10707 Homework 1

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Problem 1 (6 pts)

This question will test your general understanding of overfitting as they relate to model complexity and training set size. Consider a continuous domain and a smooth joint distribution over inputs and outputs, so that no test or training case is ever duplicated exactly.

- For a fixed training set size, sketch a graph of the typical behavior of training error rate (y-axis) versus model complexity (x-axis). Add to this graph a curve showing the typical behavior of the corresponding test error rate versus model complexity, on the same axes. (Assume that we have an infinite test set drawn independently from the same joint distribution as the training set). Mark a vertical line showing where you think the most complex model your data supports is; chose your horizontal range so that this line is neither on the extreme left nor on the extreme right. Indicate on your vertical axes where zero error is and draw your graphs with increasing error upwards and increasing complexity rightwards.

- For a fixed model complexity, sketch a graph of the typical behavior of training error rate (y-axis) versus training set size (x-axis). Add to this graph a curve showing the typical behavior of test error rate versus training set size, on the same axes (again on an iid infinite test set). Indicate on your vertical axes where zero error is and draw your graphs with increasing error upwards and increasing training set size rightwards.

- One of the commonly used regularization methods in neural networks is *early stopping*. Argue qualitatively why (or why not) early stopping is a reasonable regularization metric.

Your answer here

1. Graph shown in Figure 1.

2. Graph shown in Figure 2.

3. Yes, it is a reasonable regularization metric. As a network trains more and more, the weights tune directly to the data in the training set. The problem with this is that the network may begin to start looking at specific noise in the training set that may not be represented in the test set. The more the network trains, the more the weights are specifically tuned to the training set, and at some point it will likely be tuned to where it is overfit. Stopping early prevents the network from training to the point where it knows every detail of the test set, which can improve generalization. T

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*Use footnote for providing further information about author (webpage, alternative address)—*not* for acknowledging funding agencies.

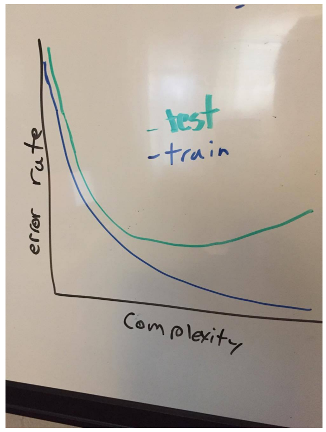


Figure 1: error rate vs complexity

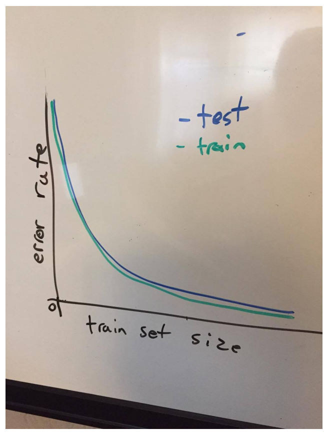


Figure 2: error rate vs dataset size

Problem 2 (8 pts)

Consider N training points (x_i, y_i) drawn i.i.d from a distribution that is characterized as:

$$x_i \sim h(x) \tag{1}$$
$$y_i = f(x_i) + \epsilon_i \tag{2}$$
$$\epsilon_i \sim (0, \sigma^2) \tag{3}$$

where f is the regression function. An estimator for this data, *linear* in y_i is given by

$$\hat{f}(x^*) = \sum_{i=1}^{N} l_i(x^*; \mathcal{X}) y_i, \tag{4}$$

where $l_i(x^*; \mathcal{X})$ depends on the entire training sequence of x_i (denoted by $\mathcal{X}$) but do not depend on y_i. Show that k-nearest-neighbor regression and linear regression are members of this class of estimators. What would be the $l_i(x^*; \mathcal{X})$ in both these regressions (knn and linear)?

Your answer here

Problem 3 (6 pts)

The form of Bernoulli distribution, given by:

$$\text{Bern}(x|\mu) = \mu^x (1-\mu)^{1-x},$$

is not symmetric between the two values of $x \in \{0, 1\}$. Often, it will be convenient to use an equivalent formulation for which $x \in \{-1, 1\}$, in which case the distribution can be written as:

$$p(x|\mu) = \left(\frac{1-\mu}{2}\right)^{(1-x)/2} \left(\frac{1+\mu}{2}\right)^{(1+x)/2},$$

where $\mu \in [-1, 1]$. Show that this new distribution is normalized and compute its mean, variance, and entropy.

Your answer here

Entropy is shown in figure below.

$$2^{\frac{1}{2}(-x-1)} (\mu + 1)^{\frac{x+1}{2}}$$

Figure 3: entropy of given distribution

Problem 4 (12 pts)

Consider a binary classification problem in which the target values are $t \in \{0, 1\}$, with a neural network output $y(x, w)$ that represents $p(t = 1|x; w)$, and suppose that there is a probability ϵ that the class label on a training data point has been incorrectly set. Assuming independent and identically distributed data, write down the error function corresponding to the negative log likelihood. What is the error function when $\epsilon = 0$? Note that this error function makes the model robust to incorrectly labelled data, in contrast to the usual error function.

Your answer here

The error function can be seen in the figure below with the function when eta=0 below it.

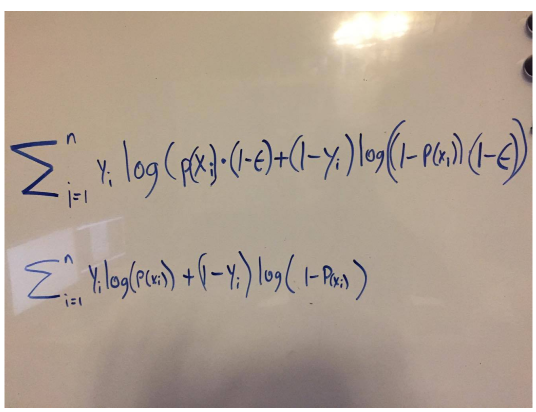


Figure 4: negative log likelyhood with uncertainty

Problem 5 (8 pts)

Consider a two-layer network function in which the hidden-unit nonlinear activation functions are given by logistic sigmoid functions of the form:

$$\sigma(a) = \frac{1}{1 + \exp(-a)} \tag{5}$$

Show that there exists an equivalent network, which computes exactly the same function, but with hidden unit activation functions given by $\tanh(a)$ where the tanh function is defined by:

$$\tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}} \tag{6}$$

Your answer here

The derivation is shown below in the figure below.

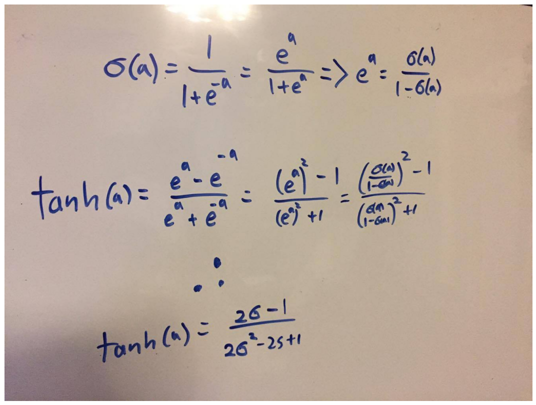


Figure 5: derivation of sigmoid into tanh

Problem 6 (60 pts)

For this question you will write your own implementation of backpropagation algorithm for training your own neural network. Please do not use any toolboxes. We recommend that you use MATLAB or Python, but you are welcome to use any other programming language if you wish.

The goal is to label images of 10 handwritten digits of “zero”, “one”,..., “nine”. The images are 28 by 28 in size (MNIST dataset), which we will be represented as a vector x of dimension 784 by listing all the pixel values in raster scan order. The labels t are 0,1,2,...,9 corresponding to 10 classes as written in the image. There are 3000 training cases, containing 300 examples of each of 10 classes, 1000 validation (100 examples of each of 10 classes), and 3000 test cases (300 examples of each of 10 classes). they can be found in the file digitstrain.txt, digitsvalid.txt and digitstest.txt:
http://www.cs.cmu.edu/∼rsalakhu/10707/assignments.html

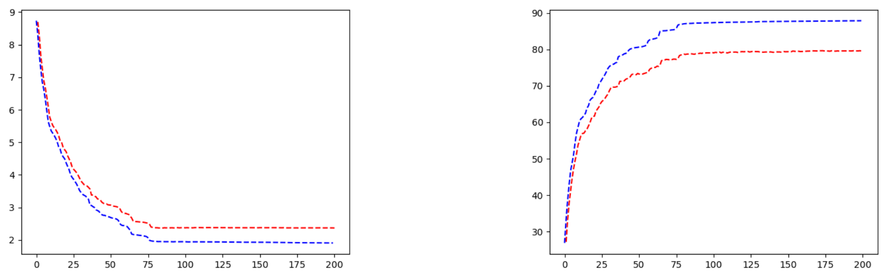
Format of the data: digitstrain.txt contains 3000 lines. Each line contains 785 numbers (comma delimited): the first 784 real-valued numbers correspond to the 784 pixel values, and the last number denotes the class label: 0 corresponds to digit 0, 1 corresponds to digit 1, etc. digitsvalid.txt and digitstest.txt contain 1000 and 3000 lines and use the same format as above. As a warm up question, load the data and plot a few examples. Decide if the pixels were scanned out in row-major or column-major order.

Backpropagation Algorithm

Implement backpropagation algorithm with sigmoid activation function in a single-layer neural network. The output layer should be a softmax output over 10 classes corresponding to 10 classes of handwritten digits. Your backprop code should minimize the cross-entropy entropy function for multi-class classification problem.

a) Basic generalization [5 points]

Train a single layer neural network with 100 hidden units (with architecture: 784 → 100 → 10). You should use initialization scheme discussed in class as well as choose a reasonable learning rate (e.g.



(a) Cross Entropy Error (b) Prediction Accuracy

Figure 6: A comparison of two error measures on validation and train data

0.1). Train the network repeatedly (more than 5 times) using different random seeds, so that each time, you start with a slightly different initialization of the weights. Run the optimization for at least 200 epochs each time. If you observe underfitting, continue training the network for more epochs until you start seeing overfitting.

Plot the average training cross-entropy error (sum of the cross-entropy error terms over the training dataset divided by the total number of training example) on the y-axis vs. the epoch number (x-axis). On the same figure, plot the average validation cross-entropy error function.

Examine the plots of training error and validation error (generalization). How does the network's performance differ on the training set versus the validation set during learning? Use the plot of error curves (training and validation) to support your argument.

Your answer here

As you can see in Figure 6,the performance of both the test set and the validation set start out fairly equal. This is the case with both measures of performance, cross-entropy loss and prediction accuracy.

Soon, however, the model begins to fit better to the training set than the validation set. While the validation set performance still improves, the improvement of train set data is faster.

Eventually, convergence is reached and performance of the validation set stays the same while the performance of the train set marginally increases over time.

When comparing cross entropy error with classification error, the charts seem very similar. The only observable difference is that the cross entropy loss seems to be more similar than the prediction accuracy. This could be because similar numerals were almost predicted correctly in validation set, but lost out to different class.

b) Classification error [5 points]

You should implement an alternative performance measure to the cross entropy, the mean classification error. You can consider the output correct if the correct label is given a higher probability than the incorrect label. You should then count up the total number of examples that are classified incorrectly (divided by the total number of examples) according to this criterion for training and validation respectively, and maintain this statistic at the end of each epoch. Plot the classification error (in percentage) vs. number of epochs, for both training and validation. Do you observe a different behavior compared to the behavior of the cross-entropy error function?

Your answer here

Question answered in section A.

c) Visualizing Parameters [5 points]

Visualize your best results of the learned W as 100 28x28 images (plot all filters as one image, as we have seen in class). Do the learned features exhibit any structure?

Your answer here

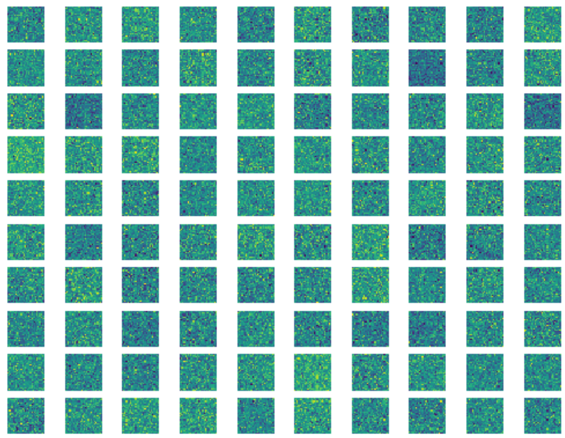


Figure 7: sample of hidden layer weights

While at first glance, the weights in Figure 7 may appear to be noisy, one can see structure taking the shape of streaks at different angles and intercepts. While we were told to use at least 200 epochs, my network seems to have completely fit in 75. For this reason, I believe that the weights would appear more structured if they were taken from this moment. As epochs went on, overfitting may have caused weights to pick up on less general details about the training set.

d) Learning rate [5 points]

Try different values of the learning rate ϵ. You should start with a learning rate of 0.1. You should then reduce it to $.01$, and increase it to 0.2 and 0.5. What happens to the convergence properties of the algorithm (looking at both average cross entropy and % Incorrect)? Try momentum of $\{0.0, 0.5, 0.9\}$. How does momentum affect convergence rate? How would you choose the best value of these parameters?

Your answer here

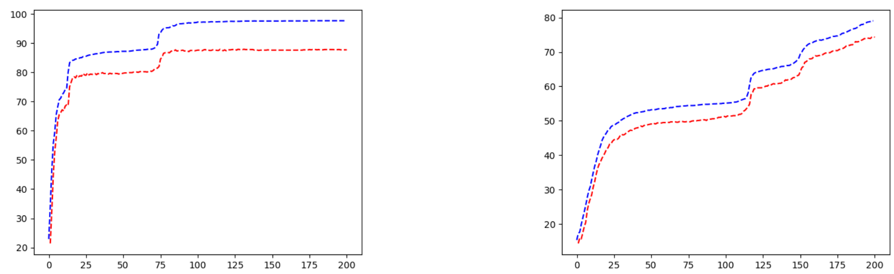
As you can see in Figure 8, the learning rate had an extremely large effect on convergence. Namely, the higher the learning rate, the faster the network converged.

When factoring in momentum, the effects were less clear. However momentum did seem to improve the convergence rate overall. Show in Figure 9, are some interesting effects caused when the momentum rate was 0.5. The network's accuracy seemed to plateau and then jump up multiple times.

e) Number of hidden units [5 points]

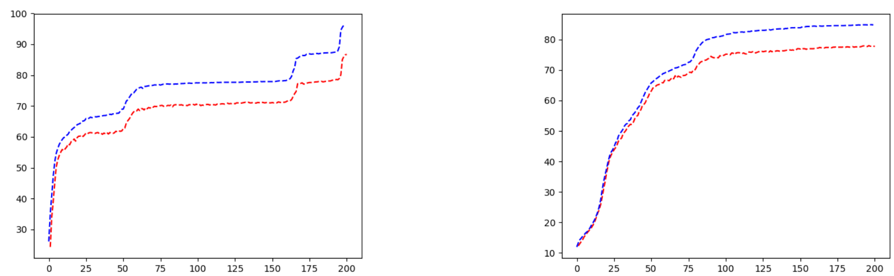
Set the learning rate ϵ to $.01$, momentum to 0.5 and try different numbers of hidden units on this problem. You should try training a network with 20, 100, 200, and 500 hidden units. Describe the effect of this modification on the convergence properties, and the generalization of the network.

To find the best parameters, I would use choose a range of each one which I thought was reasonable and perform either a random search or a grid search on these parameters.



(a) eta = 0.1 (b) eta = 0.01

Figure 8: a comparison of the conversion of different learning rates

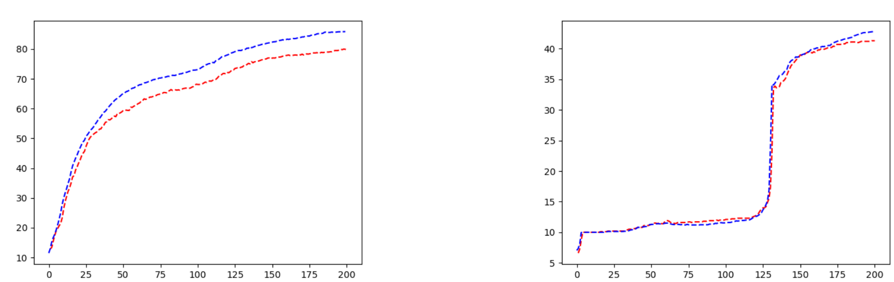


(a) momentum = 0.5 (b) momentum = 0.9

Figure 9: a comparison of the conversion of different momentum rates

Your answer here

As the number of units increased, performance actually seemed to decrease in the network. That said, even though convergence was slowed, the actual generalization of the network seemed to be improved. Figure 10 shows these effects.



(a) 20 hidden units (b) 500 hidden units

Figure 10: a comparison of the accuracy of numbers of hidden units

f) Best performing single-layer network [10 points]

Cross-validation: Explore various model hyper-parameters, including

- learning rates
- momentum
- number of hidden units in each layer
- number of epochs (early stopping)

- L_2 regularization (weight decay)

to achieve the best validation accuracy. Briefly describe your findings.

Given the best found values, report the final performance of your 1-layer neural network (both average cross entropy and % Incorrect) on the training, validation, and test sets. Visualize your best results of the learned W as 28x28 images (plot all filters as one image, as we have seen in class).

Your answer here

I found that the best learning rates tended to be higher, my best one was eta=0.5. Because I was using a high learning rate, I also employed early stopping and only ran for 18 epochs. I did not use momentum as it caused worse performance. I ended up sticking with 100 hidden units, as this had the best performance once the other hyperparameters were set. L2 regularization did help and was used. Statistics for each set of data: Train: Accuracy = 97.1 Cross Entropy = 0.28 Validation: Accuracy = 88.9 Cross Entropy = 0.60 Test: Accuracy = 87.46 Cross Entropy = 0.71 Figure 11 shows the vizualization of the weights for this network.

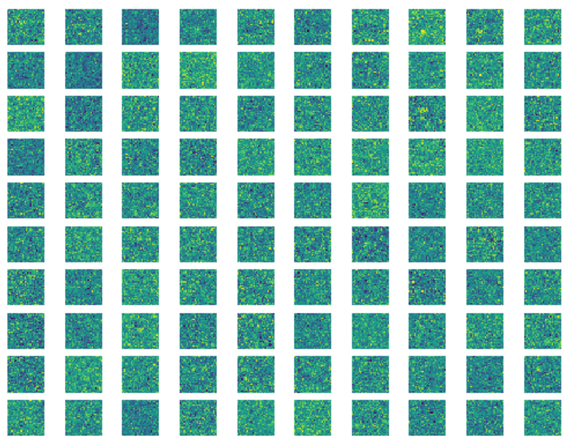


Figure 11: sample of hidden layer weights

g) Extension to multiple layers [10 points]

Implement a 2-layer neural network, starting with a simple architecture containing 100 hidden units in each layer (with architecture: $784 \rightarrow 100 \rightarrow 100 \rightarrow 10$).

Cross-validation: Explore various model hyper-parameters, including learning rates, momentum, number of hidden units in each layer, number of epochs, and weight decay to achieve the best validation accuracy. Briefly describe your findings.

Given the best found values, report the final performance of your 2-layer neural network (both average cross entropy and % Incorrect) on the training, validation, and test sets. Visualize your best results of the learned 1st-layer W as 28x28 images (plot all filters as one image, as we have seen in class). How do these filters compare to the ones you obtained when training a single-layer network?

Does 1-layer network outperform a 2-layer model in term of generalization capabilities?

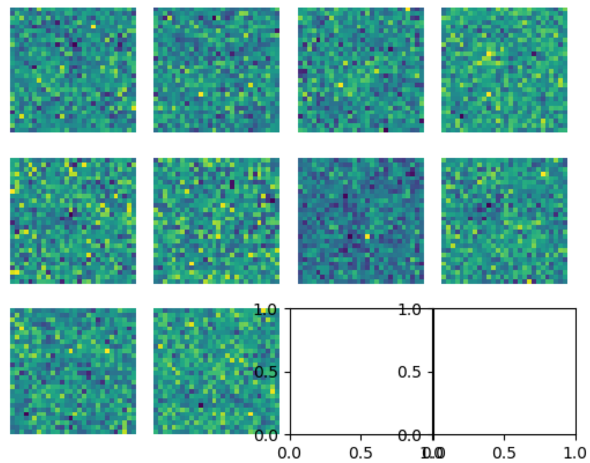


Figure 12: sample of hidden layer weights

Your answer here

While I believe that a 2-layer model should be able to outperform, I could not find hyperparameters that recieved better performance.

I found that I was able to train for many more epochs before plateauing of the validation accuracy, however I also found that it was much easier to overfit on the training data. Learning rate = .03 Epochs = 500 Momentum = 0.9 Layers = [10,20]

Statistics for each set of data: Train: Accuracy = 90.5 Cross Entropy = 0.46 Validation: Accuracy = 82.2 Cross Entropy = 0.67 Test: Accuracy = 78.9 Cross Entropy = 0.75

Figure 12 shows the weights of my first layer. The structure in these weights appears to be more complicated than the previous ones. Rather than simple lines at different angles, the weights show structures such as loops and curves. This may be because there were much fewer weights in my first layer.

h) Batch Normalization [10 points]

For your two-layer network, implement batch normalization for a batch size of 32. Describe how batch norm helps (or doesn't help) in terms of speed and accuracy (train and validation).

Your answer here

Batch normalization did not necessarily help with speed to convergence, however I did find that it helped the network with accuracy. The generalization of the network was also improved, as the loss difference between the train and validation sets were smaller.

i) Different Activation Functions [5 points]

Now, change the activation functions to ReLU and tanh instead of the original sigmoid. Do you see any difference in terms of performance or accuracy ? Report your findings.

Your answer here

ReLU seemed to perform marginally better in all aspects, however there were different optimal hyperparameters.

TanH performed horribly, and I could not find a set of hyperparameters that worked.