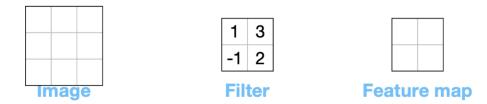
Homework 4 – Deep Neural Networks (CS/DS541, Murai, Spring 2024)

You may complete this homework assignment in teams of up to 2 people.

1. Conv to FC network [5 points]: Consider the following convolutional layer (conv2-1).



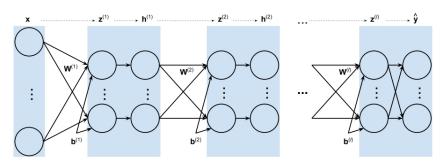
How could we encode the same operation as a fully-connected layer with weights \mathbf{W} (for $\mathbf{h} = \mathbf{W}\mathbf{x}$)? Assume that x represents the vectorized image and h represents the vectorized feature map.

2. Feed-forward neural network [15 points]:

In this problem you will train a multi-layer neural network to classify images of fashion items (10 different classes) from the Fashion MNIST dataset. Similarly to Homework 3, the input to the network will be a 28 × 28-pixel image; the output will be a real number. Specifically, the network you create should implement a function $f: \mathbb{R}^{784} \to \mathbb{R}^{10}$, where:

$$\begin{aligned} \mathbf{z}^{(1)} &=& \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)} \\ \mathbf{h}^{(1)} &=& \mathrm{relu}(\mathbf{z}^{(1)}) \\ \mathbf{z}^{(2)} &=& \mathbf{W}^{(2)}\mathbf{h}^{(1)} + \mathbf{b}^{(2)} \\ &\vdots &\vdots \\ \mathbf{z}^{(l)} &=& \mathbf{W}^{(l)}\mathbf{h}^{(l-1)} + \mathbf{b}^{(l)} \\ \hat{\mathbf{y}} &=& \mathrm{softmax}(\mathbf{z}^{(l)}) \end{aligned}$$

The network specified above is shown in the figure below:



As usual, the (unregularized) cross-entropy cost function should be

$$f_{\text{CE}}(\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \dots, \mathbf{W}^{(l)}, \mathbf{b}^{(l)}) = -\frac{1}{n} \sum_{i=1}^{n} \sum_{k=1}^{10} y_k^{(i)} \log \hat{y}_k^{(i)}$$

where n is the number of examples.

The Fashion MNIST dataset can be downloaded from:

- https://s3.amazonaws.com/jrwprojects/fashion_mnist_train_images.npy
- https://s3.amazonaws.com/jrwprojects/fashion_mnist_train_labels.npy
- https://s3.amazonaws.com/jrwprojects/fashion_mnist_test_images.npy
- https://s3.amazonaws.com/jrwprojects/fashion_mnist_test_labels.npy

Hint: Images are in grayscale and represented by values between 0 and 255. Mapping the inputs to the interval [-0.5, 0.5] will help training the neural network.

Your tasks:

- (a) Implement stochastic gradient descent (SGD; see Section 5.9 and Algorithm 6.4 in the *Deep Learning* textbook) for the multi-layer neural network shown above. **Important** #1: For SGD, reshuffle the data at the beginning of every epoch. Only permute the indices, DO NOT permute the data itself. **Important** #2: your backprop algorithm must work for *any* number of hidden layers (not just 1 hidden layer).
- (b) Verify that your gradient function is correct using the check_grad method. In particular, include in your PDF the real-valued output of the call to check_grad from your code. [UNGRADED]
- 3. Feed-forward neural network with deep learning library [15 points]:
 - (a) Implement the same network using PyTorch or Tensorflow. [6 points]
 - (b) Implement a method called findBestHyperparameters. Optimize the hyperparameters by training on the training set and selecting the parameter settings that optimize performance on the validation set. You should systematically (i.e., in code) try at least 10 (in total, not for each hyperparameter) different hyperparameter settings;

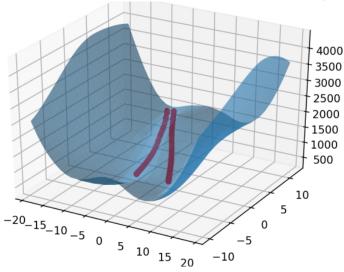
Hyperparameter tuning: In this problem, there are several different hyperparameters that will impact the network's performance: [5 points]

- Number of hidden layers (suggestions: {3, 4, 5}) (required)
- Number of units in each hidden layer (suggestions: {30, 40, 50})
- Learning rate (suggestions: {0.001, 0.005, 0.01, 0.05, 0.1, 0.5})
- Minibatch size (suggestions: 16, 32, 64, 128, 256)
- Number of epochs
- L_2 Regularization strength applied to the weight matrices (but not bias terms)

In order not to "cheat" – and thus overestimate the performance of the network – it is crucial to optimize the hyperparameters **only** on the **validation** set; do **not** use the test set. (The training set would be ok but typically leads to worse performance.) Hence, just like in Homework 3, you should fork off part of the training set into a validation portion.

- (c) After you have optimized your hyperparameters, then re-train your network again and show a screenshot displaying the training loss evolving over the last 20 iterations of SGD. (You can pick the last 20 mini-batches or last 20 epochs; it's up to you). In addition, make sure your screenshot also displays the test accuracy of the final trained classifier. The accuracy (percentage correctly classified test images) should be at least 87.5%. [4 points]
- 4. **Mountains and valleys** [15 points]: Visualize the SGD trajectory of your network when trained on Fashion MNIST:
 - (a) Plot in 3-D the cross-entropy loss f_{CE} as a function of the neural network parameters (weights and bias terms). Rather than showing the loss as a function of any particular parameters (e.g., the third component of $\mathbf{b}^{(2)}$), use the x- and y-axes to span the two directions along which your parameters vary the most during SGD training i.e., you will need to use principal component

- analysis (PCA). (In this assignment, you are free to use sklearn.decomposition.PCA.) The z-axis should represent the (unregularized) f_{CE} on training data. For each point (x, y) on a grid, compute f_{CE} and then interpolate between the points. (The interpolation and rendering are handled for you completely by the plot_surface function; see the starter code.)
- (b) Superimpose a scatter plot of the different points (in the neural network's parameter space) that were reached during SGD (just sample a few times per epoch). To accelerate the rendering, train the network and plot the surface using just a small subset of the training data (e.g., 2500 examples) to estimate f_{CE} . See the starter code, in particular the plotPath function, for an example of 3-D plotting. Submit your graph in the PDF file and the code in the Python file. Here is what I get when I superimpose two scatter plots corresponding to two different initializations and SGD runs (note that you only need to include a scatter plot for one run); as you can see, the two SGD trajectories descended into distinct local minima (though with similar cost):



In addition to your Python code (homework4_WPIUSERNAME1.py or homework4_WPIUSERNAME1.py for teams), create a PDF file (homework4_WPIUSERNAME1.pdf or homework4_WPIUSERNAME1_WPIUSERNAME2_WPIUSERNAME3.pdf for teams) containing the screenshots described above.