in version 0.22. Please use fetch_openml.

warnings.warn(msg, category=DeprecationWarning)

Train data shape: (50000, 784)
Train labels shape: (50000,)
Validation data shape: (10000, 784)
Validation labels shape: (10000,)
Test data shape: (10000, 784)
Test labels shape: (10000,)

Q2.5 Train a network on MNIST

We will now train a network on MNIST with 64 hidden units in the hidden layer. We train it using SGD, and decrease the learning rate with an exponential rate over time; this is achieved by multiplying the learning rate with a constant factor learning_rate_decay (which is less than 1) after each epoch. In effect, we are using a high learning rate initially, which is good for exploring the solution space, and using lower learning rates later to encourage convergence to a local minimum (or <u>saddle point</u> (http://www.offconvex.org/2016/03/22/saddlepoints/), which may happen more often).

• Train your MNIST network with 2 different activation functions: sigmoid and ReLU.

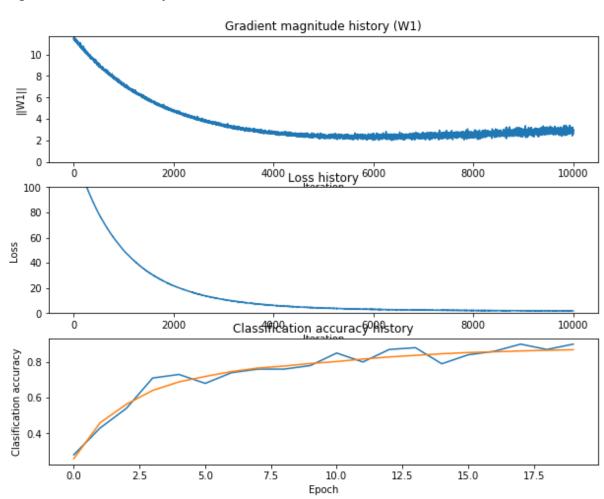
We first define some variables and utility functions. The plot_stats function plots the histories of gradient magnitude, training loss, and accuracies on the training and validation sets. The visualize_weights function visualizes the weights learned in the first layer of the network. In most neural networks trained on visual data, the first layer weights typically show some visible structure when visualized. Both functions help you to diagnose the training process.

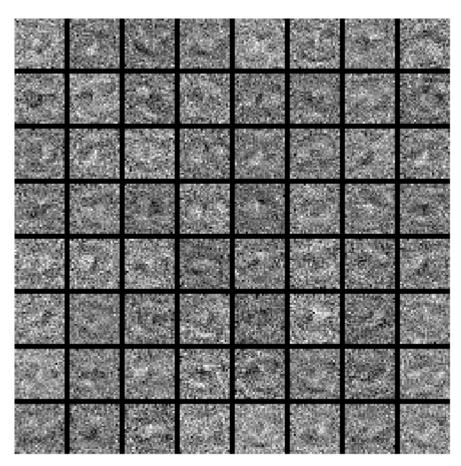
```
In [29]: | input_size = 28 * 28
         hidden size = 64
         num classes = 10
         # Plot the loss function and train / validation accuracies
         def plot_stats(stats):
             plt.subplot(3, 1, 1)
             plt.plot(stats['grad magnitude history'])
             plt.title('Gradient magnitude history (W1)')
             plt.xlabel('Iteration')
             plt.ylabel('||W1||')
             plt.ylim(0, np.minimum(100,np.max(stats['grad_magnitude_history'])))
             plt.subplot(3, 1, 2)
             plt.plot(stats['loss_history'])
             plt.title('Loss history')
             plt.xlabel('Iteration')
             plt.ylabel('Loss')
             plt.ylim(0, 100)
             plt.subplot(3, 1, 3)
             plt.plot(stats['train acc history'], label='train')
             plt.plot(stats['val_acc_history'], label='val')
             plt.title('Classification accuracy history')
             plt.xlabel('Epoch')
             plt.ylabel('Clasification accuracy')
             plt.show()
         # Visualize the weights of the network
         from utils import visualize grid
         def show net weights(net):
             W1 = net.params['W1']
             W1 = W1.T.reshape(-1, 28, 28)
             plt.imshow(visualize grid(W1, padding=3).astype('uint8'))
             plt.gca().axis('off')
             plt.show()
```

[10pts] Q2.5.1 Sigmoid network

```
In [30]: sigmoid net = TwoLayerMLP(input size, hidden size, num classes, activation=
          'sigmoid', std=1e-1)
         # Train the network
         sigmoid_stats = sigmoid_net.train(X_train, y_train, X_val, y_val,
                                            num_epochs=20, batch_size=100,
                                            learning rate=1e-3, learning rate decay=
         0.95,
                                            reg=0.5, verbose=True)
         # Predict on the training set
         train_acc = (sigmoid_net.predict(X_train) == y_train).mean()
         print('Sigmoid final training accuracy: ', train_acc)
         # Predict on the validation set
         val_acc = (sigmoid_net.predict(X_val) == y_val).mean()
         print('Sigmoid final validation accuracy: ', val acc)
         # Predict on the test set
         test acc = (sigmoid net.predict(X test) == y test).mean()
         print('Sigmoid test accuracy: ', test_acc)
         # show stats and visualizations
         plot stats(sigmoid stats)
         show_net_weights(sigmoid_net)
```

Epoch 1: loss 78.980750, train acc 0.280000, val acc 0.258300 Epoch 2: loss 49.838630, train_acc 0.430000, val_acc 0.459300 Epoch 3: loss 32.431795, train_acc 0.540000, val_acc 0.563200 Epoch 4: loss 21.732892, train_acc 0.710000, val_acc 0.640700 Epoch 5: loss 15.111877, train acc 0.730000, val acc 0.688400 Epoch 6: loss 10.906376, train_acc 0.680000, val_acc 0.718700 Epoch 7: loss 8.077669, train acc 0.740000, val acc 0.746200 Epoch 8: loss 6.229287, train acc 0.760000, val acc 0.766000 Epoch 9: loss 4.979639, train_acc 0.760000, val_acc 0.777300 Epoch 10: loss 4.108814, train acc 0.780000, val acc 0.791700 Epoch 11: loss 3.480617, train acc 0.850000, val acc 0.802500 Epoch 12: loss 3.065671, train_acc 0.800000, val_acc 0.816400 Epoch 13: loss 2.673266, train acc 0.870000, val acc 0.828100 Epoch 14: loss 2.496009, train_acc 0.880000, val_acc 0.837300 Epoch 15: loss 2.355747, train_acc 0.790000, val_acc 0.845900 Epoch 16: loss 2.138493, train acc 0.840000, val acc 0.852900 Epoch 17: loss 2.090350, train acc 0.860000, val acc 0.856900 Epoch 18: loss 1.974509, train_acc 0.900000, val_acc 0.861900 Epoch 19: loss 1.952709, train acc 0.870000, val acc 0.865300 Epoch 20: loss 1.859285, train acc 0.900000, val acc 0.868600 Sigmoid final training accuracy: 0.87384 Sigmoid final validation accuracy: Sigmoid test accuracy: 0.8676



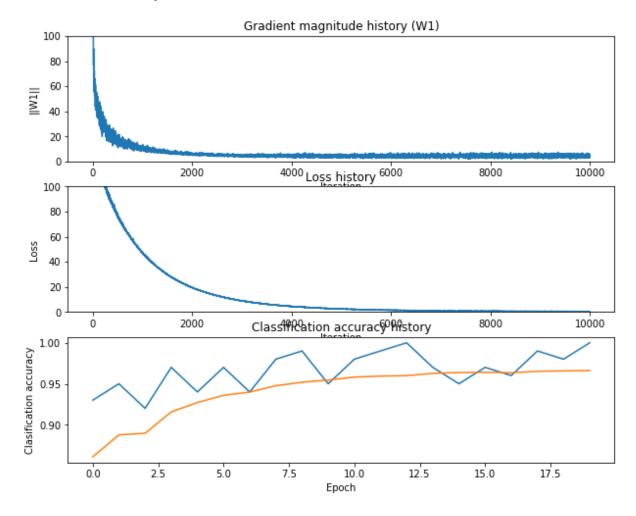


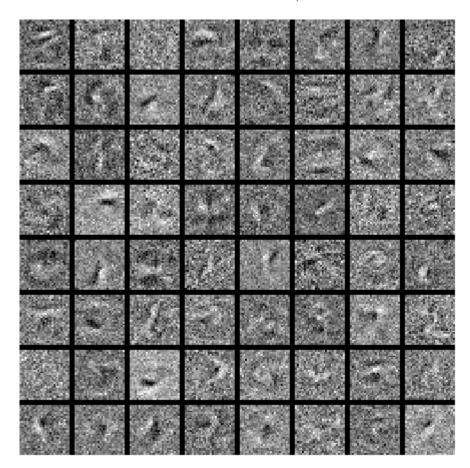
[10pts] Q2.5.2 ReLU network

```
In [31]: relu net = TwoLayerMLP(input size, hidden size, num classes, activation='re
         lu', std=1e-1)
         # Train the network
         relu_stats = relu_net.train(X_train, y_train, X_val, y_val,
                                      num_epochs=20, batch_size=100,
                                      learning_rate=1e-3, learning_rate_decay=0.95,
                                      reg=0.5, verbose=True)
         # Predict on the training set
         train_acc = (relu_net.predict(X_train) == y_train).mean()
         print('ReLU final training accuracy: ', train_acc)
         # Predict on the validation set
         val_acc = (relu_net.predict(X_val) == y_val).mean()
         print('ReLU final validation accuracy: ', val_acc)
         # Predict on the test set
         test_acc = (relu_net.predict(X_test) == y_test).mean()
         print('ReLU test accuracy: ', test_acc)
         # show stats and visualizations
         plot_stats(relu_stats)
         show_net_weights(relu_net)
```

> Epoch 1: loss 76.094922, train acc 0.930000, val acc 0.860900 Epoch 2: loss 46.876140, train_acc 0.950000, val_acc 0.887700 Epoch 3: loss 29.967661, train acc 0.920000, val acc 0.889600 Epoch 4: loss 19.382890, train_acc 0.970000, val_acc 0.915700 Epoch 5: loss 13.073030, train acc 0.940000, val acc 0.927100 Epoch 6: loss 8.889162, train_acc 0.970000, val_acc 0.935900 Epoch 7: loss 6.325204, train acc 0.940000, val acc 0.939900 Epoch 8: loss 4.410905, train acc 0.980000, val acc 0.947600 Epoch 9: loss 3.229653, train_acc 0.990000, val_acc 0.951800 Epoch 10: loss 2.440271, train acc 0.950000, val acc 0.954600 Epoch 11: loss 1.817740, train_acc 0.980000, val_acc 0.958100 Epoch 12: loss 1.411437, train_acc 0.990000, val_acc 0.959400 Epoch 13: loss 1.120475, train acc 1.000000, val acc 0.959900 Epoch 14: loss 0.994299, train_acc 0.970000, val_acc 0.962700 Epoch 15: loss 0.822049, train_acc 0.950000, val_acc 0.963700 Epoch 16: loss 0.714592, train acc 0.970000, val acc 0.964000 Epoch 17: loss 0.586014, train acc 0.960000, val acc 0.963400 Epoch 18: loss 0.475392, train_acc 0.990000, val_acc 0.965200 Epoch 19: loss 0.476712, train acc 0.980000, val acc 0.965700 Epoch 20: loss 0.379706, train acc 1.000000, val acc 0.966100 ReLU final training accuracy: 0.9734 ReLU final validation accuracy: 0.9661

ReLU test accuracy: 0.9637





[5pts] Q2.5.3

Which activation function would you choose in practice? Why?

[20pts] Problem 3: Simple Regularization Methods

You may have noticed the <code>reg</code> parameter in <code>TwoLayerMLP.loss</code>, controlling "regularization strength". In learning neural networks, aside from minimizing a loss function $\mathcal{L}(\theta)$ with respect to the network parameters θ , we usually explicitly or implicitly add some regularization term to reduce overfitting. A simple and popular regularization strategy is to penalize some *norm* of θ .

[10pts] Q3.1: L2 regularization

We can penalize the L2 norm of θ : we modify our objective function to be $\mathcal{L}(\theta)+\lambda\|\theta\|^2$ where λ is the weight of regularization. We will minimize this objective using gradient descent with step size η . Derive the update rule: at time t+1, express the new parameters θ_{t+1} in terms of the old parameters θ_t , the gradient $g_t=\frac{\partial \mathcal{L}}{\partial \theta_t}$, η , and λ .

[3.1]
$$L(\theta) + 2 \|\theta\|^2 \quad \text{minimize this with gradient observed with step size } n \cdot \text{Deriving the upclate hale for } t+L$$

$$J = L(\theta) + 2 \|\theta_t\|^2$$

$$\theta_{t+1} = \theta_t - \eta \quad \nabla \theta_t J$$

$$\theta_{t+1} = \theta_t - \eta \quad \nabla \theta_t J$$

$$\theta_{t+1} = \theta_t - \eta \quad (f_t + 2 \|\theta_t\|^2) \quad f_t = f_t$$

$$\theta_{t+1} = \theta_t - \eta \quad (f_t + 2 \|\theta_t\|^2)$$

[10pts] Q3.2: L1 regularization

Now let's consider L1 regularization: our objective in this case is $\mathcal{L}(\theta) + \lambda \|\theta\|_1$. Derive the update rule.

(Technically this becomes *Sub-Gradient* Descent since the L1 norm is not differentiable at 0. But practically it is usually not an issue.)

T3.2] Now we derive the update for:
$$L(\theta) + 2 \|\theta\|_{1}$$

$$J = L(\theta_{t}) + 2 \|\theta_{t}\|_{1}$$

$$\theta_{t+1} = \theta_{t} - n \nabla_{\theta_{t}} J$$

$$\theta_{t+1} = \theta_{t} - n \frac{t}{t\theta_{t}} (L(\theta_{t}) + 2 \|\theta\|_{1}), \frac{dL}{d\theta} = g_{t}$$

$$\theta_{t+1} = \theta_{t} - n (g_{t} + 2)$$