NYCU Pattern Recognition, Homework 4

Deadline: May 17, 23:59

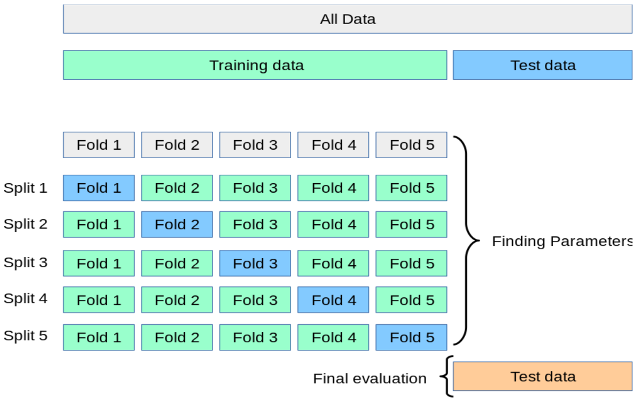
Part. 1, Coding (50%):

For this coding assignment, you are required to implement Cross-Validation and Grid Search using only NumPy. After that, you should train the SVM model from scikit-learn on the provided dataset and test the performance with the testing data. **You will get no points by simply calling sklearn.model_selection.GridSearchCV.**

(50%) K-Fold Cross-Validation & Grid Search

Requirements:

- Implement **K-Fold Cross-Validation** by creating a function that takes K as an argument and returns a list of K sublists.
    - Each sublist should contain two parts:
        - The first part contains the index of all training folds (index_x_train, index_y_train), for example, Fold 2 to Fold 5 in split 1.
        - The second part contains the index of the validation fold (index_x_val, index_y_val), for example, Fold 1 in split 1 .
    - You need to handle if the sample size is not divisible by K.
    - The first **n_samples % n_splits** folds should have a size of **n_samples // n_splits + 1**, and the other folds should have a size of **n_samples // n_splits**. Here, n_samples is the number of samples and n_splits is K.
    - Each of the samples should be used **exactly once** as the validation data.
    - Please **shuffle** your data before partition.

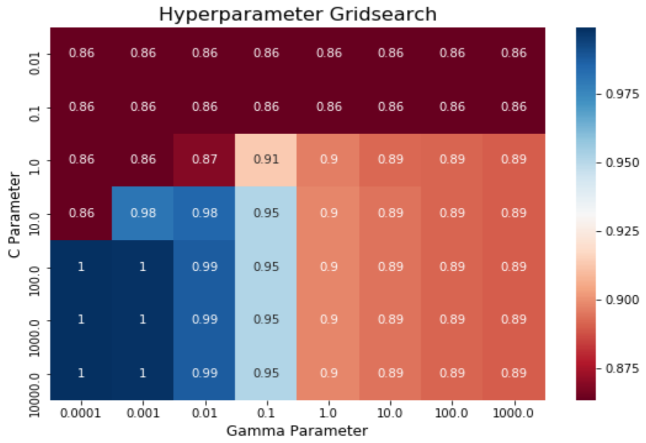


- Implement **Grid Search & Cross-Validation**:
    - Using sklearn.svm.SVC to train a classifier on the provided train set and perform **Grid Search** to find the best hyperparameters via cross-validation.

Criteria:

1. (10%) Implement K-fold data partitioning.
2. (10%) Set the kernel parameter to 'rbf' and do grid search on the hyperparameters **C** and **gamma** to find the best values through cross-validation. Print the best hyperparameters you found. Note that we suggest using K=5 for the cross-validation.

3. (10%) Plot the results of your SVM's grid search. Use "gamma" and "C" as the x and y axes, respectively, and represent the average validation score with color. Below image is just for reference.



4. (20%) Train your SVM model using the best hyperparameters found in Q2 on the entire training dataset, then evaluate its performance on the test set. Print your testing accuracy.

Points	**Testing Accuracy**
20 points	**acc > 0.9**
10 points	**0.85 <= acc <= 0.9**
0 points	**acc < 0.85**

Part. 2, Questions (50%):

1. (10%) Show that the kernel matrix $K = \left[k\left(x_n, x_m\right)\right]_{nm}$ should be positive semidefinite is the necessary and sufficient condition for $k(x, x')$ to be a valid kernel.

2. (10%) Given a valid kernel $k_1(x, x')$, explain that $k(x,\ x') = \ exp(k_1(x, x'))$ is also a valid kernel. (Hint: Your answer may mention some terms like ____ series or ____ expansion.)

3. (20%) Given a valid kernel $k_1(x, x')$, prove that the following proposed functions are or are not valid kernels. If one is not a valid kernel, give an example of $k(x, x')$ that the corresponding K is not positive semidefinite and show its eigenvalues.
   a. $k(x,\ x') = \ k_1(x,\ x') +\ x$
   b. $k(x,\ x') = \ k_1(x,\ x') -\ 1$
   c. $k(x,\ x') = \ k_1(x, x')^2 +\ exp\left(\|x\|^2\right) *\ exp(\|x'\|^2)$
   d. $k(x,\ x') = \ k_1(x, x')^2 +\ exp\left(k_1(x, x')\right) -\ 1$

4. Consider the optimization problem

$$\mathit{minimize}\ (x - 2)^2$$
$$\mathit{subject\ to}\ (x + 4)(x - 1) \leq 3$$

State the dual problem. (Full points by completing the following equations)

$L(x, \lambda) =$ ____________________

$\nabla_x L(x, \lambda) =$ ______________________

when $\nabla_x L(x, \lambda) = 0,$

$x =$ _______________

$L(x, \lambda) = L(\lambda) =$ ___________________________