NCTU Pattern Recognition, Homework 4

Deadline: May 25, 23:59

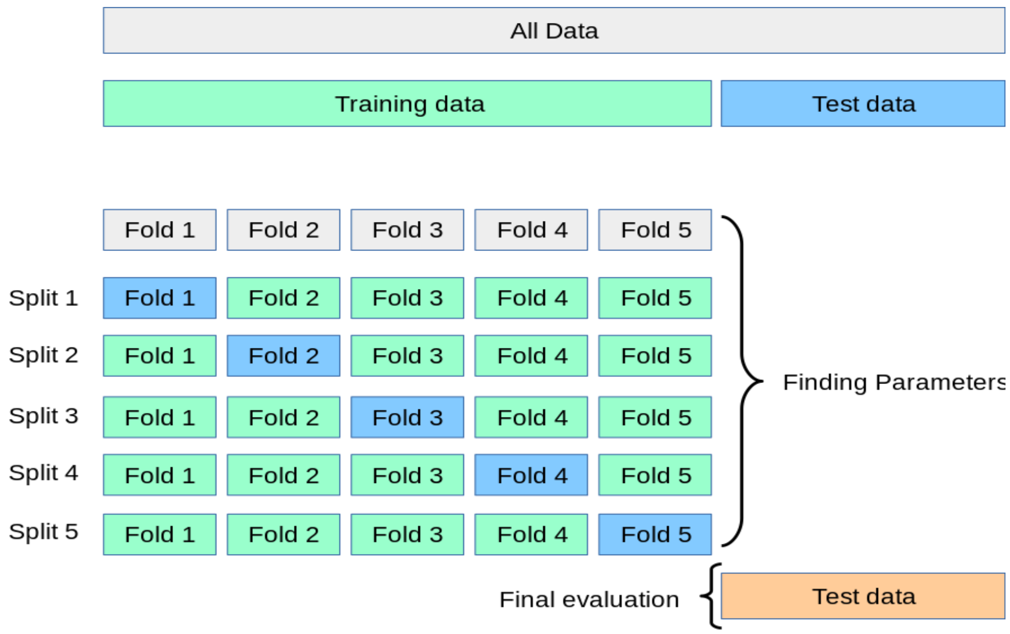
Part. 1, Coding (50%):

In this coding assignment, you need to implement the cross-validation and grid search using only NumPy, then train the SVM model from scikit-learn on the provided dataset and test the performance with testing data. Find the sample code and data on the GitHub page https://github.com/NCTU-VRDL/CS_AT0828/tree/main/HW4

Please note that only NumPy can be used to implement cross-validation and grid search. You will get no points by simply calling sklearn.model_selection.GridSearchCV.

1. (10%) K-fold data partition: Implement the K-fold cross-validation function. Your function should take K as an argument and return a list of lists (*len(list) should equal to K*), which contains K elements. Each element is a list containing two parts, the first part contains the index of all training folds (index_x_train, index_y_train), e.g., Fold 2 to Fold 5 in split 1. The second part contains the index of the validation fold, e.g., Fold 1 in split 1 (index_x_val, index_y_val)

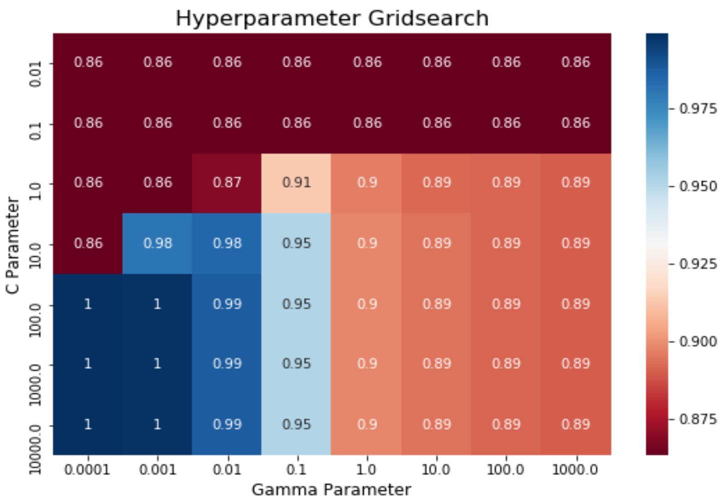
   Note: You need to handle if the sample size is not divisible by K. Using the strategy from sklearn. The first `n_samples % n_splits` folds have size `n_samples // n_splits + 1`, other folds have size `n_samples // n_splits`, where `n_samples` is the number of samples, `n_splits` is K, `%` stands for modulus, `//` stands for integer division. See this post for more details
   Note: Each of the samples should be used **exactly once** as the validation data
   Note: Please **shuffle** your data before partition



2. (20%) Grid Search & Cross-validation: using [sklearn.svm.SVC] to train a classifier on the provided train set and conduct the grid search of "C" and "gamma," "kernel'='rbf' to find the best hyperparameters by cross-validation. Print the best hyperparameters you found.
Note: We suggest using K=5

3. (10%) Plot the grid search results of your SVM. The x and y represent "gamma" and "C" hyperparameters, respectively. And the color represents the average score of validation folds.

Note: This image is for reference, not the answer
Note: matplotlib is allowed to use



4. (10%) Train your SVM model by the best hyperparameters you found from question 2 on the whole training data and evaluate the performance on the test set.

Accuracy	Your scores
acc > 0.9	**10points**
0.85 <= acc <= 0.9	**5 points**
acc < 0.85	**0 points**

Part. 2, Questions (50%):

1. (10%) Given a valid kernel $k_1(x, x')$, prove that the following proposed functions are or are not valid kernels.
   a. $k(x, x') = (k_1(x, x'))^2 + (k_1(x, x') + 1)^2$
   b. $k(x, x') = (k_1(x, x'))^2 + \exp(||x||^2) * \exp(||x'||^2)$

2. (10%) Show that the kernel matrix $\mathbf{K} = [k(\mathbf{x}_n, \mathbf{x}_m)]_{nm}$ should be positive semidefinite is the necessary and sufficient condition for $k(\mathbf{x}, \mathbf{x}')$ to be a valid kernel.

3. (10%) Consider the dual formulation of the least-squares linear regression problem given on page 6 in the ppt of Kernel Methods. Show that the solution for the components $\mathbf{a}_n$ of the vector **a** can be expressed as a linear combination of the elements of the vector $\boldsymbol{\varphi}(\mathbf{x}_n)$. Denoting these coefficients by the vector **w**, show that the dual of the dual formulation is given by the original representation in terms of the parameter vector **w**.

4. (10%) Prove that the Gaussian kernel defined by (eq 1) is valid and show the function $\boldsymbol{\varphi}(\mathbf{x})$, where $x \in R^1$.
   (eq1) $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\|\mathbf{x} - \mathbf{x}'\|^2 / 2\sigma^2\right) = \phi(x)^{\mathrm{T}}\phi(x')$

5. (10%) Consider the optimization problem

$$\text{minimize } (x - 2)^2$$
$$\text{subject to } (x+3)(x-1) \leqq 2$$

   State the dual problem.