ELEC 576 / COMP 576 - Fall 2022 Assignment 1

Due: https://elec576.rice.edu/assignments via Canvas

Submission Instructions

Every student must submit their work as a pdf file for their report, and then all supplementary code be included in a zip file in the following format: netid-assignment1.zip. You should also provide intermediate and final results as well as any necessary code. Submit your pdf file and zip file on Canvas.

GPU Resource from AWS

To accelerate the training using GPU, you can optionally use Amazon Web Services(AWS) GPU instance using AWS Education credits. You can also get additional AWS credits from Github Student Developer Pack.

After having an AWS account, You can either create a fresh ubuntu instance and install software dependencies by yourself or use off-the-shelf TensorFlow ready image from AWS Marketplace.

1 Backpropagation in a Simple Neural Network

In this problem, you will learn how to implement the backpropagation algorithm for a simple neural network. To make your job easier, we provide you with starter code in three_layer_neural_network.py. You will fill in this starter code to build a 3-layer neural network (see Fig. 1) and train it using backpropagation.

a) Dataset

We will use the Make-Moons dataset available in Scikit-learn. Data points in this dataset form two interleaving half circles corresponding to two classes (e.g. "female" and "male").

In the main() function of three_layer_neural_network.py, uncomment the "generate and visualize Make-Moons dataset" section (see below) and run the code. Include the generated figure in your report.

```
# generate and visualize Make-Moons dataset
X, y = generate_data()
plt.scatter(X[:, 0], X[:, 1], s=40, c=y, cmap=plt.cm.Spectral)
```

b) Activation Function

Tanh, Sigmoid and ReLU are popular activation functions used in neural networks. You will implement them and their derivatives.

- Implement function actFun(self, z, type) in three_layer_neural_network.py.
 This function computes the activation function where z is the net input and type ∈ {'Tanh', 'Sigmoid', 'ReLU'}.
- 2. Derive the derivatives of Tanh, Sigmoid and ReLU
- 3. Implement function diff_actFun(self, z, type) in three_layer_neural_network.py. This function computes the derivatives of Tanh, Sigmoid and ReLU.

c) Build the Neural Network

Let's now build a 3-layer neural network of one input layer, one hidden layer, and one output layer. The number of nodes in the input layer is determined by the dimensionality of our data, 2. The number of nodes in the output layer is determined by the number of classes we have, also 2. The input to the network will be x- and y- coordinates and its output will be two probabilities, one for class 0 ("female") and one for class 1 ("male"). The network looks like the following.

Mathematically, the network is defined as follows.

$$z_1 = W_1 x + b_1 \tag{1}$$

$$a_1 = \operatorname{actFun}(z_1) \tag{2}$$

$$z_2 = W_2 a_1 + b_2 \tag{3}$$

$$a_2 = \hat{y} = \operatorname{softmax}(z_2) \tag{4}$$

where z_i is the input of layer i and a_i is the output of layer i after applying the activation function. $\theta \equiv \{W_1, b_1, W_2, b_2\}$ are the parameters of this network, which we need to learn from the training data.

If we have N training examples and C classes then the loss for the prediction \hat{y} with respect to the true labels y is given by:

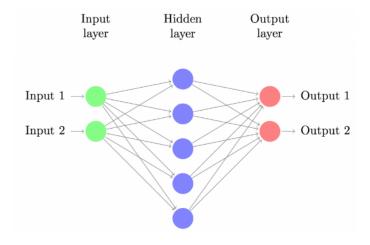


Figure 1: A three-layer neural network

$$L(y, \hat{y}) = -\frac{1}{N} \sum_{n \in N} \sum_{i \in C} y_{n,i} \log \hat{y}_{n,i}$$
 (5)

Note that y are one-hot-encoding vectors and \hat{y} are vectors of probabilities.

- 1. In three_layer_neural_network.py, implement the function feedforward(self, X, actFun). This function builds a 3-layer neural network and computes the two probabilities (self.probs in the code or a₂ in Eq. 4), one for class 0 and one for class 1. X is the input data, and actFun is the activation function. You will pass the function actFun you implemented in part b into feedforward(self, X, actFun).
- 2. In three_layer_neural_network.py, fill in the function calculate_loss(self, X, y). This function computes the loss for prediction of the network. Here X is the input data, and y is the given labels.

d) Backward Pass - Backpropagation

It's time to implement backpropagation, finally!

- 1. Derive the following gradients: $\frac{\partial L}{\partial W_2}$, $\frac{\partial L}{\partial b_2}$, $\frac{\partial L}{\partial W_1}$, $\frac{\partial L}{\partial b_1}$ mathematically
- 2. In three_layer_neural_network.py, implement the function backprop(self, X, y). Again, X is the input data, and y is the given labels. This function implements backpropagation (i.e., computing the gradients above).

e) Time to Have Fun - Training!

You already have all components needed to run the training. In three_layer_neural_network.py, we also provide you function visualize_decision_boundary(self, X, y) to visualize the decision boundary. Let's have fun with your network now.

1. Train the network using different activation functions (Tanh, Sigmoid and ReLU). Describe and explain the differences that you observe. Include the figures generated in your report. In order to train the network, uncomment the main() function in three_layer_neural_network.py, take out the following lines, and run three_layer_neural_network.py.

```
plt.scatter(X[:, 0], X[:, 1], s=40, c=y, cmap=plt.cm.Spectral)
plt.show()
```

2. Increase the number of hidden units (nn_hidden_dim) and retrain the network using Tanh as the activation function. Describe and explain the differences that you observe. Include the figures generated in your report.

f) Even More Fun - Training a Deeper Network!!!:

Let's have some more fun and be more creative now. Write your own $n_layer_neural_network.py$ that builds and trains a neural network of n layers. Your code must be able to accept as parameters (1) the number of layers and (2) layer size. We provide you hints below to help you organize and implement the code, but if you have better ideas, please feel free to implement them and ignore our hints. In your report, please tell us why you made the choice(s) you did.

Hints:

- 1. Create a new class, e.g DeepNeuralNetwork, that inherits NeuralNetwork in three_layer_neural_network.py
- In DeepNeuralNetwork, change function feedforward, backprop, calculate_loss and fit_model
- 3. Create a new class, e.g. Layer(), that implements the feedforward and backprop steps for a single layer in the network
- 4. Use Layer.feedforward to implement DeepNeuralNetwork.feedforward
- 5. Use Layer.backprop to implement DeepNeuralNetwork.backprop

6. Notice that we have L2 weight regularizations in the final loss function in addition to the cross entropy. Make sure you add those regularization terms in DeepNeuralNetwork.calculate_loss and their derivatives in DeepNeuralNetwork.fit_model.

Train your network on the Make_Moons dataset using different number of layers, different layer sizes, different activation functions and, in general, different network configurations. In your report, include generated images and describe what you observe and what you find interesting (e.g. decision boundary of deep vs shallow neural networks).

Next, train your network on another dataset different from Make_Moons. You can choose datasets provided by Scikit-learn (more details here) or any dataset of your interest. Make sure that you have the correct number of input and output nodes. Again, play with different network configurations. In your report, describe the dataset you choose and tell us what you find interesting.

Be curious and creative!!! You are exploring Deep Learning. :)

2 Training a Simple Deep Convolutional Network on MNIST

Deep Convolutional Networks (DCN) have been state-of-the-art in many perceptual tasks including object recognition, image segmentation, and speech recognition. In this problem, you will build and train a simple 5-layer DCN on MNIST Dataset. We provide you with starter in the attached .py file on the Canvas assignment page You will fill in this starter code to complete task (a), (b), and (c) below. Also, since one of the purposes of this assignment is to get you familiar with Pytorch, please review this online tutorial tutorial. You are encouraged (but not required) to re-organize the starter code but be sure to explain your code in the report.

MNIST is a dataset of handwritten digits (from 0 to 9). This dataset is one of the most popular benchmarks in machine learning and deep learning. If you develop an algorithm to learn from static images for tasks such as object recognition, most likely, you will want to debug your algorithm on MNIST first before testing it on more complicated datasets such as CIFAR10 and SVHN. There are also modified versions of MNIST, such as permutation invariant MNIST, which will come in handy for benchmarking at times.

In this lab, the MNIST data is split into 2 parts: training data and testing data. The digits have been size-normalized and centered in a fixed-size image. MNIST images are of size 28 x 28. When loaded in Tensorflow, each image is flattened into a

vector of 28x28=784 numbers. Each MNIST image will have a corresponding label which is a number between 0 and 9 corresponding to the digit that is drawn in that image.

a) Build and Train a 5-layer DCN

The architecture of the DCN that you will implement is as follows.

```
conv1(5-5-1-10) - ReLU - maxpool(2-2) - conv2(5-5-10-20) - ReLU - maxpool(2-2) - fc(320 - 50) - ReLU - DropOut(0.5) - fc(50 - 10) - Softmax(10)
```

For this part of the assignment:

- 1. **Introduction to PyTorch**: Read and try for yourself the following tutorial to get a quick introduction to PyTorch tutorial
- 2. Write Network Code: Use the following guide pytorch-mnist-guide to fill in the code skeleton provided (in the Canvas assignment posting) to build a complete DCN making sure to
 - (a) Create a logging object for tensrboard
 - (b) Import the MNIST dataset and create dataloader objects
 - (c) implement in exact structure of the 5 layer DCN described abvoe. We will have the last layer being a Softmax; therefore, unlike the pytorch-mnist-guide we will take the log of the output of our model (using torch.log) and then use nn.NLLLoss() for calculating the loss later in the training and testing loop
 - (d) Use an ADAM optimizer object for weight updates
 - (e) Implement the training and testing functions, where the statistics of each epoch is logged to later be viewed in Tensorboard
 - (f) Train over a suitable number of epochs
- 3. Visualize Training: In your terminal, type tensorboard --logdir=path/to/results where path/to/results is result_dir. Follow the instruction in your terminal to visualize the training loss in the training. You will be asked to navigate to a website to see the results, e.g. http://172.28.29.81:6006. Include the figures generated by TensorBoard in your report. If you are using Google Colab you will need to first load the tensorboard extension first and then run the commands as follows:

```
%load_ext tensorboard
%tensorboard --logdir [dir]
```

b) More on Visualizing Your Training

In part (a) of this problem, you only monitor the training loss during the training. Now, let's visualize your training more! Look at the online documentation or Github examples for PyTorch on how to monitor the statistics (min, max, mean, standard deviation, histogram) of the following terms after each 100 iterations: weights, biases, net inputs at each layer, activations after ReLU at each layer, activations after Max-Pooling at each layer. Also monitor the test and validation error after each 1100 iterations (equivalently, after each epoch). Run the training again and visualize the monitored terms in TensorBoard. Include the resultant figures in your report.

c) Time for More Fun!!!

As you have noticed, I use ReLU non-linearity, and Adam training algorithm in our sample code. In this section, run the network training with different non-linearities (tanh, sigmoid, leaky-ReLU, MaxOut,...), initialization techniques (Xavier...) and training algorithms (SGD, Momentum-based Methods, Adagrad..). Make sure you still monitor the terms specified in part (b). Include the figures generated by TensorBoard and describe what you observe. Again, be curious and creative! You are encouraged to work in groups, but you need to submit separate reports.

Collaboration Policy

Collaboration both inside and outside class is encouraged. You may talk to other students for general ideas and concepts, but individual write-ups must be done independently.

Plagiarism

Plagiarism of any form will not be tolerated. You are expected to credit all sources explicitly.