Classification Systems

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March 22, 2019

Contents

1 Classification Systems

In this practical, you are asked to compare the prediction error of:

1. The Naive Bayes Classifier
2. LDA
3. QDA
4. Nearest Shrunken Centroids Classifier

On the Breast Cancer dataset provided in the previous notebooks, and the Prostate cancer dataset attached. The details about this last dataset are found in the reference:

Singh, D., Febbo, P., Ross, K., Jackson, D., Manola, J., Ladd, C., Tamayo, P., Renshaw, A., D'Amico, A., Richie, J., Lander, E., Loda, M., Kantoff, P., Golub, T., & Sellers, W. (2002). Gene expression correlates of clinical prostate cancer behavior. Cancer Cell, 1, 203–209.

This dataset is in CSV format and the last column contains the class label. The task of interest is to discriminate between normal and tumor tissue samples.

Importantly:

Use a random split of 2 / 3 of the data for training and 1 / 3 for testing each classifier. Any hyper-parameter of each method should be tuned using a grid-search guided by an inner cross-validation procedure that uses only training data. To reduce the variance of the estimates, report average error results over 20 different partitions of the data into training and testing as described above. Submit a notebook showing the code and the results obtained. Give some comments about the results and respond to these questions:

What method performs best on each dataset? What method is more flexible? What method is more robust to over-fitting?

Script 1.0.1 (python)

```python
import warnings
warnings.filterwarnings("ignore")
%matplotlib inline
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import matplotlib.lines as mlines
import matplotlib as mpl
from matplotlib import colors
import seaborn as sns; sns.set()
import scipy.stats as stats
import scipy as sp
from scipy import linalg
from sklearn.naive_bayes import GaussianNB
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
from sklearn.discriminant_analysis import QuadraticDiscriminantAnalysis
from sklearn.naive_bayes import GaussianNB
from sklearn.neighbors import NearestCentroid
from sklearn.pipeline import Pipeline
from sklearn.model_selection import train_test_split, RepeatedStratifiedKFold, GridSearchCV
from sklearn import preprocessing
from sklearn.metrics import accuracy_score, make_scorer, confusion_matrix
```

1.1 Methods

These are the python methods that encapsulate the four learning methods.

1.1.1 Implementation details

Quadratic Discriminant Analysis

Before training the classifier we have chosen a good value for the corresponding regularization hyper-parameter with a grid-search guided by cross-validation.

The regularization parameter regularizes the covariance matrix estimate as

$$(1 - \lambda) \cdot \mathbf{\Sigma} + \lambda \cdot \mathbf{I}$$

Nearest Centroids

Before training the classifier we have chosen a good value for the shrinkage threshold hyper-parameter with a grid-search guided by cross-validation.

This procedure leads to a reduction in the number of features, by zeroing all deltas that exceed the threshold.

They take the form:

$$\mu_{kj} = m_j + \Delta_{kj} \,,$$

where Δ_{kj} is the shrunken component

Selecting the best parameter value

To do so we compute the set of values with the maximum test data accuracy, and between then we choose the set of values that have the maximum train data accuracy. From this set we choose the lowest value.

Script 1.1.1 (python)

```python
def create_datasets_from_file(data_file, header, random_state, label_pos,
                              label_value, features_ini, features_fin=None):
    """Create training and test sets from file

        Args:
            data_file (string): Name of the data file (csv) of samples a features
            header (string): None or position of the header (pandas read_csv parameter)
            random_state (int): Seed for the random split (as needed for sklearn
↪   train_test_split)
            label_pos (int): Column of the labels in data_file
            label_value (int): Value of the label to asign internal '1' value
            features_ini (int): First column of features in data_file
            features_fin (int): Last column + 1 of features in data_file. If None, last
↪   column of file.

        Returns:
            (np.array): train set scaled
            (np.array): test set scaled
            (np.array): class labels for the train set
            (np.array): class labels for the test set

    """
    data = pd.read_csv(data_file, header = header)
    if features_fin == None:
        X = data.values[ :, features_ini:].astype(np.float)
    else:
        X = data.values[ :, features_ini:features_fin].astype(np.float)
    y = (data.values[ :, label_pos ] == label_value).astype(np.int)
    # Split dataset between training and test
    x_train, x_test, y_train, y_test = train_test_split(X, y,
                                                        test_size=1.0/3, random_state=random_state)
    # Data standardization
    scaler = preprocessing.StandardScaler().fit(x_train)
    x_train_scaled = scaler.transform(x_train)
    x_test_scaled = scaler.transform(x_test)

    # Check standardization
    for i in range (1, np.size(x_train_scaled,1)):
        assert round(np.var(x_train_scaled[:,0]),3) == round(np.var(x_train_scaled[:,i]),3),\
        "Warning: revise data standardization"

    return x_train_scaled, x_test_scaled, y_train, y_test

def prediction_accuracy(x_train, x_test, y_train, y_test, method_func, method_param, param_value):
    """Estimate parameter given training and test sets:
        Args:
            x_train (np.array): train set
            x_test (np.array): test set
            y_train (np.array): class labels for the train set
            y_test (np.array): class labels for the test set
            method_func (string) : name of the learning method
            param (string): name of learning method parameter
            param_value (float): value of parameter to try
        Returns:
            float: best parameter value to use in prediction

    """
    if method_param != "" :
        params = {method_param : param_value}
    else:
        params ={}
    method = globals()[method_func](**params)

    # Training
    method.fit(x_train, y_train)

    # Prediction
    y_pred = method.predict(x_test)
    conf = confusion_matrix(y_test, y_pred)
    TN = conf[0][0]
    TP = conf[1][1]
    FP = conf[0][1]
    FN = conf[1][0]
    print(conf)
    print('Predicion accuracy is: %f' % ((TP + TN) / (TN + TP + FP + FN)))
    print('True postive rate is: %f' % (TP / (TP + FN)))
    print('True negative rate is: %f\n' % (TN / (TN + FP)))

def estimate_parameter(x_train, x_test, y_train, y_test, method_func, param, param_values):
    """Estimate parameter given training and test sets:
        Args:
            x_train (np.array): train set
            x_test (np.array): test set
            y_train (np.array): class labels for the train set
            y_test (np.array): class labels for the test set
            method_func (string) : name of the learning method
            param (string): name of learning method parameter
            param_values (list of float): list of parameter values to try
        Returns:
            (float): best parameter value to use in prediction

    """
    # Pipeline for estimate the regularization parameter
    pipeline = Pipeline([ ('method', globals()[method_func]()) ])

    # Construct the grid the hyperparameter candidate shronk theshold
    param_grid = { 'method__' + param : param_values }

    # Evaluating
    skfold = RepeatedStratifiedKFold(n_splits=10, n_repeats=1, random_state=0)
    gridcv = GridSearchCV(pipeline, cv=skfold, n_jobs=1, param_grid=param_grid,\
            scoring=make_scorer(accuracy_score))
    result = gridcv.fit(x_train, y_train)

    # Accuracies
    accuracies = gridcv.cv_results_['mean_test_score']
    std_accuracies = gridcv.cv_results_['std_test_score']

    test_accuracies = np.ones(len(param_values))

    for i in range(len(param_values)):
        method_params = {param : param_values[ i ]}
        method = globals()[method_func](**method_params)
        method.fit(x_train, y_train)
        test_accuracies[ i ] = accuracy_score(method.predict(x_test), y_test)

    max_test_accuracy = max(test_accuracies)

    # Obtain best_param_value as max
    best_param_value = 0
    best_train_accuracy = 0
    for i in range(len(param_values)):
        if test_accuracies[ i ] == max_test_accuracy:
            if accuracies[i] > best_train_accuracy:
                best_train_accuracy = accuracies[i]
                best_param_value = param_values[i]

    # Plot
    plt.figure(figsize=(15, 10))
    line1, = plt.plot(param_values, accuracies, 'o-', color="g")
    line2, = plt.plot(param_values, test_accuracies, 'x-', color="r")
    plt.fill_between(param_values, accuracies - std_accuracies / np.sqrt(10), \
        accuracies + std_accuracies / np.sqrt(10), alpha=0.1, color="g")
    plt.grid()
    plt.title("Different hyper-parameter " + param + " values for " + method_func)
    plt.xlabel('Hyper-parameter')
    plt.xticks(np.round(np.array(param_values), 2))
    plt.ylabel('Classification Accuracy')
    plt.ylim((min(accuracies) - 0.1, min(1.02, max(accuracies) + 0.1)))

    plt.xlim((min(param_values), max(param_values)))
    legend_handles = [ mlines.Line2D([], [], color='g', marker='o', \
                              markersize=15, label='CV-estimate'), \
                    mlines.Line2D([], [], color='r', marker='x', \
                              markersize=15, label='Test set estimate')]
    plt.legend(handles=legend_handles, loc = 3)
    plt.show()

    print("Best param value:", best_param_value)
    return best_param_value

def learn_dataset(data_file, header, random_state, label_pos,
                  label_value, features_ini, features_fin=None):
    """Learn data sets from file, methods:
            1. The Naive Bayes Classifier
            2. LDA
            3. QDA
            4. Nearest Shrunken Centroids Classifier
        Args:
            data_file (string): Name of the data file (csv) of samples a features
            header (string): None or position of the header (pandas read_csv parameter)
            random_state (int): Seed for the random split of sets (as needed for sklearn
 ↪  train_test_split)
            label_pos (int): Column of the labels in data_file
            label_value (int): Value of the label to asign internal '1' value
            features_ini (int): First column of features in data_file
            features_fin (int): Last column + 1 of features in data_file. If None, last
 ↪  column of file

    """
    X_train_scaled, X_test_scaled, y_train, y_test = \
        create_datasets_from_file(data_file, header, random_state,
                                  label_pos, label_value, features_ini, features_fin=None)
    print(X_train_scaled.shape)

    # Naive Bayes accuracy
    prediction_accuracy(X_train_scaled, X_test_scaled, y_train, y_test, "GaussianNB", "", "")

    # LDA accuracy
    prediction_accuracy(X_train_scaled, X_test_scaled, y_train, y_test,
     ↪  "LinearDiscriminantAnalysis", "", "")

    # QDA estimate reg parameter
    param_values = np.linspace(0, 1, 10).tolist()
    best_param_value = estimate_parameter(X_train_scaled, X_test_scaled, y_train, y_test,\
                       "QuadraticDiscriminantAnalysis", "reg_param", param_values)
    # QDA accuracy
    # Best parameter reg value according CV estimate
    prediction_accuracy(X_train_scaled, X_test_scaled, y_train, y_test, \
                        "QuadraticDiscriminantAnalysis", "reg_param", best_param_value)

    # Centroids
    # Best parameter shrink_threshold value according CV estimate
    param_values = np.linspace(0, 8, 20).tolist()
    best_param_value = estimate_parameter(X_train_scaled, X_test_scaled, y_train, y_test,\
                       "NearestCentroid", "shrink_threshold", param_values)
    # Centroids accuracy
    prediction_accuracy(X_train_scaled, X_test_scaled, y_train, y_test, "NearestCentroid",
     ↪  "shrink_threshold", best_param_value)
```

1.2 Breast cancer

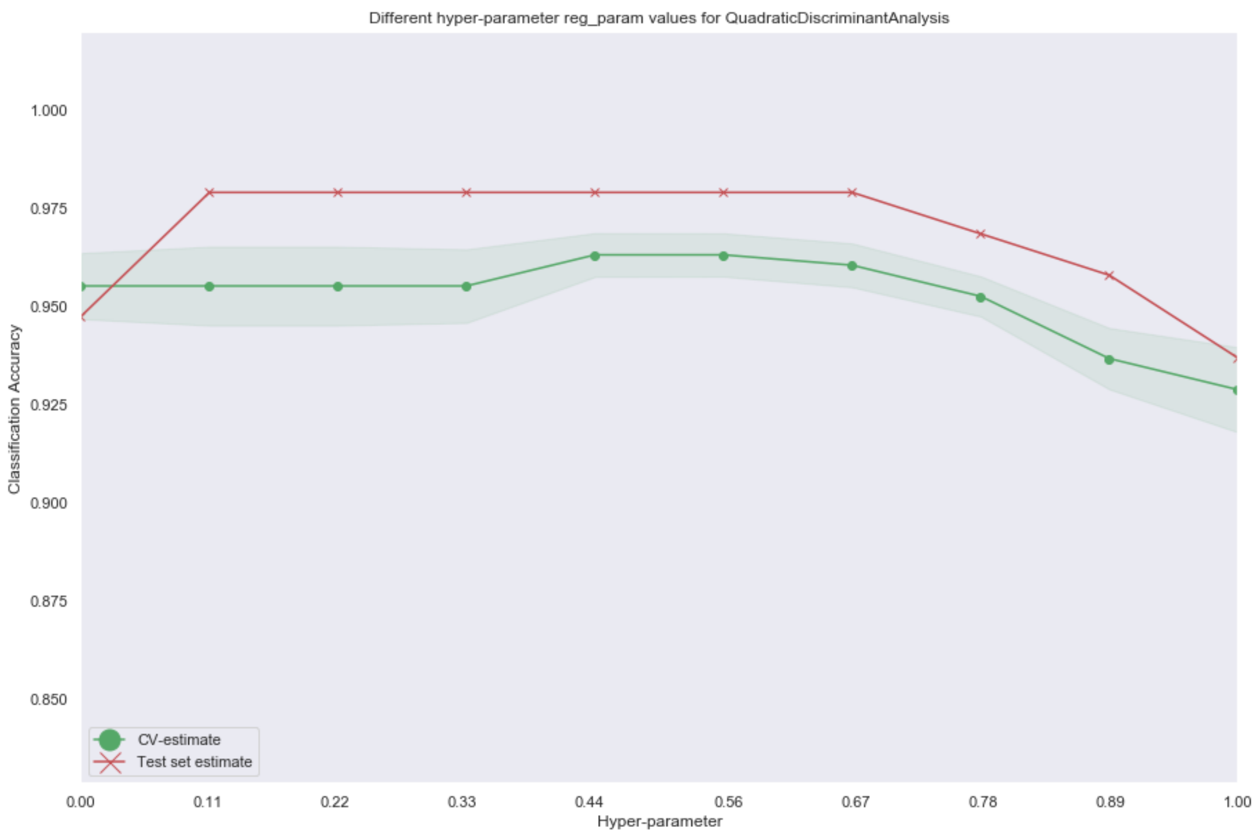
Script 1.2.1 (python)

```python
# Breast Cancer
data_file = './data/wdbc.csv'
learn_dataset(data_file, None, 1, 1, "B", 2)
```

Output

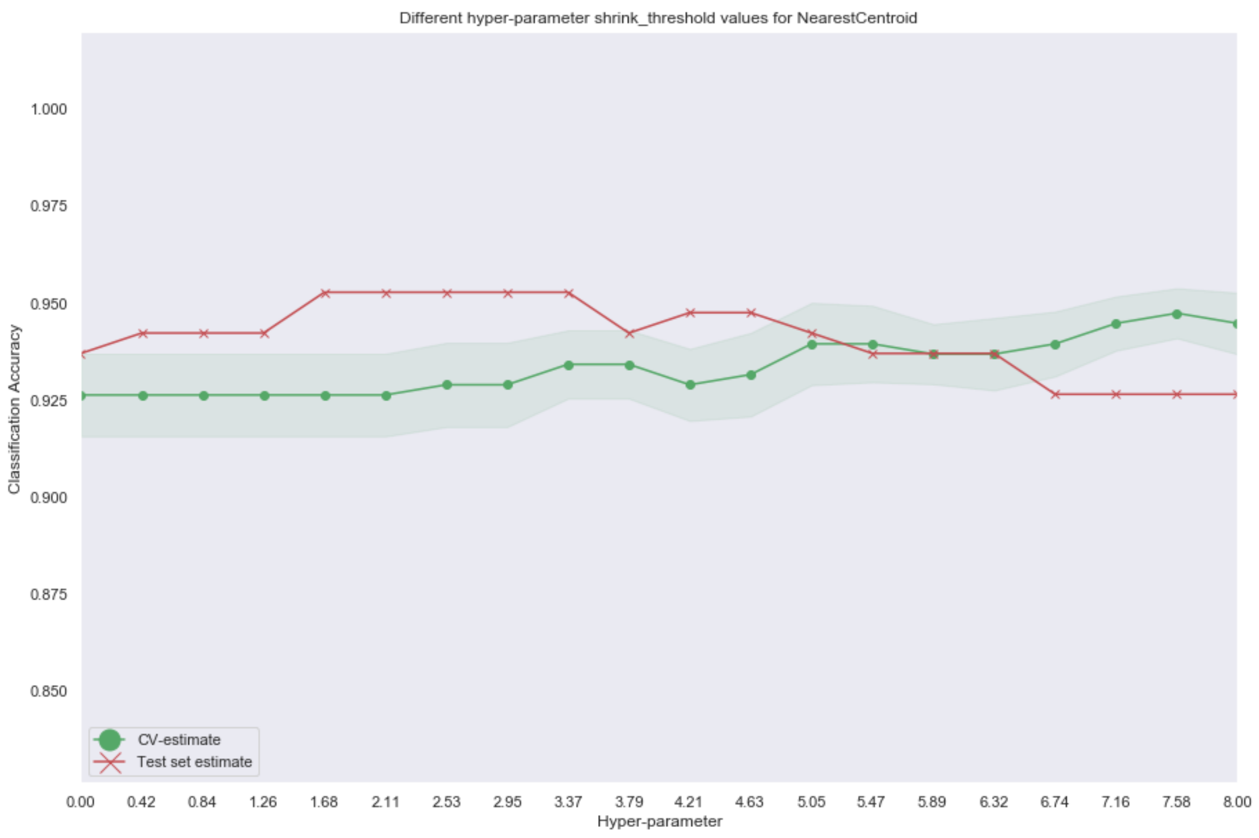
```
(379, 30)
[[ 61   5]
 [  7 117]]
Predicion accuracy is: 0.936842
True postive rate is: 0.943548
True negative rate is: 0.924242

[[ 60   6]
 [  1 123]]
Predicion accuracy is: 0.963158
True postive rate is: 0.991935
True negative rate is: 0.909091
```



Output

```
Best param value: 0.4444444444444444
[[ 62   4]
 [  0 124]]
Predicion accuracy is: 0.978947
True postive rate is: 1.000000
True negative rate is: 0.939394
```



Output

```
Best param value: 3.3684210526315788
[[ 60   6]
 [  3 121]]
Predicion accuracy is: 0.952632
True postive rate is: 0.975806
True negative rate is: 0.909091
```

1.3 Prostate cancer

Script 1.3.1 (python)

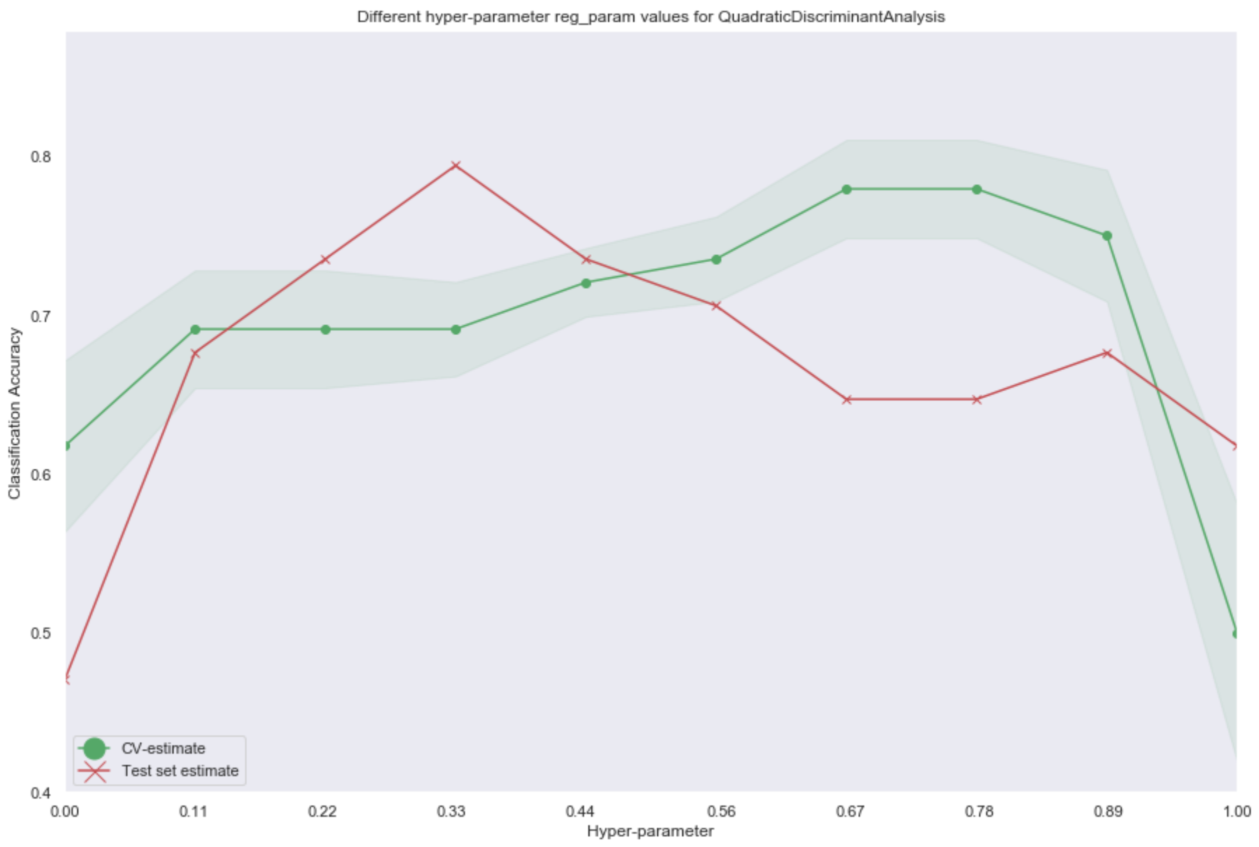
```python
# Prostate Cancer
data_file = './data/prostate.csv'
learn_dataset(data_file, 0, 1, -1, 1, 0, -1)
```

Output

```
(68, 12626)
[[16  0]
```

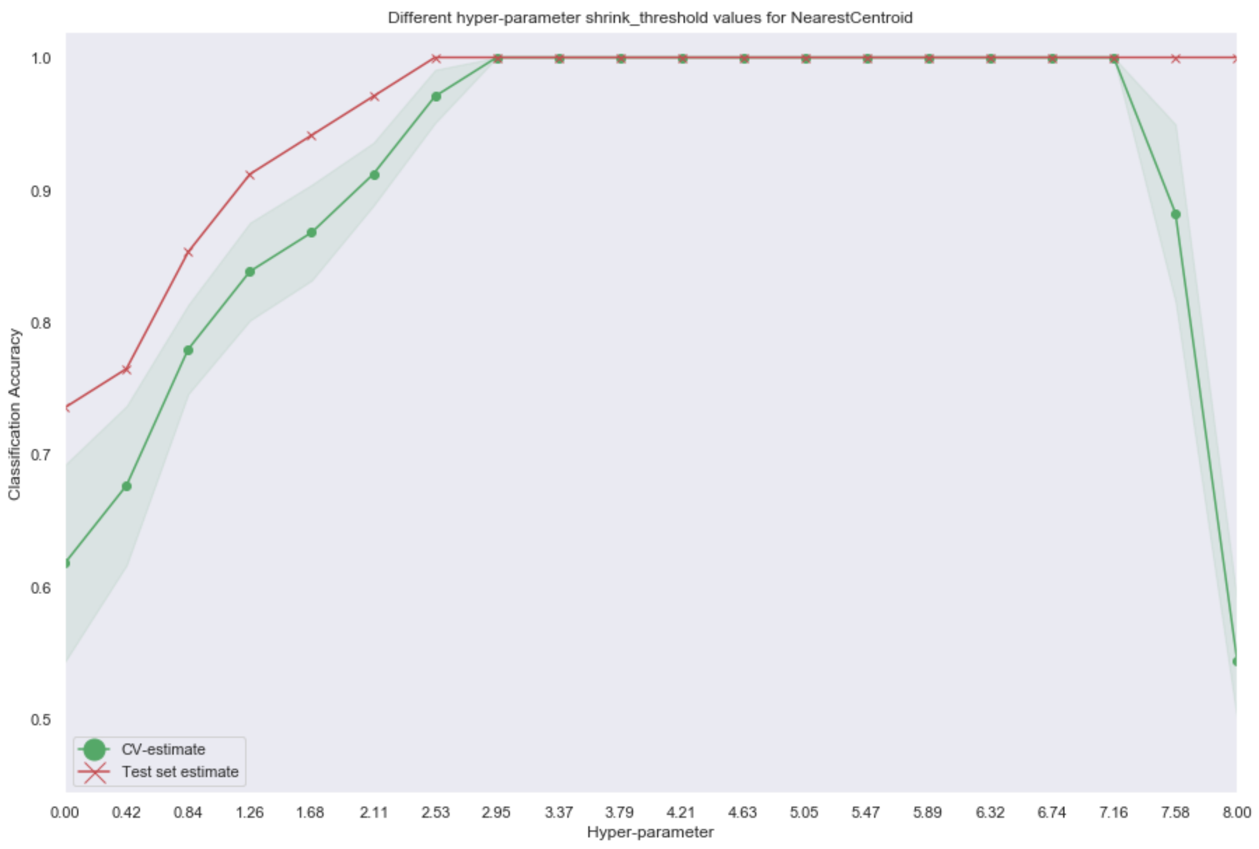
```
 [ 0 18]]
Predicion accuracy is: 1.000000
True postive rate is: 1.000000
True negative rate is: 1.000000

[[15  1]
 [ 4 14]]
Predicion accuracy is: 0.852941
True postive rate is: 0.777778
True negative rate is: 0.937500
```



Output

```
Best param value: 0.3333333333333333
[[13  3]
 [ 4 14]]
Predicion accuracy is: 0.794118
True postive rate is: 0.777778
True negative rate is: 0.812500
```



Output

```
Best param value: 2.9473684210526314
[[16  0]
 [ 0 18]]
Predicion accuracy is: 1.000000
True postive rate is: 1.000000
True negative rate is: 1.000000
```

1.4 Conclusions

We observe that **QDA** performs very poorly in the prostate dataset, given the high dimensionality of this dataset, which do not ease the accurate computation of the covariance matrices. Perhaps if we perform previously a dimensionality reduction by PCA, we'll improve this result.

NSC performs in this case much better due to the reduced number of parameters and the feature selection properties of this classifier and more consistently between both cases (prostate and breast).