

Homework Assignment 5

COGS 118A: Introduction to Machine Learning I

Due: 11:59pm, Sunday, Nov. 11st, 2018 (Pacific Time).

Instructions: Answer the questions below, attach your code, and insert figures to create a PDF file; submit your file via Gradescope. You may look up the information on the Internet, but you must write the final homework solutions by yourself.

Late Policy: 5% of the total points will be deducted on the first day past due. Every 10% of the total points will be deducted for every extra day past due.

Grade: ____ out of 100 points

1 (10 points) Multiple Choices

1. Which of the following statements is **false** regarding structural risk minimization?
 - (A) It is a method to perform model selection, i.e., choosing an optimal classifier to reduce the test errors.
 - (B) The goal is to balance fitting the training data against the model complexity.
 - (C) Different algorithms often have different model complexities.
 - (D) We always need to compute the testing error for each model to perform structural risk minimization.
2. Which of the following statements is **false** regarding cross validation?
 - (A) It is a method to perform model selection, i.e., choosing the optimal parameters for a classifier.
 - (B) It works for both regression and classification models.
 - (C) Cross validation can be used to perform structural risk minimization.
 - (D) To perform k-fold cross validation, the greater the k is, the more optimal the result will be.

2 (20 points) Linear Discriminant Analysis

Linear discriminant analysis has many applications, such as dimensionality reduction and feature extraction. In this problem, we consider a simple task. In data file `lda.npy`, there are two classes: class 0 and class 1. The data are expressed as matrices X_0 for class 0 and X_1 for class 1. Each $X_j = [\mathbf{x}_1^{(j)}, \mathbf{x}_2^{(j)}, \dots, \mathbf{x}_n^{(j)}]$. Note that in this problem we use **column vector** $\mathbf{x}_i^{(j)}$ for a single data point to simplify the calculation. Please fill the blanks in skeleton code `HW5.ipynb` to solve the following sub-problems:

(a) Compute the mean for each class, μ_0 and μ_1 .

(b) Compute the covariance matrix for each class, Σ_0 and Σ_1 .

The Fisher's linear discriminant analysis is defined to maximize criterion function:

$$S(\mathbf{w}) = \frac{\sigma_{\text{between}}^2}{\sigma_{\text{within}}^2} = \frac{(\mathbf{w}^\top \mu_0 - \mathbf{w}^\top \mu_1)^2}{\mathbf{w}^\top (\Sigma_0 + \Sigma_1) \mathbf{w}}$$

An optimal solution \mathbf{w}^* is:

$$\mathbf{w}^* = (\Sigma_0 + \Sigma_1)^{-1}(\mu_0 - \mu_1)$$

(c) Find the optimal $\tilde{\mathbf{w}}^*$ with unit length.

Hint: The optimal \mathbf{w}^* above is unnormalized. To normalize \mathbf{w}^* to unit length in order to get $\tilde{\mathbf{w}}^*$, you need to divide \mathbf{w}^* by $\|(\Sigma_0 + \Sigma_1)^{-1}(\mu_0 - \mu_1)\|_2$, which is the L_2 norm of \mathbf{w}^* .

(d) Compute the projection on $\tilde{\mathbf{w}}^*$ for each data point. Plot such projected data points with original data points in one figure.

Hint: Suppose we have a data point $\mathbf{x} = (x_1, x_2)^\top$, here, the data point \mathbf{x} and $\tilde{\mathbf{w}}^*$ are both column vectors. The projection on vector $\tilde{\mathbf{w}}^*$ for \mathbf{x} is simply the dot product:

$$\mathbf{x}_{\text{projected}} = ((\tilde{\mathbf{w}}^*)^\top \mathbf{x}) \tilde{\mathbf{w}}^*$$

3 (10 points) Shattering

Use shattering to derive the VC-dimension for classifiers below. Show your work.

1) $f(x; w, b) = \text{sign}(x \times w + b)$

2) $f(x; w, b) = \text{sign}((x \times w + b)^2)$

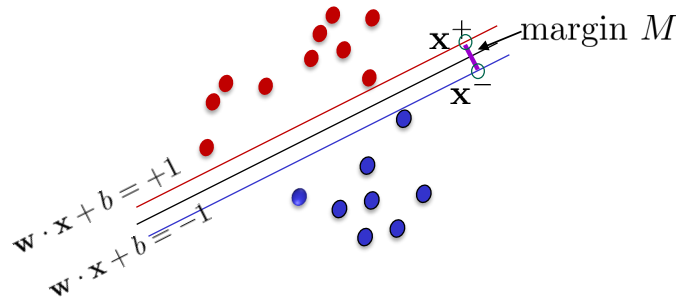
where $x, w, q, b \in \mathbb{R}$, and w, q and b are free parameters.

4 (10 points) Support Vector Machine 1

As shown in the figure, two boundaries are shifted to be parallel to the decision boundary in black, which is $\mathbf{w} \cdot \mathbf{x} + b = 0$. The equations of the boundaries are given in the figure. We first pick an arbitrary point \mathbf{x}^- on the negative plane such that $\mathbf{w} \cdot \mathbf{x}^- + b = -1$; we then draw a line that passes \mathbf{x}^- and is perpendicular to the negative plane; the intersection between this line and the positive plane can be denoted as \mathbf{x}^+ with $\mathbf{w} \cdot \mathbf{x}^+ + b = 1$. We thus have the following equations:

$$\begin{aligned}\mathbf{w} \cdot \mathbf{x}^- + b &= -1, \\ \mathbf{w} \cdot \mathbf{x}^+ + b &= +1, \\ \mathbf{x}^+ &= \mathbf{x}^- + \lambda \mathbf{w},\end{aligned}$$

where \mathbf{x}^- is any point that lies on the blue boundary and \mathbf{x}^+ is any point that lies on the red boundary, \mathbf{w}, b are given, and λ is an unknown parameter. Margin, M , is the distance between the two boundaries, which can be calculated as $M = \|\mathbf{x}^+ - \mathbf{x}^-\|_2 = \sqrt{\langle \lambda \mathbf{w}, \lambda \mathbf{w} \rangle}$. Please derive M to be parameterized by known parameters only (not containing λ).



Hint: (1) Derive λ based on the three equations given above (2) Plug in the value of λ you derive in (1) to $M = \|\mathbf{x}^+ - \mathbf{x}^-\|_2 = \sqrt{\langle \lambda \mathbf{w}, \lambda \mathbf{w} \rangle}$.

5 (20 points) Support Vector Machine 2

In this problem, you are required to solve a series of questions using support vector machine (SVM). You will use Arrhythmia dataset that contains 452 data points. Each data point has a 279-dimensional feature vector and an 1-dimensional label (either 0 or 1), which means it is a binary classification task and can be solved by SVM. Please download the `arrhythmia.npy` as data source and `HW5.ipynb` to fill the blanks. You can use the functions from `sklearn` in your implementation unless in some case we ask you to implement a few built-in functions by yourself.

In this problem, you need to use the linear SVM to conduct the binary classification.

- 1) Load data from `arrhythmia.npy` and randomly shuffle the data points.
- 2) Select 80% of the data points as your **training and validation set**. The rest 20% is regarded as your **test set**. Actually, in the cross-validation, the training and validation set can be called as “training set”. However, in order to be consistent with the code, we still call it “training and validation set” here.
- 3) Train the SVM classifier using a linear kernel. In linear SVM, there is a parameter C which adjusts the cost of outliers. You would need to use a grid search method to find the best parameter C^* . In fact, such grid search will utilize the cross-validation (3-fold) to get all the **average training accuracies** and **average validation accuracies** from the linear SVM model with different parameter C on training and validation set. The parameter $C = C^*$ which maximizes the **average validation accuracy** will be selected as the best. In fact, here “average” means the average accuracy over the folds in cross-validation, not the average accuracy over the different parameter C .

Hint 1: You are allowed to use `svm.SVC()` and `GridSearchCV()` in your code.

Hint 2: You can perform grid search on the following list of C :

$$C \in \{10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}\}$$

- 4) Draw heatmaps for the result of grid search and find the best C^* for average validation accuracy. Report the heatmaps and best C^* .
- 5) Use the the best C^* to train a linear SVM classifier on training and validation set. Then, use the trained classifier to calculate the accuracy on test set. Report the test accuracy.

6 (30 points) Implement Grid Search and Cross-validation

In this problem, you need to implement the grid search and cross-validation functions by yourself. You are **NOT** allowed to use `GridSearchCV()` here.

- 1) Implement a cross-validation function. In this function, you should divide your training and validation set into several subsets which have roughly the same size (the number of subsets is given by variable `fold`). Train the SVM with RBF kernel for `fold` rounds and each round choose one different subset as validation set and all the other data points (all the other `fold - 1` subsets) as training set. Calculate the **training accuracy** and **validation accuracy** every round. Finally, return the **average training accuracy** and **average validation accuracy** over all rounds.
- 2) Implement a grid search function. In this function you need to traverse all combinations of C and γ . For each combination of C and γ , you should call your implemented cross-validation function above to get the average training accuracy and average validation accuracy. Finally, you need to return **average training accuracy matrix** and **average validation accuracy matrix** for all combinations of C and γ .
- 3) Like what you have done in SVM, perform your implemented grid search with cross-validation (3-fold) to find the best combination of parameter C^* and γ^* . Draw heatmaps for result of grid search and get the best C^* and γ^* . Report the heatmaps and the best C^* and γ^* .

Hint: You can compare your heatmaps with the heatmaps from `GridSearchCV()` in the above sub-problem to confirm the correctness of your implementation. Both heatmaps should share similar behavior.