Homework Set 5, CPSC 8420, Fall 2024

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Problem 1

Recall the classification models we discussed in class: **SVM** and **Logistic Regression**, seems both of them work on binary classification task. However, in real-world applications, multi-classification is everywhere, thus in this problem we explore how to extend vanilla **Logistic Regression** for multi-classification. Assume we have K different classes and the input $\mathbf{x} \in \mathcal{R}^d$, and the probability to each class is defined as:

$$P(Y = k | X = \mathbf{x}) = \frac{exp(\mathbf{w}_k^T \mathbf{x})}{1 + \sum_{l=1}^{K-1} exp(\mathbf{w}_l^T \mathbf{x})} \quad for \quad k = 1, 2, \dots, K-1;$$

$$P(Y = K | X = \mathbf{x}) = \frac{1}{1 + \sum_{l=1}^{K-1} exp(\mathbf{w}_l^T \mathbf{x})}$$
(1)

If we define $\mathbf{w}_K = \mathbf{0}$, then we can combine the two cases above as one:

$$P(Y = k|X = \mathbf{x}) = \frac{exp(\mathbf{w}_k^T \mathbf{x})}{1 + \sum_{l=1}^{K-1} exp(\mathbf{w}_l^T \mathbf{x})} \quad for \quad k = 1, \dots, K$$
 (2)

- 1. What and how many parameters are there to be optimized?
- 2. The training data is given as: $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, please simplify the log likelihood function to your best:

$$L(\mathbf{w}_1, \dots, \mathbf{w}_{K-1}) = \sum_{i=1}^n ln P(Y = y_i | X = \mathbf{x}_i)$$
(3)

- 3. Now please find the gradient of L w.r.t. \mathbf{w}_k .
- 4. If we add regularization term and formulate new objective function as:

$$f(\mathbf{w}_1, \dots, \mathbf{w}_{K-1}) = L(\mathbf{w}_1, \dots, \mathbf{w}_{K-1}) - \frac{\lambda}{2} \sum_{l=1}^{K-1} ||\mathbf{w}_l||_2^2,$$
 (4)

now please determine the new gradient.

5. You are given USPS handwritten recognition digit dataset, with image size 16×16 . For each digit $(i.e.\ 0,1,\ldots,9)$ there are 600 training samples in addition to 500 testing ones. You may use: imshow(reshape($\mathbf{x},16,16$)) to view the image in Matlab. (Non-Matlab user may utilize .txt files to conduct experiments.)

- (a) Please use gradient ascent algorithm (you are expected to complete log_grad.m) to train the model and plot 1) vanilla objective function L in Eq.(3); 2) training accuracy and 3) testing accuracy with updates respectively. Also indicate the final testing accuracy score. (Please choose a proper learning rate and stopping criterion). The folder include figures for your reference.
- (b) Now if we add the regularization term as Eq.(4), please show the final accuracy when $\lambda = \{0, 1, 10, 100, 200\}$ respectively.
- (c) What conclusion can we draw from the above experiments?

P1.1, Answer:

For the given multi-class logistic regression model, the parameters to be optimized are the weight vectors $\{\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_{K-1}\}$, where each $\mathbf{w}_k \in \mathbb{R}^d$ is a d-dimensional vector corresponding to one of the K-1 classes. The parameter \mathbf{w}_K is fixed to $\mathbf{0}$, so it does not need to be optimized. As a result, the total number of parameters to estimate is given by $(K-1) \times d$, where K-1 represents the number of weight vectors to optimize, and d is the number of features in the input \mathbf{x} . These parameters are learned during the training process to maximize the likelihood of the observed data.

P1.2, Answer:

Using the probability definition from the model, for $y_i = k$, where $k \in \{1, ..., K-1\}$, the conditional probability is given by:

$$P(Y = k | X = \mathbf{x}_i) = \frac{\exp(\mathbf{w}_k^{\top} \mathbf{x}_i)}{1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i)}.$$

For $y_i = K$, the conditional probability is:

$$P(Y = K | X = \mathbf{x}_i) = \frac{1}{1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i)}.$$

The log-likelihood can then be expressed as:

$$L(\mathbf{w}_1, \dots, \mathbf{w}_{K-1}) = \sum_{i=1}^n \ln P(Y = y_i | X = \mathbf{x}_i).$$

Substituting the expressions for $P(Y = y_i | X = \mathbf{x}_i)$:

$$L(\mathbf{w}_1, \dots, \mathbf{w}_{K-1}) = \sum_{i=1}^n \left[\mathbf{I}_{\{y_i < K\}} \ln \left(\frac{\exp(\mathbf{w}_{y_i}^\top \mathbf{x}_i)}{1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^\top \mathbf{x}_i)} \right) + \mathbf{1}_{\{y_i = K\}} \ln \left(\frac{1}{1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^\top \mathbf{x}_i)} \right) \right],$$

where $\mathbf{1}_{\{y_i < K\}}$ is the indicator function that is 1 if $y_i \in \{1, \dots, K-1\}$, and $\mathbf{1}_{\{y_i = K\}}$ is 1 if $y_i = K$. For $y_i < K$, the first term simplifies to:

$$\ln \left(\frac{\exp(\mathbf{w}_{y_i}^{\top} \mathbf{x}_i)}{1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i)} \right) = \mathbf{w}_{y_i}^{\top} \mathbf{x}_i - \ln \left(1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i) \right).$$

For $y_i = K$, the second term simplifies to:

$$\ln\left(\frac{1}{1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i)}\right) = -\ln\left(1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i)\right).$$

Combining these, the log-likelihood simplifies to:

$$L(\mathbf{w}_1, \dots, \mathbf{w}_{K-1}) = \sum_{i=1}^n \left[\mathbf{w}_{y_i}^\top \mathbf{x}_i \mathbf{I}_{\{y_i < K\}} - \ln \left(1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^\top \mathbf{x}_i) \right) \right].$$

Here, the first term contributes only when $y_i < K$, while the second term applies to all data points.

P1.3, Answer:

The first term in the summation contributes only when $y_i = k$. Therefore:

$$\frac{\partial}{\partial \mathbf{w}_k} \left(\mathbf{w}_{y_i}^{\top} \mathbf{x}_i \right) = \begin{cases} \mathbf{x}_i & \text{if } y_i = k, \\ 0 & \text{if } y_i \neq k. \end{cases}$$

The second term is the log of the denominator:

$$\frac{\partial}{\partial \mathbf{w}_k} \ln \left(1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i) \right).$$

Let:

$$f(\mathbf{w}_k) = \ln\left(1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i)\right).$$

The derivative of f with respect to \mathbf{w}_k is:

$$\frac{\partial f}{\partial \mathbf{w}_k} = \frac{\exp(\mathbf{w}_k^{\top} \mathbf{x}_i) \mathbf{x}_i}{1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i)}.$$

Combining these, the gradient of L with respect to \mathbf{w}_k is:

$$\frac{\partial L}{\partial \mathbf{w}_k} = \sum_{i=1}^n \left[\mathbf{I}_{\{y_i = k\}} \mathbf{x}_i - \frac{\exp(\mathbf{w}_k^{\top} \mathbf{x}_i) \mathbf{x}_i}{1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i)} \right],$$

where $\mathbf{1}_{\{y_i=k\}}$ is the indicator function that equals 1 if $y_i=k$, and 0 otherwise. Simplifying further, let:

$$P(Y = k | \mathbf{x}_i) = \frac{\exp(\mathbf{w}_k^{\top} \mathbf{x}_i)}{1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i)}.$$

Then the gradient can be written as:

$$\frac{\partial L}{\partial \mathbf{w}_k} = \sum_{i=1}^n \mathbf{x}_i \left[\mathbf{I}_{\{y_i = k\}} - P(Y = k | \mathbf{x}_i) \right].$$

This is the gradient of the log-likelihood L with respect to \mathbf{w}_k . It consists of the difference between the observed indicator for class k and the predicted probability for class k, scaled by the feature vector \mathbf{x}_i .

P1.4, Answer:

To determine the gradient of the regularized objective function, we begin with the definition of f, which is given by:

$$f(\mathbf{w}_1, \dots, \mathbf{w}_{K-1}) = L(\mathbf{w}_1, \dots, \mathbf{w}_{K-1}) - \frac{\lambda}{2} \sum_{l=1}^{K-1} ||\mathbf{w}_l||_2^2,$$

where $L(\mathbf{w}_1, \dots, \mathbf{w}_{K-1})$ is the log-likelihood function:

$$L(\mathbf{w}_1, \dots, \mathbf{w}_{K-1}) = \sum_{i=1}^n \left[\mathbf{w}_{y_i}^\top \mathbf{x}_i - \ln \left(1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^\top \mathbf{x}_i) \right) \right].$$

To compute the gradient of f with respect to \mathbf{w}_k , we compute the derivative of each term in f. First, the gradient of L with respect to \mathbf{w}_k is:

$$\nabla L(\mathbf{w}_k) = \sum_{i=1}^n \mathbf{x}_i \left[I(y_i = k) - P(Y = k | X = \mathbf{x}_i) \right],$$

where $P(Y = k | X = \mathbf{x}_i) = \frac{\exp(\mathbf{w}_k^{\top} \mathbf{x}_i)}{1 + \sum_{l=1}^{K-1} \exp(\mathbf{w}_l^{\top} \mathbf{x}_i)}$, and $I(y_i = k)$ is the indicator function that equals 1 if $y_i = k$, and 0 otherwise.

The gradient of the regularization term $-\frac{\lambda}{2}\sum_{l=1}^{K-1}\|\mathbf{w}_l\|_2^2$ with respect to \mathbf{w}_k is:

$$\nabla \left(-\frac{\lambda}{2} \sum_{l=1}^{K-1} \|\mathbf{w}_l\|_2^2 \right) = -\lambda \mathbf{w}_k.$$

Combining these results, the gradient of f with respect to \mathbf{w}_k is:

$$\nabla f(\mathbf{w}_k) = \nabla L(\mathbf{w}_k) - \lambda \mathbf{w}_k.$$

Substituting the expression for $\nabla L(\mathbf{w}_k)$:

$$\nabla f(\mathbf{w}_k) = \sum_{i=1}^n \mathbf{x}_i \left[I(y_i = k) - P(Y = k | X = \mathbf{x}_i) \right] - \lambda \mathbf{w}_k.$$

P1.5.a, Answer:

For the Matlab code in 1.5.a, I used a stepsize of 0.0001 and iterations of 5000. For lambda = 0, I graphed my objective value, training accuracy, and testing accuracy v.s. iterations. The results can be seen in Figures 1, 2, and 3. The final accuracy for lambda = 0 can be seen in Figure 4.

P1.5.b, Answer:

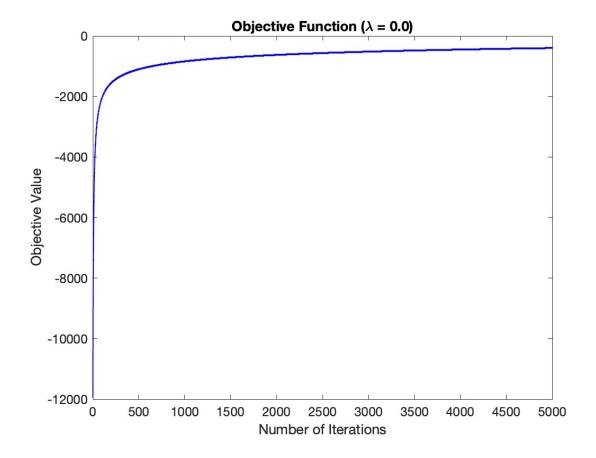


Figure 1: Objective Value

The final accuracy for the given lambdas can be seen in Figure 4.

P1.5.c, Answer:

From the results of the experiments, we observe that adding a regularization term can help avoid overfitting and improve generalization performance. For example, with a moderate regularization parameter such as $\lambda=10$, the model achieves better performance on the testing set while maintaining high accuracy on the training set. This indicates that regularization helps control the complexity of the model, preventing it from memorizing the training data and instead promoting generalization to unseen data. However, it is also evident that the regularization parameter cannot be too large. Excessive regularization, as seen with higher values of λ (e.g., $\lambda=100$ or $\lambda=200$), overly constrains the model, leading to underfitting and a decrease in both training and testing accuracy. Therefore, an optimal balance in the choice of λ is crucial to achieve the best generalization performance.

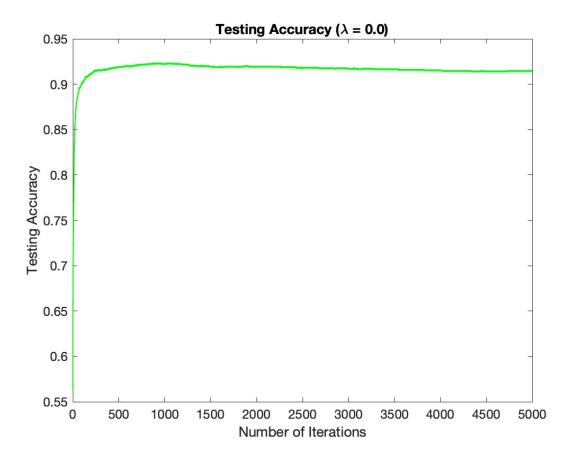


Figure 2: Test Accuracy

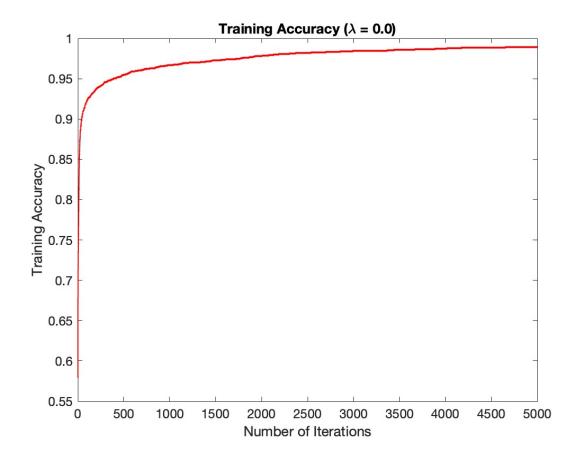


Figure 3: Train Accuracy

Lambda	Final Train Accuracy	Final Test Accuracy
0.0	0.9892	0.9144
0.1	0.9890	0.9144
1.0	0.9865	0.9158
10.0	0.9628	0.9192
100.0	0.9193	0.8974
200.0	0.9032	0.8818

Figure 4: Final Accuracy

A Appendix: MATLAB Code

```
function G=log_grad (y, X, B)
%compute gradient
        K_1 = size(B, 2);
        eXB = exp(X*B);
        s_eXB = 1./(sum(eXB, 2) + 1);
        eXB=eXB.*repmat(s_eXB, 1, K_1);
        for k=1: K_{-1}
                eXB(:,k)=(y=k)-eXB(:,k);
        end
        G=(X'*eXB);
end
clear; clc; close all;
load usps_digital.mat;
learning_rate = 1e-4;
max_{iterations} = 5000;
lambdas = [0, 0.1, 1, 10, 100, 200];
final_test_accuracies = zeros(size(lambdas));
final_train_accuracies = zeros(size(lambdas));
for idx = 1:length(lambdas)
        lambda = lambdas(idx);
        [B, test_error, train_error, objective_values] = log_reg(tr_y, tr_X
        final_test_accuracies(idx) = test_error(end);
        final_train_accuracies(idx) = train_error(end);
        figure;
        plot (1: length (objective_values)-1, objective_values (1:end-1), 'b-o
        title (sprintf('Objective Function (\\lambda = \%.1f)', lambda), 'Fo
        xlabel('Number of Iterations', 'FontSize', 15);
        ylabel('Objective Value', 'FontSize', 15);
        set(gca, 'FontSize', 12);
        saveas(gcf, sprintf('objective_lambda_%.1f.fig', lambda));
```

```
figure;
         plot(1:length(train_error)-1, train_error(1:end-1), 'r-o', 'LineWie
         title(sprintf('Training Accuracy (\\lambda = \%.1f)', lambda), 'Fon
         xlabel('Number of Iterations', 'FontSize', 15);
         ylabel('Training Accuracy', 'FontSize', 15);
         set(gca, 'FontSize', 12);
         saveas(gcf, sprintf('train_accuracy_lambda_%.1f.fig', lambda));
         figure;
         \mathbf{plot} (1: \mathbf{length} ( \mathbf{test\_error}) - 1, \ \mathbf{test\_error} (1: \mathbf{end} - 1), \ \mathbf{'g-o'}, \ \mathbf{'LineWidth})
         title (sprintf('Testing - Accuracy - (\\lambda -= - %.1f)', lambda), 'Font
         xlabel('Number of Iterations', 'FontSize', 15);
         ylabel('Testing Accuracy', 'FontSize', 15);
         set (gca, 'FontSize', 12);
         saveas(gcf, sprintf('test_accuracy_lambda_%.1f.fig', lambda));
end
fprintf('Final-Testing-and-Training-Accuracies-for-Each-\\lambda:\n');
\mathbf{fprintf}(\ 'Lambda \setminus tFinal \cdot Train \cdot Accuracy \setminus tFinal \cdot Test \cdot Accuracy \setminus n');
fprintf('—
for idx = 1:length(lambdas)
         fprintf('\%.1f\t\t\%.4f\t\t\t\%.4f\n', lambdas(idx), final_train_accur
end
fprintf('-
                                                                           —\n ' ) ;
save ('final_accuracies.mat', 'lambdas', 'final_train_accuracies', 'final_te
```