Machine Learning 6.867 - Pset 3

November 10, 2015

1 Multi-Class SVM

Due to time constraint we did not do this problem.

2 Neural Networks

Neural networks are used in machine learning to make predictions, similar to logistic regression, SVM, or linear regression. We can represent neural networks using a graph with nodes and edges (see Bishop figure 5.1). Assume that we observe data $(\mathbf{x}^{(n)}, \mathbf{y}^{(n)}), n = 1, \ldots, N$, where $\mathbf{x}^{(n)} \in \mathbb{R}^{D+1}$ (including the bias term) and $\mathbf{y}^{(n)} \in \{0,1\}^K$. Let $(\mathbf{x}, \mathbf{y}) = ([x_0, x_1, \ldots, x_D], [y_1, \ldots, y_K])$ be a general observation, where $x_0 = 1$ is a constant term for the bias. In this example, only one term of $[y_1, \ldots, y_K])$ can be one; the rest are zero. We create nodes for each of the features x_i, referred to as *inputs*, and nodes for each of the class labels y_i, referred to as *outputs*. Next, we introduce a series of nodes in the middle of the graph, called *hidden units*, and we draw edges connecting the **inputs** $\rightarrow$**hidden units**$\rightarrow$ **outputs**. The key idea in neural networks is that we can model the hidden units as functions of the inputs, and model the outputs as functions of the hidden units.

For 2-layer neural networks, we have one layer of hidden units denoted by $[z_0, z_1, \ldots, z_M]$. There are weights $\mathbf{w}_{ji}^{(1)}$ for each edge $x_i \rightarrow z_j$ and $\mathbf{w}_{kj}^{(2)}$ for each edge $z_j \rightarrow y_k$, which are unknown and will be learned through training the model. However, there are no edges from the inputs to z_0, because we assume $z_0 = 1$ is a constant term for the bias. Let $\sigma(\cdot)$ denote the logistic function, which we will use as the *activation function* for both the hidden and output layers of our neural network. The predicted value for output k given parameters $\mathbf{w} = (\mathbf{w}^{(1)}, \mathbf{w}^{(2)})$ and input $\mathbf{x}$ will be:

$$h_k(\mathbf{x}, \mathbf{w}) = \sigma\left(\sum_{j=1}^{M} w_{kj}^{(2)} \sigma\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right) + w_{k0}^{(2)}\right). \tag{1}$$

2.1 Implementation

2.1.1 Gradient Descent

We implemented a 2-layer regularized neural network using gradient descent. The loss function, which is the negative log-likelihood, is equal to:

$$\ell(\mathbf{w}) \equiv \sum_{n=1}^{N} \sum_{k=1}^{K} \left[-y_k^{(n)} \log(h_k(\mathbf{x}^{(n)}, \mathbf{w})) - (1 - y_k^{(n)}) \log(1 - h_k(\mathbf{x}^{(n)}, \mathbf{w}))\right] \tag{2}$$

Let $\tilde{\mathbf{w}}^{(1)} = (\mathbf{w}_{ji}^{(1)})_{i \neq 0}$ and $\tilde{\mathbf{w}}^{(2)} = (\mathbf{w}_{kj}^{(2)})_{j \neq 0}$. We add a regularizer term, and the final cost function becomes:

$$J(\mathbf{w}) \equiv \frac{1}{N}\ell(\mathbf{w}) + \lambda(\|\tilde{\mathbf{w}}^{(1)}\|_F^2 + \|\tilde{\mathbf{w}}^{(2)}\|_F^2), \tag{3}$$

where $\|A\|_F = \sqrt{\sum_{i,j} A_{ij}^2}$ is the matrix Frobenius norm, and λ is a fixed parameter chosen via cross-validation. Note that we exclude the bias terms from our regularizer in order to avoid penalty if the data is shifted. To take the derivative of this function, we introduce some more notation:

$$a_j^{(1)}(\mathbf{x}) \equiv \sum_{i=0}^{D} w_{ji}^{(1)} x_i \tag{4}$$

$$z_j(\mathbf{x}) \equiv \begin{cases} \sigma(a_j^{(1)}(\mathbf{x})), & j = 1, \dots, M \\ 1, & j = 0 \end{cases} \tag{5}$$

$$a_k^{(2)}(\mathbf{x}) \equiv \sum_{j=0}^{M} w_{kj}^{(2)} z_j(\mathbf{x}) \tag{6}$$

We refer to $a_j^{(1)}(\mathbf{x})$ and $a_k^{(2)}(\mathbf{x})$ as the *activations* for a fixed value of $\mathbf{x}$. It follows that $h_k(\mathbf{x}, \mathbf{w}) = \sigma(a_k^{(2)}(\mathbf{x}))$. Taking partial derivatives of J with respect to $\mathbf{w}_{kj}^{(2)}$ and $\mathbf{w}_{ji}^{(1)}$ for $i \neq 0$ and $j \neq 0$, we find:

$$\begin{aligned} \frac{\partial J(\mathbf{w})}{\partial \mathbf{w}_{kj}^{(2)}} &= 2\lambda \mathbf{w}_{kj}^{(2)} + \frac{1}{N} \sum_{n=1}^{N} \left(\frac{-y_k^{(n)}}{h_k(\mathbf{x}^{(n)}, \mathbf{w})} + \frac{1 - y_k^{(n)}}{1 - h_k(\mathbf{x}^{(n)}, \mathbf{w})} \right) h_k(\mathbf{x}^{(n)}, \mathbf{w})(1 - h_k(\mathbf{x}^{(n)}, \mathbf{w})) z_j(\mathbf{x}^{(n)}) && (7) \\ &= 2\lambda \mathbf{w}_{kj}^{(2)} + \frac{1}{N} \sum_{n=1}^{N} \left(-y_k^{(n)}(1 - h_k(\mathbf{x}^{(n)}, \mathbf{w})) + (1 - y_k^{(n)}) h_k(\mathbf{x}^{(n)}, \mathbf{w}) \right) z_j(\mathbf{x}^{(n)}) && (8) \end{aligned}$$

$$\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}_{ji}^{(1)}} = 2\lambda \mathbf{w}_{ji}^{(1)} + \frac{1}{N} \sum_{n=1}^{N} \sum_{k=1}^{K} \left(-y_k^{(n)}(1 - h_k(\mathbf{x}^{(n)}, \mathbf{w})) + (1 - y_k^{(n)}) h_k(\mathbf{x}^{(n)}, \mathbf{w}) \right) w_{kj}^{(2)} z_j(\mathbf{x}^{(n)})(1 - z_j(\mathbf{x}^{(n)})) \mathbf{x}^{(n)} \tag{9}$$

For the bias terms, there is no regularizer penalty, so we obtain:

$$\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}_{k0}^{(2)}} = \frac{1}{N} \sum_{n=1}^{N} \left(-y_k^{(n)}(1 - h_k(\mathbf{x}^{(n)}, \mathbf{w})) + (1 - y_k^{(n)}) h_k(\mathbf{x}^{(n)}, \mathbf{w}) \right) \tag{10}$$

$$\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}_{j0}^{(1)}} = \frac{1}{N} \sum_{n=1}^{N} \sum_{k=1}^{K} \left(-y_k^{(n)}(1 - h_k(\mathbf{x}^{(n)}, \mathbf{w})) + (1 - y_k^{(n)}) h_k(\mathbf{x}^{(n)}, \mathbf{w}) \right) w_{kj}^{(2)} z_j(\mathbf{x}^{(n)})(1 - z_j(\mathbf{x}^{(n)})) \mathbf{x}^{(n)} \tag{11}$$

Therefore, we have calculated analytic expressions for the gradients of J with respect to the different groups of parameters $\mathbf{w}^{(2)}$ and $\mathbf{w}^{(1)}$. From these expressions, we coded a function in MATLAB to train a our neural network using *batch gradient descent*. The function takes in all the input data $(\mathbf{x}^{(n)}, \mathbf{y}^{(n)}), n = 1, \dots, N$ at once, and does gradient descent on the total objective value over the N data points each time, until convergence. Model parameters are regularization parameter λ, number of nodes in the hidden layer M, and initial solution $(\mathbf{w}_{init}^{(1)}, \mathbf{w}_{init}^{(2)})$. The function outputs the optimal solution $\mathbf{w} = (\mathbf{w}^{(1)}, \mathbf{w}^{(2)})$ that minimizes the final cost function $J(\mathbf{w})$. The formula for the update is as follows:

$$\mathbf{w}_{new}^{(1)} = \mathbf{w}_{old}^{(1)} - \eta \nabla_{w^{(1)}} J(\mathbf{w}_{old}), \qquad \mathbf{w}_{new}^{(2)} = \mathbf{w}_{old}^{(2)} - \eta \nabla_{w^{(2)}} J(\mathbf{w}_{old}), \tag{12}$$

where η is the step size. We will discuss the choice of η in the next sections. Because the objective function is non-convex, we run our training function with multiple initial solutions to avoid reporting a single local optimum. After running multiple times, we report the optimal solution $\mathbf{w} = (\mathbf{w}^{(1)}, \mathbf{w}^{(2)})$ that minimizes $J(\mathbf{w})$ over all trials.

2.1.2 Stochastic Gradient Descent

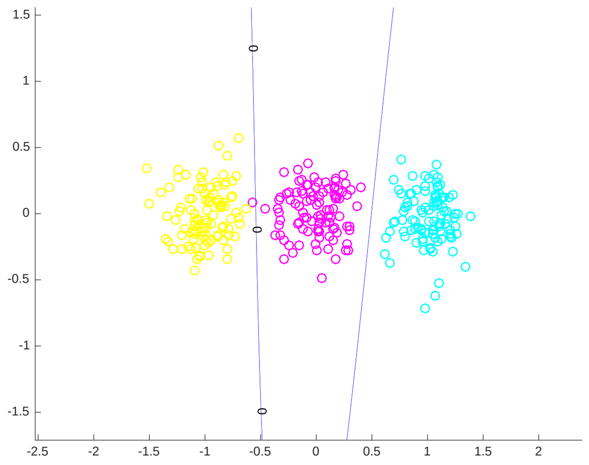
We implemented an alternate function in MATLAB to train our neural network using *stochastic gradient descent*. We first take one training point and run gradient descent on the objective function on this point. With the output $\mathbf{w}^{(1)}$ and $\mathbf{w}^{(2)}$ as new initial values, we then take a second training point and run gradient descent on the objective function on this point. Repeat the process until convergence. If necessary, we can reshuffle the data and loop through the data multiple times.

2.2 Computational Results

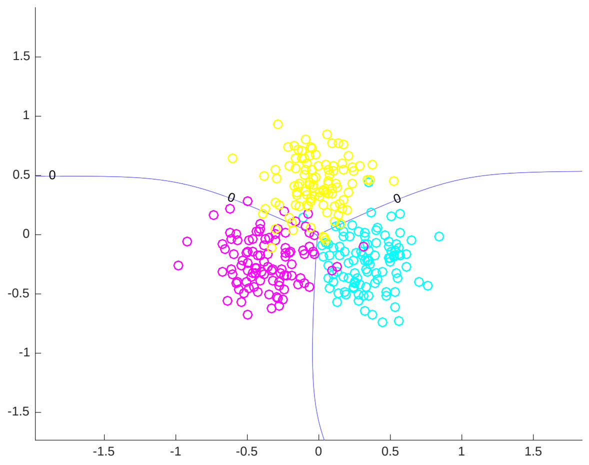
We tested our neural network on various data sets, including toy problems and real-world MNIST data on hand-written digits. Both batch gradient descent and stochastic gradient descent methods are tested on the sets.

2.2.1 Toy Problems

The first toy problem is on a linearly separable 3-class data. The decision boundary of a good ANN classifier we found is illustrated in Figure 1a. We present the validation set accuracy results in Table 1, under different number of units in the hidden layer and the trade-off parameter in regularization. We see from the table that we achieve highest validation accuracy under $\lambda = 0.001$ and $M = 2$. This gives us test accuracy of 99.3%.



(a) Toy Data 1



(b) Toy Data 2

Figure 1: Plots of decision boundaries from Artificial Neural Networks on training toy data.

The second problem we considered is another 3-class data with points that are more closely spaced. The decision boundary of our ANN classifier is presented in Figure 1b. Similarly, the accuracy from cross-validation is given in Table 2. The best validation accuracy is obtained when $M = 4$ and $\lambda = 0.001$. The accuracy decreases when $\lambda \geq 0.005$, which are not included in the table but this was observed during experiments. For $M = 4$ and $\lambda = 0.001$, we obtain testing set accuracy of 90.7%.

Table 1: Validation accuracy on Toy Data 1 under different parameter specification

λ / M	2	3	4	5	6
0	0.9933	0.9900	0.9933	0.9900	0.9933
0.001	0.9967	0.9833	0.9867	0.9800	0.9933
0.01	0.9833	0.9733	0.9667	0.9833	0.9900

Table 2: Validation accuracy on Toy Data 2 under different parameter specification

λ / M	2	3	4	5	6
0	0.9100	0.9167	0.9267	0.9167	0.9267
0.0001	0.9267	0.9100	0.9133	0.9167	0.9233
0.001	0.8967	0.8233	0.9333	0.9167	0.9333
0.005	0.9100	0.8833	0.9133	0.8967	0.8933

There are some computational considerations when choosing the parameters for the model. In particular, it is very important to choose reasonable initial values for $\mathbf{w}$ and the step size. We chose the initial values to be random numbers between $[-0.05, 0.05]$ because when the initial values are close to zero, the gradient on the logistic function would have a sizable magnitude. We use a symmetric range around zero so that the sign of the initial solution is not biased. The step size is chosen to satisfy the Robbins-Monro criterion: we chose $\eta = ss/(iter + 100)^{0.6}$, where $iter$ is the number of current iteration, and ss is chosen to be 25 for these toy data sets. Regarding the convergence criteria, the lower it is, the better accuracy we have generally; however the longer run-time it takes as well.

Between batch and stochastic gradient descent implementations, we found that the batch method is more sensitive to the choice of initial $\mathbf{w}$. Because stochastic gradient descent optimizes the objective for one data point at a time, some data points can pull the current solution from local minima during the training process. On the other hand, batch gradient descent optimizes the objective for all data points simultaneously, and therefore tends to get stuck in local minima more easily. In addition, stochastic gradient descent is more computationally tractable for large problems with high number of data points, because the complexity for the updates remain constant for each data point, even as $n \to \infty$. In practice, for the Toy data problems, we also observe that stochastic gradient descent is the faster method. The numbers we present here are from stochastic gradient descent, but can also replicated by batch method if the parameters are chosen carefully.

2.2.2 MNIST Data

The MNIST dataset is a set of handwritten digits (0-9) that is widely used in the machine learning community to benchmark classification methods. Each observation is a single digit 0-9 written in a 28 x 28 pixel square, and the task is to classify new digits using the pixel intensities as predictive features. Therefore, there are 10 possible classes (the digits 0-9) and 784 features (total number of pixels), so this a high-dimensional, challenging classification problem.

For this paper, we used a subset of MNIST data containing digits (1-6), which has been pre-split into a training, validation, and test set. We implemented our neural network using stochastic gradient descent on this dataset, using the analytic formula for the gradient for computational purposes. We used a multistep procedure to determine the multiple input parameters that must be specified for the neural network. First, we fixed λ (regularization parameter), M (number of hidden nodes), and $iter\_lim$ (maximum number of iterations) to arbitrary values $(\lambda, M, iter\_lim) = (10^{-10}, 20, 6000)$ which were reasonable parameter values found through trial-and-error exploration. Then, we varied the step size by modifying the ss parameter in the Robbins-Monro criterion, and we found $ss = 10$ to be the best value. Therefore, we determined the solver parameters for our implementation of stochastic gradient descent to be $ss = 10$, $iter\_lim = 6000$. We chose convergence threshold 10^{-6} which resulted in reasonable run time and high precision.

With these fixed solver parameters, we then used cross-validation techniques to select the optimal parameter values for the λ and M. We trained our neural network model on the training dataset using stochastic gradient descent for various pairs of parameters λ and M, and the validation results are presented in Figure 2. For the ranges that we searched over, $\lambda \in \{0, 10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}, 10^{-10}\}$ and $M \in \{5, 10, 15, 25, 30, 35, 40\}$, we found the optimal parameter pair to be $(\lambda, M) = (10^{-4}, 35)$. (Note that 0 is not included in the heatmap for consistency, however, we explored the non-regularized option but it was suboptimal). We did cross-validation procedures for model parameters (λ, M) separately from the solver parameters $(ss, iter\_lim)$ because there are

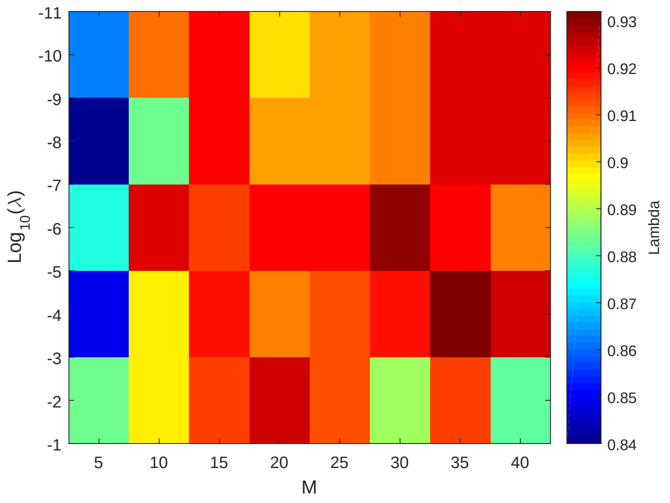


Figure 2: Heatmap of cross-validation accuracy for Artificial Neural Networks on MNIST data.

not significant interactions between these groups of variables. In particular, we made the assumption that the optimal choice of step-size will be constant for any choice of (λ, M) within a large range of possible values.

Finally, we ran our model with $(\lambda, M, ss, iter\_lim) = (10^{-6}, 30, 10, 6000)$ on the training set with a smaller convergence criterion 10^{-10}, in order to achieve higher accuracy. This model did not reach the convergence criterion, but the stochastic gradient algorithm terminated when the iteration limit was attained instead. Our 2-layer neural network using stochastic gradient descent with these parameter values and random seed=0 yielded training accuracy: 98.8%, validation accuracy: 93.4%, and test accuracy: 94.0% on the MNIST data set. We also tested the implementation of our neural network using batch gradient descent. This method yielded comparable results, although it was much slower on the MNIST dataset, so we did not rerun the cross-validation procedure which took several hours.