LMP1210H Winter 2025 Assignment 1

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By turning in this assignment, I agree by the UofT honor code and declare that all of this is my own work.

Problem 1 - Basics about Machine Learning

(a) Answers

Definition:

overfitting means that the model is trained to have very good and detailed understanding of hidden patterns on training data but does not have good generalization on the test or unseen data. This usually comes with good learning of the noises of the data.

Techniques to prevent overfitting:

- 1. Introduce cross-validation strategy to the training so that model can be evaluated on the validation dataset.
- 2. Add the regularization loss to the cost function.
- 3. Reduce the complexity of the model architecture.
- 4. Add dropout layers to the model to reduce the dependencies of features.

(b) Answers

Impacts:

The magnitude of k controls the performance of the model.

- 1. k is small, the model learns a good underlying pattern of the data and thus predicts strong boundaries to label the data, but this may cause the model to over-fitting because it is sensible to a random sample in the training data.
- 2. k is large, it makes a stable/smooth prediction by averaging over many examples, but the model may be under-fitting since it does not capture important regularities.

How to choose k:

- 1. Choose optimal k based on the number of data points or the size of data pool n, use the rule of thumb: $k = n^{\frac{2}{2+d}}$ (d refers to dimensionality).
- 2. Measure the generalization error on the unseen data set with different choices of k.

(c) Answers

• Regression category

- Goal: explore the relationship between independent variables (age, gender, BMI, height, etc) with the volume of hippocampus.
- Method: we can use <u>linear regression</u> to model the continuous outcome
 which represents the volume of hippocampus and thus provides better judgment for neurodegenerative diseases.

- Risk:

- * The linear regression may not capture accurate relationship between independent variables and volume of hippocampus, since volume of hippocampus may have non-linear relationship with independent variables.
- * The model may be over-fitting if there are too many independent variables or features using to predict outcomes while the data size is small.
- * The model may be poor and has bias if the variances of errors among each independent variables in data are not constant.
- * The model may be sensitive to outliers for both independent and dependent variables.

• Classification category

- Goal: make a judgment if the patient will have the stroke given the current and previous medical records like (systolic blood pressure, BMI, age, etc).
- **Method:** we can use <u>logistic regression</u> to model the binary outcomes which tells whether or not the stroke will happen.

- Risk:

- * The logistic regression results may not be accurate since it relies on the threshold which is a hyper-parameter to predict binary results. Picking an optimal threshold is a challenge work.
- * The model may be over-fitting if there are too many independent variables or features using to predict outcomes while the data size is small.
- * The data set is imbalanced. The distribution of stroke patients is not approximate to that of non-stroke one. The model could predict the majority class (no stroke) more often, ignoring the minority class (stroke).

Problem 2 - Python Familiarity

Answers: please click and check this Google Colab Notebook.

Problem 3 - Regularized Linear Regression

(a) Answers

$$\frac{\partial \mathcal{J}_{\text{reg}}^{\beta}}{\partial w_j} = \frac{\partial \mathcal{J}}{\partial w_j} + \frac{\partial \mathcal{R}}{\partial w_j} = \frac{\partial \mathcal{J}}{\partial y} \frac{\partial y}{\partial w_j} + \frac{\partial \mathcal{R}}{\partial w_j}$$
(1)

$$\frac{\partial \mathcal{J}}{\partial y} \frac{\partial y}{\partial w_j} = \frac{1}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)}) x_j^{(i)} = \frac{1}{N} \sum_{i=1}^{N} (\sum_{j=1}^{D} w_j x_j^{(i)} - t^{(i)}) x_j^{(i)}$$
(2)

$$\frac{\partial \mathcal{R}}{\partial w_j} = \frac{\partial}{\partial w_j} \left(\frac{1}{2} \sum_{j=1}^D \beta_j w_j^2\right) = \beta_j w_j \tag{3}$$

Place Eq. (2) and Eq. (3) to Eq. (1), we will get

$$\frac{\partial \mathcal{J}_{\text{reg}}^{\beta}}{\partial w_j} = \frac{1}{N} \sum_{i=1}^{N} \left(\sum_{j=1}^{D} w_j x_j^{(i)} - t^{(i)} \right) x_j^{(i)} + \beta_j w_j \tag{4}$$

To update the gradient with respect to w_i , we can use the equation

$$w_j \leftarrow w_j - \eta \frac{\partial \mathcal{J}_{\text{reg}}^{\beta}}{\partial w_j} \tag{5}$$

Place Eq. (4) to Eq. (5) and we get final answer

$$w_j \leftarrow w_j - \eta \left(\frac{1}{N} \sum_{i=1}^{N} \left(\sum_{j=1}^{D} w_j x_j^{(i)} - t^{(i)}\right) x_j^{(i)} + \beta_j w_j\right)$$
 (6)

Where η is the learning rate which is a hyper-parameter defined by users.

If we know that j-th feature is less important which means this feature should be removed or ignored in the forward process to predict outcomes. To achieve this, changing the value of w_j to a very small value is rational. Therefore, we can assign a large value to β_j to penalize the w_j toward to 0 and thus reduce the importance of that variable contributing to the model.

(b) Answers

Given the Eq. (4) we got in question (a), we can make some mathematical transformation to obtain expected format,

$$\frac{\partial \mathcal{J}_{\text{reg}}^{\beta}}{\partial w_{j}} = \frac{1}{N} \sum_{i=1}^{N} \left(\sum_{j=1}^{D} w_{j} x_{j}^{(i)} - t^{(i)} \right) x_{j}^{(i)} + \beta_{j} w_{j} = 0$$

$$= \frac{1}{N} \sum_{i=1}^{N} \sum_{j'=1}^{D} w_{j'} x_{j'}^{(i)} x_{j}^{(i)} - \frac{1}{N} \sum_{i=1}^{N} t^{(i)} x_{j}^{(i)} + \beta_{j} w_{j} = 0$$
(7)

Transfer the term $(\frac{1}{N}\sum_{i=1}^{N}t^{(i)}x_{j}^{(i)})$ in Eq. (7) to right hand side

$$\frac{1}{N} \sum_{i=1}^{N} \sum_{j'=1}^{D} w_{j'} x_{j'}^{(i)} x_j^{(i)} + \beta_j w_j = \frac{1}{N} \sum_{i=1}^{N} t^{(i)} x_j^{(i)}$$
(8)

Since only variable $x_j^{(i)}$ is dependent on parameter i instead of j', we can swap the order of the summation in Eq. (8).

$$\sum_{j'=1}^{D} w_{j'} \left(\frac{1}{N} \sum_{i=1}^{N} x_{j'}^{(i)} x_{j}^{(i)}\right) + \beta_{j} w_{j} = \frac{1}{N} \sum_{i=1}^{N} t^{(i)} x_{j}^{(i)}$$

$$\tag{9}$$

For the regularization term $\beta_j w_j$, we know that this term only contribute when j' = j. Therefore, we can create a diagonal matrix $\delta_{jj'}$ where $\delta_{jj'} = 1$ only when j' = j otherwise it is 0. Indeed, we can combine the $\beta_j w_j$ with first term in Eq. (9),

$$\sum_{j'=1}^{D} w_{j'} \left(\frac{1}{N} \sum_{i=1}^{N} x_{j'}^{(i)} x_{j}^{(i)} + \beta_{j} \delta_{jj'}\right) = \frac{1}{N} \sum_{i=1}^{N} t^{(i)} x_{j}^{(i)}$$
(10)

Finally we can write the Eq. (10) in the expected format,

$$\sum_{j'=1}^{D} \left(\frac{1}{N} \sum_{i=1}^{N} x_{j'}^{(i)} x_{j}^{(i)} + \beta_{j} \delta_{jj'}\right) w_{j'} - \frac{1}{N} \sum_{i=1}^{N} t^{(i)} x_{j}^{(i)} = 0$$
(11)

where

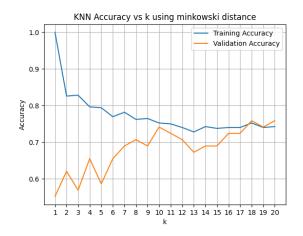
$$A_{jj'} = \frac{1}{N} \sum_{i=1}^{N} x_{j'}^{(i)} x_{j}^{(i)} + \beta_{j} \delta_{jj'}$$

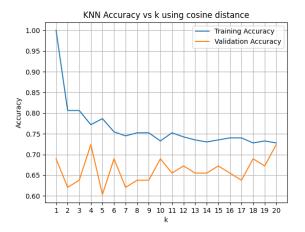
$$c_{j} = \frac{1}{N} \sum_{i=1}^{N} t^{(i)} x_{j}^{(i)}$$
(12)

Problem 4 - Classification with Nearest Neighbours

Please check the README.md and run the code A1_code.py file.

The plots and accuracy report of training and validation accuracy with different k selections and metrics are showed:





KNN Report				
metric	best k	accuracy		
minkowski	18	0.684		
cosine	4	0.709		

Table 1: Test accuracy of KNN model with different metrics

Problem 5 - Classification with Decision Tree

Please check the README.md and run the code A1_code.py file.

The screenshots and accuracy report of first 2 decision tree layers with different min_sample_leaf are showed:

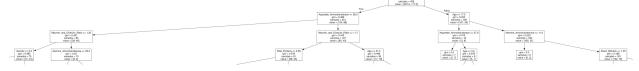


Figure 1: Screenshot of first 2 decision tree layers with min_sample_leaf=1

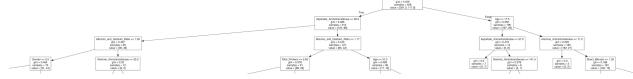


Figure 2: Screenshot of first 2 decision tree layers with min_sample_leaf=2

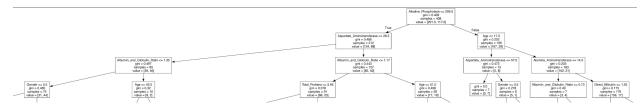


Figure 3: Screenshot of first 2 decision tree layers with min_sample_leaf=3

Decision Tree Report				
min_sample_leaf	acc_train	acc_valid	acc_test	
1	1.00	0.603	0.598	
2	0.949	0.603	0.667	
3	0.926	0.569	0.607	

Table 2: Train, validation and test accuracy of decision tree model with different min_sample_leaf

Problem 6 - Classification with Logistic Regression

Please check the README.md and run the code A1_code.py file. The accuracy report of logistic regression is showed:

Logistic Regression Report				
acc_train	acc_valid	acc_test		
0.740	0.741	0.718		

Table 3: Train, validation and test accuracy of logistic regression model