Department of Computer Science and Technology

Machine Learning

Homework 1

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1 Mathematics Basics

1.1 Optimization

Use the Lagrange multiplier method to solve the following problem:

$$\begin{aligned} \min_{x_1,x_2} \quad & x_1^2 + x_2^2 - 1 \\ s.t. \quad & x_1 + x_2 - 1 = 0 \\ & x_1 - 2x_2 \geq 0 \end{aligned}$$

Solution:

The Lagrangian equation can be written as $L(x_1, x_2, \lambda_1, \lambda_2)$, where λ_1 and λ_2 are the Lagrange multipliers. Therefore, Lagrangian function would be written as:

$$\mathcal{L}(x_1, x_2, \lambda_1, \lambda_2) = x_1^2 + x_2^2 - 1 - \lambda_1(x_1 + x_2 - 1) - \lambda_2(x_1 - 2x_2)$$

Hence, we can have that:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial x_1} = 0 \quad => \quad 2x_1 - \lambda_1 - \lambda_2 = 0 \quad => \quad x_1^* = \frac{\lambda_1 + \lambda_2}{2} \\ \frac{\partial \mathcal{L}}{\partial x_2} = 0 \quad => \quad 2x_2 + \lambda_2 + 2\lambda_2 = 0 \quad => \quad x_2^* = \frac{\lambda_1 - 2\lambda_2}{2} \end{aligned}$$

Accordingly, using the above equations, we can expand and rewrite the Lagrangian equation as follows:

$$\begin{aligned} \mathcal{L}(\lambda_1, \lambda_2) = & \frac{1}{4}\lambda_1^2 + \frac{1}{2}\lambda_1\lambda_2 + \frac{1}{4}\lambda_2^2 + \frac{1}{4}\lambda_1^2 - \lambda_1\lambda_2 + \lambda_2^2 \\ & -1 - \lambda_1^2 + \frac{1}{2}\lambda_1\lambda_2 + \lambda_1 + \frac{1}{2}\lambda_1\lambda_2 - \frac{5}{2}\lambda_2^2 \\ = & -\frac{1}{2}\lambda_1^2 - \frac{5}{4}\lambda_2^2 + \frac{1}{2}\lambda_1\lambda_2 + \lambda_1 - 1 \end{aligned}$$

Therefore, we can have that:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \lambda_1} = 0 \quad => -\lambda_1 + \frac{1}{2}\lambda_2 + 1 = 0 \\ \frac{\partial \mathcal{L}}{\partial \lambda_2} = 0 \quad => -\frac{5}{2}\lambda_2 + \frac{1}{2}\lambda_1 = 0 \end{aligned}$$

Solving the above two equations gives $\lambda_1 = \frac{10}{9}$ and $\lambda_2 = \frac{2}{9}$. Accordingly, we use these values to obtain $x_1 = \frac{2}{3}$ and $x_2 = \frac{1}{3}$ based on the initial two derivations. Since (1) both Lagrange multipliers satisfy $\lambda \geq 0$; (2) $g(x) = x_1 + x_2 - 1 = \frac{2}{3} + \frac{1}{3} - 1 = 0$ and $h(x) = x_1 - 2x_2 = \frac{2}{3} - 2(\frac{1}{3}) = 0 \geq 0$; (3) $\lambda_2 h(x) = \frac{2}{9}(\frac{2}{3} - 2(\frac{1}{3})) = 0$; KKT conditions are satisfied and therefore, the solutions $x_1 = \frac{2}{3}$ and $x_2 = \frac{1}{3}$ are valid.

1.2 Stochastic Process

We toss a fair coin for a number of times and use H(head) and T(tail) to denote the two sides of the coin. Please compute the expected number of tosses we need to observe a first time occurrence of the following consecutive pattern

H, T, T, ..., T

Solution:

Let x denote the number of tosses we need to get n consecutive turns of the same side (i.e n heads or n tails). For the first toss, if we get the side we want immediately, then the probability would be $\frac{1}{2}$. Otherwise, this turn is useless and the number of turns would be x+1. In the second toss, the probability of getting the order we want is $\frac{1}{2} \times \frac{1}{2} = \frac{1}{4}$ and the case that we don't get what we want, the number of turns would be x+2. This gives us the following sequence for the expected number of tosses before observing our desired pattern for a coin side:

$$x = \frac{1}{2}(x+1) + \frac{1}{4}(x+2) + \frac{1}{8}(x+3) + ...$$

Accordingly, solving the above equation gives $x_{S(n)} = 2(2^n - 1)$, where S is the side we want to observe n times. Hence, if we think of this problem as number of tosses to see one consecutive head and k consecutive tails, we would need $x_{H(1)} + x_{T(k)} = 2(2^1 - 1) + 2(2^k - 1) = 2 + 2^{k+1} - 2 = 2^{k+1}$ tosses to observe this pattern.

2 SVM

Consider the regression problem with training data $\{(x_i, y_i)\}_{i=1}^{N} (x_i \in R^d, y_i \in R)$. $\epsilon < 0$ denotes a fixed small value. Derive the dual problem of the following primal problem of linear SVM:

$$\begin{aligned} \min_{w,b,\xi,\hat{\xi}} \quad & \frac{1}{2}||w||^2 \quad + \quad C\sum_{i=1}^{N}(\xi_i + \hat{\xi}_i) \\ s.t. \quad y_i \quad & \leq \quad w^T x_i + b + \epsilon + \xi_i, i = 1, ..., N \\ y_i \quad & \geq \quad w^T x_i + b - \epsilon - \xi_i, i = 1, ..., N \\ \xi_i \quad & \geq \quad 0 \quad \forall i = 1, ..., N \\ \hat{\xi}_i \quad & \geq \quad 0 \quad \forall i = 1, ..., N \end{aligned}$$

Solution:

Let $a, c, d,$ and $e \geq 0$ be the Lagrange multipliers. Then, the Lagrangian function would be

$$\begin{aligned}\mathcal{L}(w, b, \xi, \hat{\xi}, a, c, d, e) = \frac{1}{2}||w||^2 + C\sum_i(\xi_i + \hat{\xi}_i) - \sum_i a_i(w^T x_i + b + \epsilon + \xi_i - y_i) \\ - \sum_i c_i(y_i - w^T x_i - b + \epsilon + \hat{\xi}_i) - \sum_i d_i\xi_i - \sum_i e_i\hat{\xi}_i\end{aligned}$$

Therefore, we can have that

$$\frac{\partial \mathcal{L}}{\partial w} = \hat{w} - \sum_{i=1}^{N} a_i x_i + \sum_{i=1}^{N} c_i x_i = 0 \quad giving \quad \hat{w} = \sum_{i=1}^{N}(a_i - c_i)x_i \tag{1}$$

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{i=1}^{N} a_i x_i + \sum_{i=1}^{N} c_i x_i = 0 \quad giving \quad \sum_i a_i - c_i = 0 \tag{2}$$

$$\frac{\partial \mathcal{L}}{\partial \xi} = C1 - \sum_i a_i - \sum_i d_i = 0 \quad giving \quad C = a + d \tag{3}$$

$$\frac{\partial \mathcal{L}}{\partial \hat{\xi}} = C1 + \sum_i c_i - \sum_i e_i = 0 \quad giving \quad C = c + e \tag{4}$$

Therefore, we initially expand the Lagrangian function as below

$$\begin{aligned}\mathcal{L}(w, b, \xi, \hat{\xi}, a, c, d, e) &= \frac{1}{2}||w||^2 + C\sum_i(\xi_i + \hat{\xi}_i) - \sum_i a_i w^T x_i - \sum_i a_i b - \sum_i a_i\epsilon \\ &- \sum_i a_i\xi_i + \sum_i a_i y_i - \sum_i c_i y_i + \sum_i c_i w^T x_i + \sum_i c_i b \\ &- \sum_i c_i\epsilon - \sum_i c_i\hat{\xi}_i - \sum_i d_i\xi_i - \sum_i e_i\hat{\xi}_i \\ &= \frac{1}{2}||w||^2 + C\sum_i(\xi_i + \hat{\xi}_i) - \sum_i(a_i - c_i)w^T x_i \\ &- \sum_i(a_i - c_i)b - \sum_i(a_i + c_i)\epsilon - \sum_i(a_i + d_i)\xi_i \\ &+ \sum_i(a_i - c_i)y_i - \sum_i(c_i + e_i)\hat{\xi}_i\end{aligned}$$

Then, using equations 5-8 ,we can write the Lagrangian function as

$$\begin{aligned}\mathcal{L}(w,b,\xi,\hat{\xi},a,c,d,e) &= \frac{1}{2}||w||^2 - \hat{w}w^T - b(0) - \epsilon\sum_i(a_i+c_i) + \sum_i(a_i-c_i)y_i \\ &\quad +C\sum_i(\xi_i+\hat{\xi}_i) - \sum_i(a_i+d_i)(\xi_i+\hat{\xi}_i) \\ &= -\frac{1}{2}||w||^2 - \epsilon\sum_i(a_i+c_i) + \sum_i(a_i-c_i)y_i\end{aligned}$$

Hence, the dual optimization problem would be

$$\begin{aligned}\underset{a,c}{argmax} -\frac{1}{2}\sum_i\sum_j(a_i-c_i)(a_j-c_j)x_i^Tx_j - \epsilon\sum_i(a_i+c_i) + \sum_i(a_i-c_i)y_i \\ s.t \qquad \sum_i(a_i-c_i) = 0 \\ 0 \le a_i, c_i \le C\end{aligned}$$

3 Deep Neural Networks

To make neural networks work well in practice is not easy in general, since there are too many hyper-parameters to tune such as the choice of the number of hidden layers, the activation function, the learning rate and so on. Besides some general guidelines (some standard techniques which are useful at most cases such as dropout, data augmentation), experience is of great importance.
Though a beginner may often be confused with them, luckily, there are some software available on the internet to help you build up a good sense on tuning neural networks. In this problem, you need to train the neural networks with different choices of hyper-parameters from the following link - A Neural Network Playground (you may need a VPN) - and answer the following questions:

1. Identify the best configuration you find for different problems and datasets. Here you only need to list you configuration for the bottom-right dataset of the classification problem.

2. List your findings that how the learning rate, the activation function, the number of hidden layers and the regularization influence the performance and convergence rate.

Solution:

1. The values for the best configuration are provided respectively below:

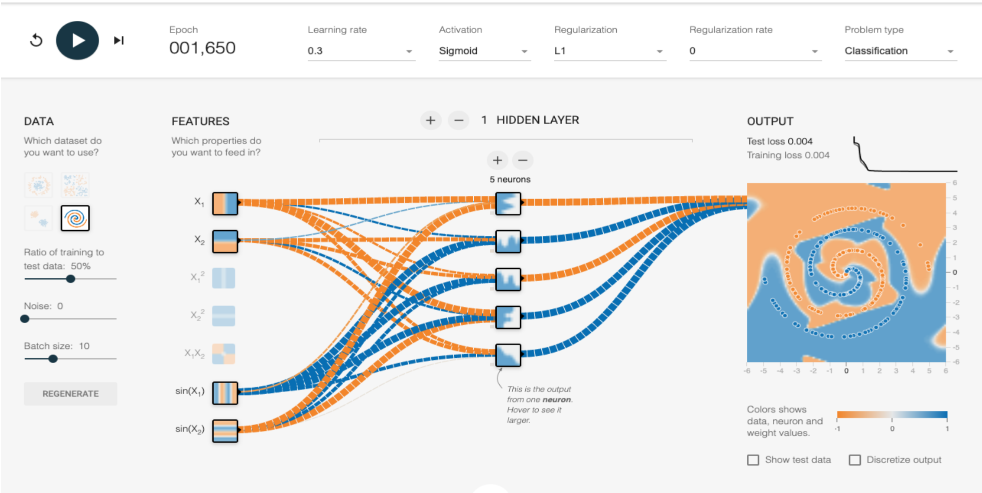


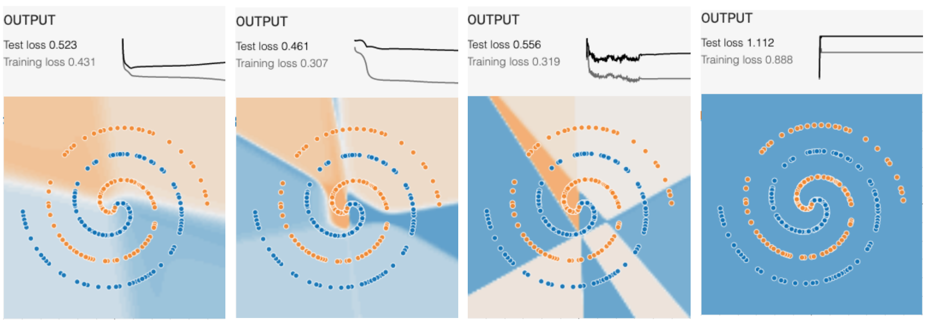
Figure 1: Best playground configuration

Learning Rate	Activation	Regularization	Features	Hidden parameters
0.03	Sigmoid	None	$x_1, x_2, sin(x_1), sin(x_2)$	1 layer - 5 neurons

Table 1: Best configuration parameters

2. The analyzed parameters and their influence for the performance and convergence rate are discussed respectively below:

   Learning Rate: as the name suggests, the learning rate relates to the rate at which the model learns; i.e. the amount of correction that is applied to weights with each training example.

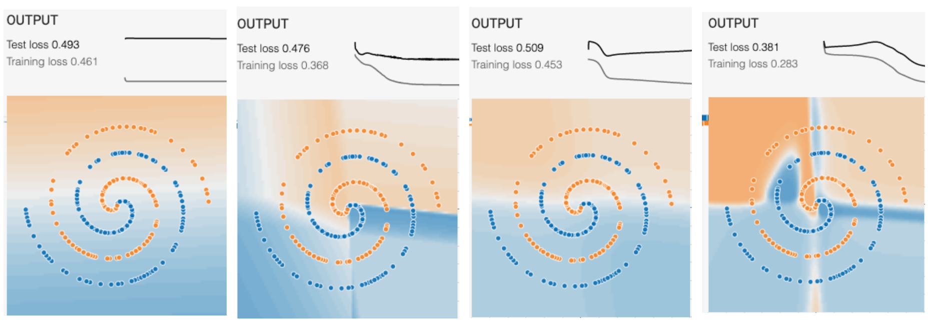


(a) $lr = 0.01$ (b) $lr = 0.1$ (c) $lr = 1$ (d) $lr = 10$

Figure 2: Four different learning rates

Hence, smaller values of the learning rate may result in a considerably slow convergence while larger values of learning rate may result in over-shooting as the local minima point may be missed due to large changes. Therefore, the learning rate should be set to a small enough value to ensure that it does not miss its convergence point, but a large enough value to reach convergence in a reasonable amount of time (i.e. avoid slow convergence). In practice, the learning set is initially rate is set to 0.01 and may be slightly modified depending on the given application. This is further shown by the above illustrations as too small and too large learning rates led to increased loss.

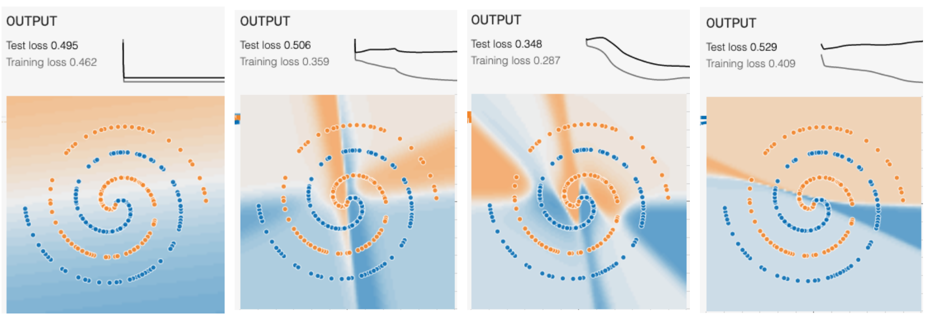
Activation Function: this is a function that determines the final output of the model and it could either a linear or a nonlinear function. Accordingly, since linear functions only work with linear data, they are insufficient for producing nonlinear outputs. Since activation functions have different complexities, execution times, etc., a fitting activation function should be chosen based on the characteristics of the data for which we are building the model.



(a) *Linear* (b) *Relu* (c) *Sigmoid* (d) *Tanh*

Figure 3: Four different activation functions

Number of Hidden Layers: the number of hidden layers determines the amount of information available for the model for producing the output.

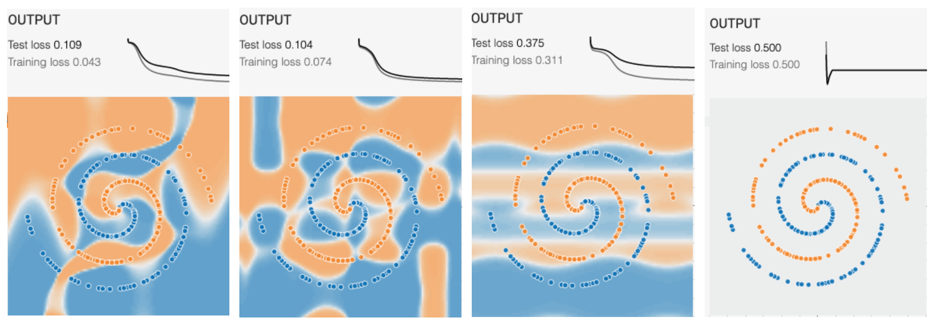


(a) 0 layers (b) 1 layers (c) 2 layers (d) 3 layers

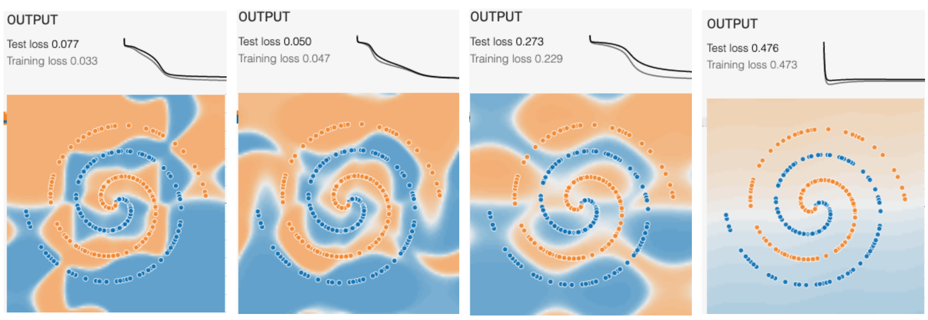
Figure 4: Four different number of hidden layers

Hence, too few hidden layers may not provide enough information for the model to produce a reasonable output, which results in under-fitting. If we implement too many hidden layers, there would be too much information for the model to process, which results in over-fitting as there may not be enough training examples to properly train a model of this scale. As demonstrated in the above figures, 2 hidden layers showed satisfactory results. However, the number of hidden neurons plays an important role in the results likewise.

Regularization: the main usage of regularization is to add a penalty term to the change of weights as a means of avoiding over-fitting. The two generally used types of regularization are L1 and L2, which both follow the similar structure for the cost function: loss + regularization term. However, the regularization term in L1 is $\frac{\lambda}{2m}\sum||w||$ ($\frac{\lambda}{2m}$ being the regularization rate) whereas it is $\frac{\lambda}{2m}\sum||w||^2$ in L2. Therefore, L1 tends to move the weights to 0 whereas L2 focuses on decreasing the weights evenly, which makes L1 better for feature selection tasks and L2 useful in tasks where a number of features are dependent on one another. The figures below display the results obtained by both the L1 and L2 regularization methods with respective different regularization rates. Hence, it can be observed that for the given dataset, a rate of 0.003 would be satisfactory with L2 regularization performing better.



(a) L1 - 0.001 (b) L1 - 0.003 (c) L1 - 0.01 (d) L1 - 0.1



(a) L2 - 0.001 (b) L2 - 0.003 (c) L2 - 0.01 (d) L2 - 0.1

Figure 6: Different regularization implementations

4 IRLS for Logistic Regression

Solution:

1. Data pre-processing:

The provided datasets follows the below format:

Label [feature id]:[feature] [feature id]:[feature] ......

where we have 123 features (x) in total, 32,561 samples for testing and 16,281 samples for training. Initially, an extra feature (x_0) known as the bias would be added, giving 124 features for each sample. Accordingly, since the labels for the provided samples are either -1 or 1, the label of all -1 samples are changed to 0 to make this a binary classification task.

2. Weight update rule with L2 regularization:

By Newton's method, we aim to maximize the following

$$\mathcal{L}(w) = \sum_i [y_i w^T x_i - log(1 + exp(w^T x_i))] \tag{5}$$

By adding L2-regularization to the above equation, we get

$$\mathcal{L}(w) = \sum_i [y_i w^T x_i - log(1 + exp(w^T x_i))] - \frac{\lambda}{2}||w||_2^2 \tag{6}$$

Accordingly, we need to find w^* such that

$$\nabla_w \mathcal{L}(w^*) = \sum_i (y_i - \mu_i) x_i - \lambda w^* = 0 \tag{7}$$

The hessian matrix ($H = \nabla_w^2 \mathcal{L}(w)|_{w_t} = \nabla_w [\nabla_w \mathcal{L}(w)]^T$) would be

$$\nabla_w [\sum_i (y_i - \mu_i) x^T - \lambda w^T] = -\sum_i \mu_i (1 - \mu_i) x_i x_i^T - \lambda = -XRX^T - \lambda I \tag{8}$$

Where $R_{ii} = \mu_i(1 - \mu_i)$. Therefore, the weight update rule ($w_{t+1} \leftarrow w_t - H^{-1} \nabla_w \mathcal{L}(w)|_{w_t}$) would be as follows

$$w_{t+1} \leftarrow w_t - [(-XRX^T - \lambda I)^{-1}][X^T(y_i - \mu_i) - \lambda w_t] \tag{9}$$

However, it should be noted that by getting closer to the point of convergence, R slowly converges to 0, which causes the hessian matrix to be non-invertable. Hence, the inverse of H should be changed to its pseudo-inverse (H^+).

3. Data analysis:

Initially, in order to find a beneficial value of λ the training data is split into 10 folds (k=10). Accordingly, for a given array of lambda values (0.01, 0.1, 1, 2, 5, 10, 20, 50, 100), one of the folds is used as the testing data while the remaining 9 folds are used for training. The model would be trained for 10 epochs, and each of the 10 folds would be used once to test the model. Consequently, the average mean squared error (MSE) for each value of λ during different folds and epochs was recorded and is provided in the below chart.

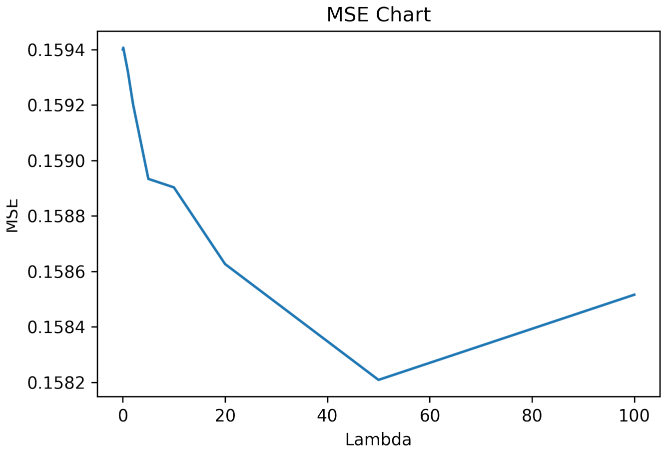


Figure 7: MSE chart for different values of λ

Consequently, as $\lambda = 50$ produced the lowest MSE in cross-validation, λ for L2-regularization was set to this value. The following two figures illustrate the accuracy chart for the training and testing data for both normal and regularized logistic regressions respectively.

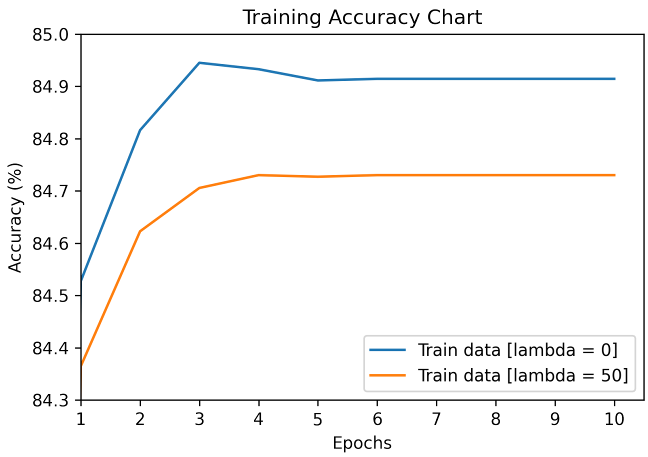


Figure 8: Accuracy chart for training data

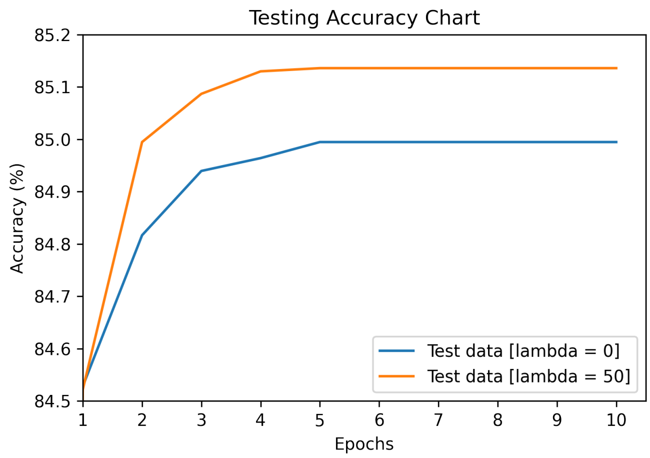


Figure 9: Accuracy chart for testing data

According to the above figures, both types of logistic regression converge nearly at the same number of epochs (=5). In addition, it can be seen that by regularization, the model achieves a lower accuracy on the training data while experiencing an increased accuracy with the test data. Therefore, it can be postulated that the regularized model would be able to generalize its predictions comparatively better than the normal logistic regression model.

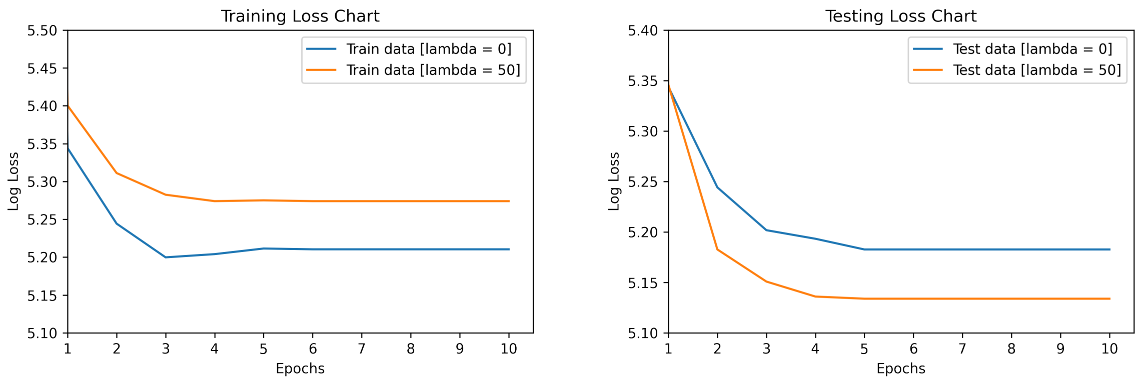


Figure 10: Loss charts for training and testing data

Moreover, the logarithmic loss for both training and testing data was recorded during each epoch likewise. Figures 10 and 11 demonstrate the obtained results. As shown in the figures, similar to the recorded values of accuracy, the calculated loss for the training data was lower for the normal logistic regression model while the regularized model experienced less loss on the testing data. Hence, the previously drawn conclusion, which stated that the regularized model is able to perform better generalization, still stands.