Classification Systems

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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.decomposition import PCA
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,
↪  classification_report, precision_score
```

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, as a first idea, 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.

We compare this method defined in the global parameter *gp_best_hyper_method = "max_in_test"* to the method than simply computes the parameter for maximum cross validation data accuracy (*gp_best_hyper_method = "max_in_cv"*) and we obtain better accuracies in test data. But we came into account that because we use test data to adjust the hyper-parameter perhaps we are introducing some bias improving the accuracy of this particular test data, and so a optimistic evaluation of the accuracy.

Thus, we compute the hyperparameters with "max_in_cv" choose method.

Script 1.1.1 (python)

```python
# Global parameters
# Verbose flag
gp_verbose = False
# Show progress  flag
gp_show_progress = True
# Disable plots
gp_disable_plots = True
# Activate QDA with hyper-parameter reg_param
gp_qda_hyper = True
# Activate NSC with hyper-parameter shrink_threshold
gp_nsc_hyper = True
# Dimensionality reduction(PCA)
gp_dim_red = False
# Retained variance (PCA)
gp_retained_variance = 99
# Number of iterations
gp_iterations = 1
```

```python
# Test size = number of samples / gp_test_size
gp_test_size = 3
# Best_hyper_param_method
gp_best_hyper_method = "max_in_cv"
# Skfold splits for hyperparameter guessing
gp_skfold_splits = 10

# Global execution parameters
# New dimensions after PCA
ge_features_reduction = 0

#Number of params of learning methods
ge_complexity = []

# Methods
def get_component_number(df_data, desired_variance=99.0, scaling=False):
    """
    Obtain the number of components that explains a %desired_variance
    Args:
        df_data (dataframe): dataframe of features in cols and samples in rows
        desired_variance (float): desired explained variance
        scaling (boolean): True if pre-scaling is needed prior to compute PCA
    Returns:
        int: number of components to maintain to have a explained variance >=
    ↪   desired_variance
        float: variance explained for the number of components returned
        numpy array: cumulative variance by number of components retained
    """
    if scaling:
        df_data_2 = preprocessing.StandardScaler().fit_transform(df_data)
    else:
        df_data_2 = df_data
    # project the data into this new PCA space
    pca = PCA().fit(df_data_2)
    desired_variance = desired_variance/100.0
    explained_variance = np.cumsum(pca.explained_variance_ratio_)
    component_number = 0
    for cumulative_variance in explained_variance:
        component_number += 1
        if cumulative_variance >= desired_variance:
            break
    return component_number, cumulative_variance, explained_variance


def create_datasets_from_file(data_file, header, random_state, label_pos,
                              label_value, features_ini, features_fin=None,
                              with_dim_red=False, retained_variance=99.0,
                              reuse=False, dataset=None, labels=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.
            with_dim_red (bool): If True, it performs a dimensionality reduction by PCA
            retained_variance (float): If dimensionality reduction, variance to retain
            reuse (bool): Reuse previous dataset
            dataset: Dataset to reuse
            labels: Labels to reuse

        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
            (np.array): dataset
            (np.array): labels

    """
    global ge_features_reduction
    if not reuse:
        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)
    else: #reuse previous dataset
        X = dataset
        y = labels

    # Split dataset between training and test
    x_train, x_test, y_train, y_test = train_test_split(X, y,
                                                        test_size=1.0/gp_test_size,
                                                         ↪   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"

    if with_dim_red:
        desired_variance = retained_variance
        component_number, _, _ =\
            get_component_number(x_train_scaled, desired_variance, scaling=None)
        if gp_verbose: print("Features reduced to", component_number)
        ge_features_reduction = component_number
        pca = PCA(n_components = component_number)
        pca.fit(x_train_scaled)
        x_train_scaled = pca.transform(x_train_scaled)
        x_test_scaled = pca.transform(x_test_scaled)

    return x_train_scaled, x_test_scaled, y_train, y_test, X, y

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
            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)

    ge_complexity.append([method_func, len(method.get_params())])
    # Prediction of test
    y_pred = method.predict(x_test)
    conf_test = confusion_matrix(y_test, y_pred, labels=[1,0])

    # Prediction of train
    y_pred = method.predict(x_train)
    conf_train = confusion_matrix(y_train, y_pred, labels=[1,0])

    return conf_train, conf_test

def estimate_parameter(x_train, x_test, y_train, y_test,
                       method_func, param, param_values,
                       best_param_value_method="max_in_test"):
    """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
            best_param_value_method: if "max_in_test" gives the value with the maximum
↪   accuracy
                                        in test data.
        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=gp_skfold_splits, 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)

    # Obtain best_param_value as max
    max_test_accuracy = max(test_accuracies)
    if best_param_value_method == "max_in_test":
        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]
    else:
        best_param_value = param_values[ np.argmax(accuracies) ]
    # Plot
    if not gp_disable_plots:
        plt.figure(figsize=(9, 9))
        line1, = plt.plot(param_values, accuracies, 'o-', color="g")
        line2, = plt.plot(param_values, test_accuracies, 'x-', color="r")
```

```python
        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(min(accuracies), min(test_accuracies)) - 0.1,
                  min(1.02, max(max(accuracies), max(test_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()
    if gp_verbose:
        print("Best param value %s Method %s: %s" % (method_func, best_param_value_method, best_param_value))
    return best_param_value

def calculate_avg_results(train_results, test_results, classifier_name):
    """Calculate the average accuracy, TPN and TNR for the n=gp_iterations of a classifier
        Args:
            train_results (array nx2x2): Each of the n confusions matrix generated for the train set
            test_results (array nx2x2): Each of the n confusions matrix generated for the test set
            classifier_name (string): Classifier name gp_iterations print the results
        Returns:
            (np.array 3): Average accuracy, TPR and TNR of the n iterations of the train set
            (np.array 3): Average accuracy, TPR and TNR of the n iterations of the test set
            (np.array 3): Stdev accuracy, TPR and TNR of the n iterations of the train set
            (np.array 3): Stdev accuracy, TPR and TNR of the n iterations of the test set

    """

    measures_train = np.zeros(shape = (gp_iterations,3)) # Each row is an ex. and each column is the accuracy, TPR and TNR
    measures_test = np.zeros(shape =(gp_iterations,3))

    avg_results_train = np.zeros(3) # Each element is the average accuracy, the TPR and the TNR
    avg_results_test = np.zeros(3)
    #   TP in 0,0
    #   FN in 0,1
    #   TN in 1,1
    #   FP in 1,0
    for i in range(gp_iterations):
        # For train set
        TN = train_results[i,1,1]
        TP = train_results[i,0,0]
        FP = train_results[i,1,0]
        FN = train_results[i,0,1]
        measures_train[i][0] = (TP + TN) / (TN + TP + FP + FN)
        measures_train[i][1] = (TP / (TP + FN))
        measures_train[i][2] = (TN / (TN + FP))

        #For the test set
        TN = test_results[i,1,1]
        TP = test_results[i,0,0]
        FP = test_results[i,1,0]
        FN = test_results[i,0,1]
        measures_test[i][0] = (TP + TN) / (TN + TP + FP + FN)
        measures_test[i][1] = (TP / (TP + FN))
        measures_test[i][2] = (TN / (TN + FP))

    avg_results_train = measures_train.mean(axis = 0)
    avg_results_test = measures_test.mean(axis = 0)
    std_results_train = measures_train.std(axis = 0)
    std_results_test = measures_test.std(axis = 0)
    if gp_verbose:
        print("\nResults for the ", classifier_name, " classifier\n")

        print('For the train set:')
        print('Predicion accuracy of train set is: %f' % avg_results_train[0])
        print('True postive rate of train set is: %f' % avg_results_train[1])
        print('True negative rate of train set is: %f\n' % avg_results_train[2])

        print('For the test set:')
        print('Predicion accuracy of train set is: %f' % avg_results_test[0])
        print('True postive rate of train set is: %f' % avg_results_test[1])
        print('True negative rate of train set is: %f\n' % avg_results_test[2])

    return avg_results_train, avg_results_test, std_results_train, std_results_test

def print_parameters():
    print("Parameters")
    pdata = {'Parameters' : [gp_qda_hyper, gp_nsc_hyper,
                             gp_dim_red, gp_retained_variance,
                             gp_iterations, 100.0/gp_test_size,
                             gp_best_hyper_method]}
    pdataf = pd.DataFrame(data = pdata, index = ['QDA hyper-parameter reg_param',
                                                 'NSC Hyper-parameter shrink_threshold',
                                                 'Dimensionality Reduction',
                                                 'Retained variance',
                                                 'Number of iterations',
                                                 'Test set size',
                                                 'Best hyperparameter select method'])
    display(pdataf)
    print("")

def print_execution_data():
```

```python
    print("Execution data")
    data = [ge_samples, ge_features, ge_features_reduction]
    index = ['Number of samples', 'Number of features', 'Features reduction']
    for [method, complexity] in ge_complexity:
        data.append(complexity)
        index.append("Params " + method)
    pdata = {'Execution Data' : data}
    pdataf = pd.DataFrame(data = pdata, index = index)
    display(pdataf)
    print("")

def print_accuracies(accuracy_NBC, accuracy_LDA, accuracy_QDA, accuracy_NSC, metric):
    print(metric)
    d = {}
    for m in [accuracy_NBC, accuracy_LDA, accuracy_QDA, accuracy_NSC]:
        overfit_indicator = 1000 * round(abs(m[1] - m[0]) / (m[0] + 0.0000001), 4)
        #overfit_indicator = round(abs(m[1] - m[0]),3)
        m[0] = (round(m[0],2), round(m[2],2))
        m[1] = (round(m[1],2), round(m[3],2))
        m[2] = overfit_indicator
    d = {'NBC': accuracy_NBC[:3],
         'LDA': accuracy_LDA[:3],
         'QDA': accuracy_QDA[:3],
         'NSC': accuracy_NSC[:3]}
    df = pd.DataFrame(data = d, index = ['Train', 'Test', 'Overfit degree'])
    display(df)
    print("")

def learn_dataset(data_file, header, random_state, label_pos,
                  label_value, features_ini, features_fin=None,
                  best_param_value_method="max_in_test",
                  with_dim_red=False, retained_variance=99.0):
    """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. We consider
↪   this label as
            the positive label in prediction validation. We asign malign or cancer status to
↪   this label.
            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
            best_param_value_method (str): if "max_in_test" gives the value with the maximum
↪   accuracy
```

```
                                    in test data
            with_dim_red (bool): If True, it performs a dimensionality reduction by PCA
            retained_variance (float): If dimensionality reduction, variance to retain

    """
    global ge_features_reduction
    global ge_features
    global ge_samples
    global ge_complexity
    ge_features_reduction = 0
    nbc_train = np.zeros(shape=(gp_iterations,2,2))
    nbc_test = np.zeros(shape=(gp_iterations,2,2))
    lda_train = np.zeros(shape=(gp_iterations,2,2))
    lda_test = np.zeros(shape=(gp_iterations,2,2))
    qda_train = np.zeros(shape=(gp_iterations,2,2))
    qda_test = np.zeros(shape=(gp_iterations,2,2))
    nsc_train = np.zeros(shape=(gp_iterations,2,2))
    nsc_test = np.zeros(shape=(gp_iterations,2,2))


    for i in range(gp_iterations):
        ge_complexity = []
        if gp_show_progress: print("\nIteration: ",i)
        if i == 0:
            reuse = False
            X = None
            y = None
        else:
            reuse = True
        X_train_scaled, X_test_scaled, y_train, y_test, X, y = \
            create_datasets_from_file(data_file, header, random_state + i,
                                      label_pos, label_value, features_ini, features_fin =
                                       ↪  features_fin,
                                      with_dim_red = with_dim_red, retained_variance =
                                       ↪  retained_variance,
                                      reuse = reuse, dataset = X, labels = y)
        ge_samples = X.shape[0]
        ge_features = X.shape[1]
        if gp_verbose: print(X_train_scaled.shape)

        if gp_verbose: print("NBC")
        # Naive Bayes accuracy
        nbc_train[i], nbc_test[i] = prediction_accuracy(X_train_scaled, X_test_scaled,
         ↪  y_train, y_test, "GaussianNB")

        # LDA accuracy
        if gp_verbose: print("LDA")
        lda_train[i], lda_test[i] = prediction_accuracy(X_train_scaled, X_test_scaled,
         ↪  y_train, y_test, "LinearDiscriminantAnalysis")

        # QDA estimate reg parameter
        if gp_verbose: print("QDA")
        if gp_qda_hyper:
            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,\
                                 best_param_value_method)
            # QDA accuracy
            # Best parameter reg value according CV estimate
            qda_train[i], qda_test[i] = prediction_accuracy(X_train_scaled, X_test_scaled,
            ↪  y_train, y_test,\
                                 "QuadraticDiscriminantAnalysis", "reg_param",
                                  ↪  best_param_value)
        else:
            qda_train[i], qda_test[i] = prediction_accuracy(X_train_scaled, X_test_scaled,
            ↪  y_train, y_test,\
                                 "QuadraticDiscriminantAnalysis")
        # Centroids
        if gp_verbose: print("NSC")
        if gp_nsc_hyper:
            # 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,\
                                 best_param_value_method)
            # Centroids accuracy
            nsc_train[i], nsc_test[i] = prediction_accuracy(X_train_scaled, X_test_scaled,
            ↪  y_train, y_test,\
                                                "NearestCentroid", "shrink_threshold",
                                                 ↪  best_param_value)
        else:
            nsc_train[i], nsc_test[i] = prediction_accuracy(X_train_scaled, X_test_scaled,
            ↪  y_train, y_test,\
                                                "NearestCentroid")
    # Calculate and print the average results
    avg_results_train_NBC, avg_results_test_NBC, std_results_train_NBC, std_results_test_NBC
    ↪  = calculate_avg_results(nbc_train, nbc_test, "NBC")
    avg_results_train_LDA, avg_results_test_LDA, std_results_train_LDA, std_results_test_LDA
    ↪  = calculate_avg_results(lda_train, lda_test, "LDA")
    avg_results_train_QDA, avg_results_test_QDA, std_results_train_QDA, std_results_test_QDA
    ↪  = calculate_avg_results(qda_train, qda_test, "QDA")
    avg_results_train_NSC, avg_results_test_NSC, std_results_train_NSC, std_results_test_NSC
    ↪  = calculate_avg_results(nsc_train, nsc_test,"NSC")

    print_parameters()
    i = 0
    for metric in ["Accuracy", "TPR", "TNR"]:
        print_accuracies([avg_results_train_NBC[i], avg_results_test_NBC[i],
        ↪  std_results_train_NBC[i], std_results_test_NBC[i]],
                         [avg_results_train_LDA[i], avg_results_test_LDA[i],
                          ↪  std_results_train_LDA[i], std_results_test_LDA[i]],
```

```python
                      [avg_results_train_QDA[i], avg_results_test_QDA[i],
                      ↪  std_results_train_QDA[i], std_results_test_QDA[i]],
                      [avg_results_train_NSC[i], avg_results_test_NSC[i],
                      ↪  std_results_train_NSC[i], std_results_test_NSC[i]], metric)
        i += 1
    print_execution_data()
```

1.2 Breast cancer

Script 1.2.1 (python)

```python
gp_disable_plots = True
gp_verbose = False
gp_dim_red = False
gp_retained_variance = 99
gp_qda_hyper = True
gp_nsc_hyper = True
gp_iterations = 20
gp_show_progress = False
gp_best_hyper_method = "max_in_cv"
gp_skfold_splits = 10

learn_dataset(data_file = './data/wdbc.csv', header = None, random_state=0,
              label_pos=1, label_value="M", features_ini = 2, features_fin = None,
              best_param_value_method = gp_best_hyper_method,
              with_dim_red = gp_dim_red, retained_variance = gp_retained_variance)

gp_dim_red = True
learn_dataset(data_file = './data/wdbc.csv', header = None, random_state=0,
              label_pos=1, label_value="M", features_ini = 2, features_fin = None,
              best_param_value_method = gp_best_hyper_method,
              with_dim_red = gp_dim_red, retained_variance = gp_retained_variance)
```

Output

```
Parameters
```

```
                                       Parameters
QDA hyper-parameter reg_param                True
NSC Hyper-parameter shrink_threshold         True
Dimensionality Reduction                    False
Retained variance                              99
Number of iterations                           20
Test set size                             33.3333
Best hyperparameter select method       max_in_cv
```

Output

```
Accuracy
```

```
                         NBC           LDA           QDA           NSC
Train           (0.94, 0.01)  (0.97, 0.01)  (0.97, 0.01)  (0.94, 0.01)
Test            (0.93, 0.01)  (0.96, 0.01)  (0.97, 0.01)  (0.94, 0.01)
Overfit degree           5.4           7.5           9.4             7
```

Output

```
TPR
```

```
                        NBC           LDA           QDA          NSC
Train           (0.9, 0.01)  (0.92, 0.01)  (0.95, 0.01)  (0.9, 0.02)
Test            (0.9, 0.03)  (0.89, 0.03)  (0.93, 0.03)  (0.9, 0.04)
Overfit degree         10.1          23.3          14.7          3.6
```

Output

```
TNR
```

```
                         NBC          LDA          QDA           NSC
Train           (0.97, 0.01)  (1.0, 0.0)   (0.99, 0.0)  (0.97, 0.01)
Test            (0.95, 0.02)  (1.0, 0.0)  (0.98, 0.02)  (0.96, 0.02)
Overfit degree          14.3            0          6.8           9.2
```

Output

```
Execution data
```

```
                                      Execution Data
Number of samples                                569
Number of features                                30
Features reduction                                 0
Params GaussianNB                                  2
Params LinearDiscriminantAnalysis                  6
Params QuadraticDiscriminantAnalysis               5
Params NearestCentroid                             2
```

Output

```
Parameters
```

```
                                         Parameters
QDA hyper-parameter reg_param                  True
NSC Hyper-parameter shrink_threshold           True
Dimensionality Reduction                       True
Retained variance                                99
Number of iterations                             20
Test set size                               33.3333
Best hyperparameter select method         max_in_cv
```

Output

```
Accuracy
```

```
                          NBC           LDA           QDA           NSC
Train              (0.9, 0.01)   (0.96, 0.0)  (0.98, 0.01)  (0.93, 0.01)
Test              (0.89, 0.02)  (0.96, 0.01)  (0.97, 0.01)  (0.93, 0.02)
Overfit degree            10.2           7.4           8.8           5.7
```

Output

```
TPR
```

```
                          NBC           LDA           QDA           NSC
Train             (0.84, 0.02)  (0.91, 0.01)  (0.95, 0.02)  (0.87, 0.01)
Test              (0.83, 0.04)  (0.89, 0.02)  (0.94, 0.03)  (0.87, 0.03)
Overfit degree             5.4          18.6          17.2             4
```

Output

```
TNR
```

```
                          NBC           LDA           QDA           NSC
Train             (0.94, 0.01)    (1.0, 0.0)   (0.99, 0.0)  (0.97, 0.01)
Test              (0.93, 0.03)  (0.99, 0.01)  (0.99, 0.01)  (0.96, 0.02)
Overfit degree            13.1           2.1           4.6           7.6
```

Output

```
Execution data
```

```
                                         Execution Data
Number of samples                                   569
Number of features                                   30
Features reduction                                   17
Params GaussianNB                                     2
Params LinearDiscriminantAnalysis                     6
Params QuadraticDiscriminantAnalysis                  5
Params NearestCentroid                                2
```

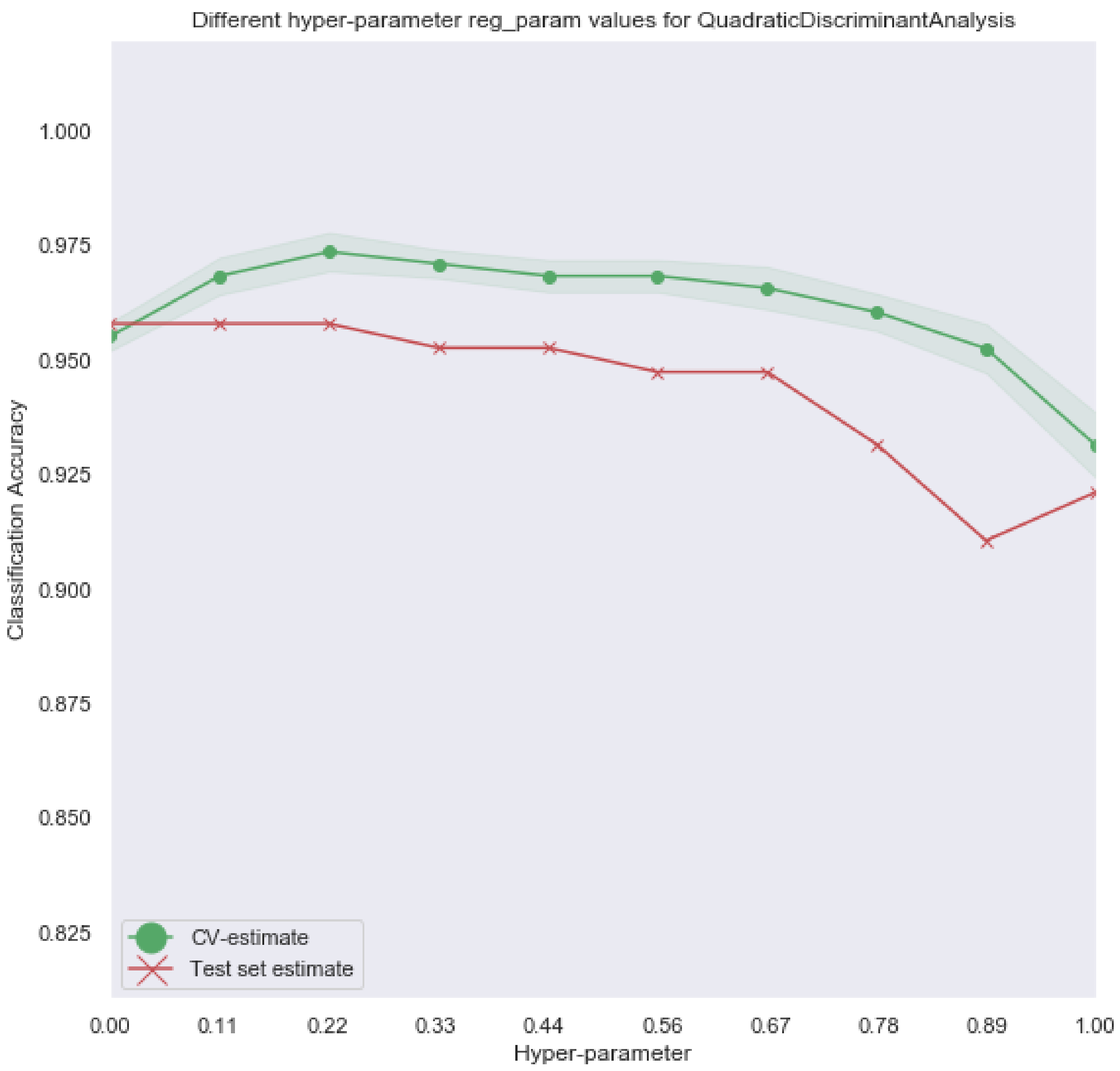
Output

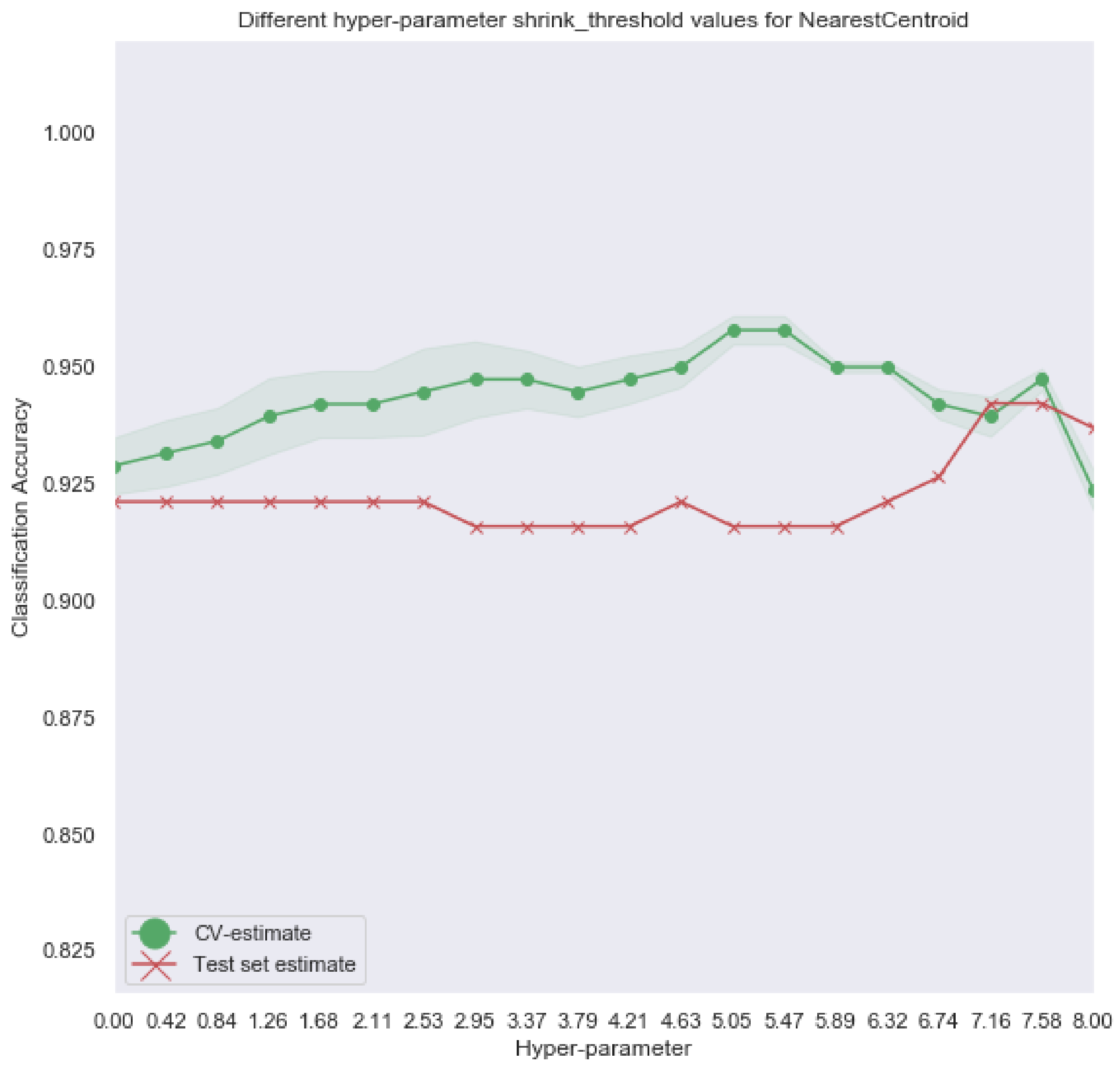
1.2.1 Hyper-parameter guessing plots

Script 1.2.2 (python)

```python
gp_disable_plots = False
gp_verbose = False
gp_dim_red = False
gp_retained_variance = 99
gp_qda_hyper = True
gp_nsc_hyper = True
gp_iterations = 1
gp_show_progress = False
gp_best_hyper_method = "max_in_cv"
ge_features_reduction = 0

learn_dataset(data_file = './data/wdbc.csv', header = None, random_state=0,
              label_pos=1, label_value="M", features_ini = 2, features_fin = None,
              best_param_value_method = gp_best_hyper_method,
              with_dim_red = gp_dim_red, retained_variance = gp_retained_variance)
```


Different hyper-parameter reg_param values for QuadraticDiscriminantAnalysis
Classification Accuracy
1.000
0.975
0.950
0.925
0.900
0.875
0.850
0.825
0.00
0.11
0.22
0.33
0.44
0.56
0.67
0.78
0.89
1.00
Hyper-parameter
CV-estimate
Test set estimate



Output

```
Parameters
```

```
                                         Parameters
QDA hyper-parameter reg_param                  True
NSC Hyper-parameter shrink_threshold           True
Dimensionality Reduction                      False
Retained variance                                99
Number of iterations                              1
Test set size                               33.3333
```

```
Best hyperparameter select method     max_in_cv
```

Output

```
Accuracy
```

```
                         NBC          LDA          QDA          NSC
Train           (0.95, 0.0)  (0.96, 0.0)  (0.98, 0.0)  (0.94, 0.0)
Test             (0.9, 0.0)  (0.97, 0.0)  (0.96, 0.0)  (0.92, 0.0)
Overfit degree         49.9           11         18.8         30.5
```

Output

```
TPR
```

```
                         NBC          LDA          QDA          NSC
Train            (0.9, 0.0)  (0.91, 0.0)  (0.94, 0.0)  (0.91, 0.0)
Test            (0.85, 0.0)  (0.93, 0.0)  (0.91, 0.0)  (0.87, 0.0)
Overfit degree         55.2         18.4         34.6         46.3
```

Output

```
TNR
```

```
                         NBC         LDA          QDA          NSC
Train           (0.97, 0.0)  (1.0, 0.0)   (1.0, 0.0)  (0.97, 0.0)
Test            (0.93, 0.0)  (1.0, 0.0)  (0.98, 0.0)  (0.94, 0.0)
Overfit degree         49.5         4.3         12.2         24.2
```

Output

```
Execution data
```

```
                                     Execution Data
Number of samples                               569
Number of features                               30
Features reduction                                0
Params GaussianNB                                 2
Params LinearDiscriminantAnalysis                 6
Params QuadraticDiscriminantAnalysis              5
Params NearestCentroid                            2
```

Output

1.3 Prostate cancer

Script 1.3.1 (python)

```python
# Prostate Cancer
gp_disable_plots = True
gp_verbose = False
gp_dim_red = False
gp_retained_variance = 99
gp_qda_hyper = True
gp_nsc_hyper = True
gp_iterations = 20
gp_best_hyper_method = "max_in_cv"
ge_features_reduction = 0
gp_skfold_splits = 5

learn_dataset(data_file = './data/prostate.csv', header = 0, random_state = 1,
              label_pos = -1, label_value = 1, features_ini = 0, features_fin = -1,
              best_param_value_method = gp_best_hyper_method,
              with_dim_red = gp_dim_red, retained_variance = gp_retained_variance)

gp_best_hyper_method = "max_in_cv"
gp_dim_red = True
gp_retained_variance = 99
ge_features_reduction = 0
learn_dataset(data_file = './data/prostate.csv', header = 0, random_state = 1,
              label_pos = -1, label_value = 1, features_ini = 0, features_fin = -1,
              best_param_value_method = gp_best_hyper_method,
              with_dim_red = gp_dim_red, retained_variance = gp_retained_variance)

gp_best_hyper_method = "max_in_cv"
gp_dim_red = True
gp_retained_variance = 80
ge_features_reduction = 0
learn_dataset(data_file = './data/prostate.csv', header = 0, random_state = 1,
              label_pos = -1, label_value = 1, features_ini = 0, features_fin = -1,
              best_param_value_method = gp_best_hyper_method,
              with_dim_red = gp_dim_red, retained_variance = gp_retained_variance)
```

Output

```
Parameters
```

```
                                      Parameters
QDA hyper-parameter reg_param               True
NSC Hyper-parameter shrink_threshold        True
```

```
Dimensionality Reduction                 False
Retained variance                           99
Number of iterations                        20
Test set size                          33.3333
Best hyperparameter select method    max_in_cv
```

Output

```
Accuracy
```

```
                         NBC           LDA           QDA           NSC
Train           (0.72, 0.06)  (0.86, 0.02)  (0.14, 0.25)  (0.91, 0.02)
Test            (0.64, 0.12)  (0.85, 0.04)   (0.64, 0.1)  (0.89, 0.05)
Overfit degree         106.3          17.9        3557.9          26.5
```

Output

```
TPR
```

```
                         NBC           LDA           QDA           NSC
Train           (0.68, 0.07)  (0.83, 0.03)  (0.12, 0.24)  (0.88, 0.03)
Test            (0.66, 0.12)   (0.8, 0.07)  (0.62, 0.18)  (0.85, 0.07)
Overfit degree          29.6          36.8        4243.1          26.7
```

Output

```
TNR
```

```
                         NBC           LDA           QDA           NSC
Train           (0.76, 0.08)  (0.89, 0.03)  (0.16, 0.27)  (0.95, 0.03)
Test            (0.62, 0.18)   (0.9, 0.08)  (0.63, 0.23)  (0.93, 0.06)
Overfit degree         178.1          16.7        2863.6          19.8
```

Output

```
Execution data
```

```
                                      Execution Data
Number of samples                                102
Number of features                             12625
```

```
Features reduction                                  0
Params GaussianNB                                   2
Params LinearDiscriminantAnalysis                   6
Params QuadraticDiscriminantAnalysis                5
Params NearestCentroid                              2
```

Output

```
Parameters
```

```
                                     Parameters
QDA hyper-parameter reg_param              True
NSC Hyper-parameter shrink_threshold       True
Dimensionality Reduction                   True
Retained variance                            99
Number of iterations                         20
Test set size                           33.3333
Best hyperparameter select method     max_in_cv
```

Output

```
Accuracy
```

```
                        NBC          LDA           QDA           NSC
Train           (0.92, 0.04)   (1.0, 0.0)  (0.87, 0.15)  (0.75, 0.08)
Test            (0.74, 0.12)  (0.9, 0.04)  (0.71, 0.09)  (0.72, 0.11)
Overfit degree         200.6          100         181.1          41.3
```

Output

```
TPR
```

```
                        NBC           LDA           QDA           NSC
Train           (0.92, 0.05)    (1.0, 0.0)  (0.83, 0.19)  (0.75, 0.08)
Test            (0.95, 0.05)  (0.87, 0.07)  (0.71, 0.14)  (0.73, 0.12)
Overfit degree          40.9         128.7         140.4          22.2
```

Output

```
TNR
```

```
                          NBC            LDA            QDA            NSC
Train            (0.93, 0.05)    (1.0, 0.0)  (0.92, 0.13)   (0.74, 0.1)
Test             (0.48, 0.29)  (0.93, 0.07)   (0.7, 0.19)  (0.69, 0.17)
Overfit degree          483.8          66.9         235.8          62.9
```

Output

```
Execution data
```

```
                                       Execution Data
Number of samples                                 102
Number of features                              12625
Features reduction                                 63
Params GaussianNB                                   2
Params LinearDiscriminantAnalysis                   6
Params QuadraticDiscriminantAnalysis                5
Params NearestCentroid                              2
```

Output

```
Parameters
```

```
                                      Parameters
QDA hyper-parameter reg_param               True
NSC Hyper-parameter shrink_threshold        True
Dimensionality Reduction                    True
Retained variance                             80
Number of iterations                          20
Test set size                            33.3333
Best hyperparameter select method      max_in_cv
```

Output

```
Accuracy
```

```
                          NBC            LDA            QDA            NSC
Train            (0.89, 0.06)  (0.96, 0.02)  (0.98, 0.01)  (0.72, 0.08)
Test             (0.78, 0.08)  (0.85, 0.05)  (0.87, 0.05)  (0.67, 0.12)
Overfit degree          116.8         110.6         116.8          76.3
```

Output

```
TPR
```

```
                      NBC           LDA           QDA           NSC
Train          (0.83, 0.1)  (0.93, 0.04)  (0.97, 0.02)   (0.7, 0.09)
Test          (0.66, 0.13)  (0.82, 0.07)  (0.88, 0.07)  (0.69, 0.12)
Overfit degree       200.4         122.7          91.3          11.2
```

Output

```
TNR
```

```
                      NBC           LDA           QDA           NSC
Train         (0.94, 0.03)  (0.98, 0.02)  (0.99, 0.01)  (0.75, 0.08)
Test          (0.93, 0.07)    (0.9, 0.1)  (0.86, 0.11)   (0.64, 0.2)
Overfit degree        15.2          82.4         133.7         137.2
```

Output

```
Execution data
```

```
                                        Execution Data
Number of samples                                  102
Number of features                               12625
Features reduction                                  19
Params GaussianNB                                    2
Params LinearDiscriminantAnalysis                    6
Params QuadraticDiscriminantAnalysis                 5
Params NearestCentroid                               2
```

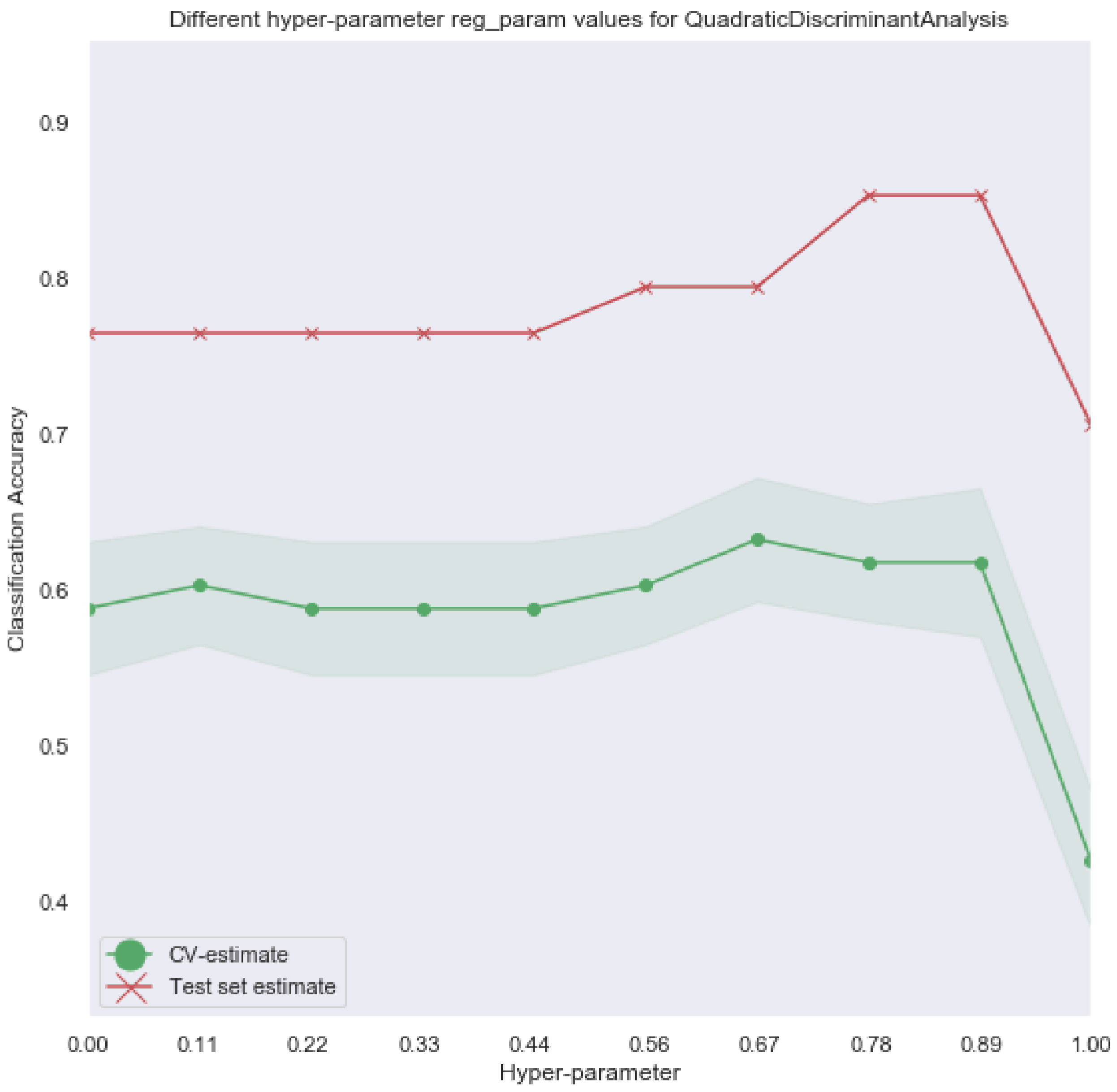
Output

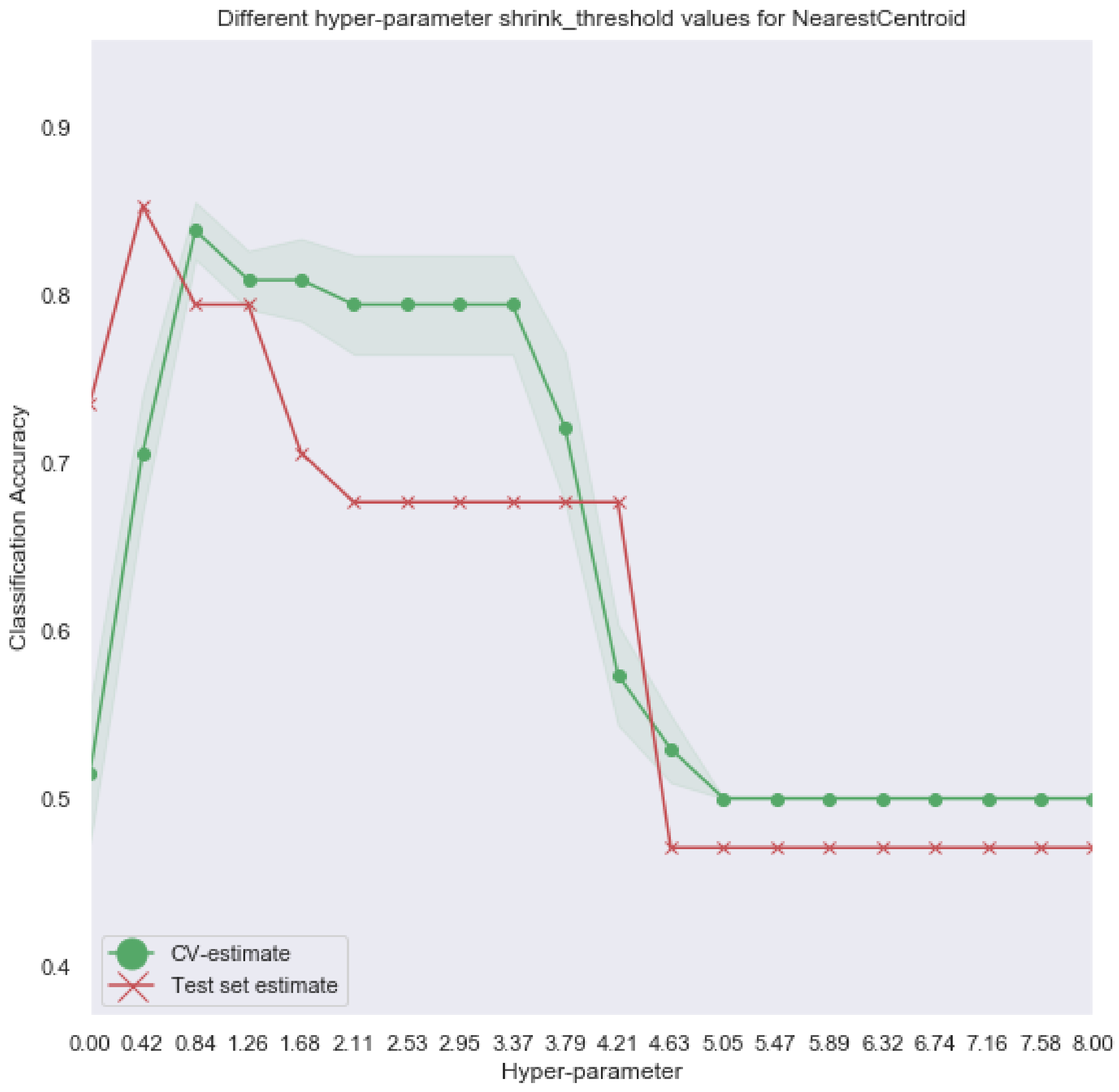
1.3.1 Hyper-parameter guessing plots

Script 1.3.2 (python)

```python
gp_disable_plots = False
gp_verbose = False
```

```
gp_dim_red = True
gp_retained_variance = 99
gp_qda_hyper = True
gp_nsc_hyper = True
gp_iterations = 1
gp_best_hyper_method = "max_in_cv"
ge_features_reduction = 0
gp_skfold_splits = 5
learn_dataset(data_file = './data/prostate.csv', header = 0, random_state = 1,
              label_pos = -1, label_value = 1, features_ini = 0, features_fin = -1,
              best_param_value_method = gp_best_hyper_method,
              with_dim_red = gp_dim_red, retained_variance = gp_retained_variance)
```





Output

```
Parameters
```

```
                                    Parameters
QDA hyper-parameter reg_param             True
NSC Hyper-parameter shrink_threshold      True
```

```
Dimensionality Reduction                 True
Retained variance                          99
Number of iterations                        1
Test set size                         33.3333
Best hyperparameter select method   max_in_cv
```

Output

```
Accuracy
```

```
                       NBC          LDA          QDA          NSC
Train           (0.94, 0.0)   (1.0, 0.0)  (0.93, 0.0)  (0.85, 0.0)
Test            (0.82, 0.0)  (0.91, 0.0)  (0.79, 0.0)  (0.79, 0.0)
Overfit degree          125         88.2        142.9           69
```

Output

```
TPR
```

```
                       NBC          LDA          QDA          NSC
Train           (0.97, 0.0)   (1.0, 0.0)  (0.91, 0.0)  (0.85, 0.0)
Test            (0.94, 0.0)  (0.83, 0.0)  (0.94, 0.0)  (0.72, 0.0)
Overfit degree         26.9        166.7         35.8        153.3
```

Output

```
TNR
```

```
                       NBC         LDA          QDA          NSC
Train           (0.91, 0.0)  (1.0, 0.0)  (0.94, 0.0)  (0.85, 0.0)
Test            (0.69, 0.0)  (1.0, 0.0)  (0.62, 0.0)  (0.88, 0.0)
Overfit degree          246           0        335.9         25.9
```

Output

```
Execution data
```

```
                                       Execution Data
Number of samples                                 102
Number of features                              12625
```

```
Features reduction                          63
Params GaussianNB                            2
Params LinearDiscriminantAnalysis            6
Params QuadraticDiscriminantAnalysis         5
Params NearestCentroid                       2
```

Output

1.4 Conclusions

Executions

We have two executions in breast, one without PCA and another with PCA (99 percent variance retained), and three in prostate, without PCA, with PCA 99 percent variance retention and PCA 80 percent variance. There is a parameter that indicates the level of possible overfit. The more his value, less robust to overfiting is the learning method, thus more flexible as more closed to the training data.

We have defined this *overfiting indicator* as the ratio of the difference of accuracies between train and test as numerator, and as denominator the test accuracy

The tables show the means of 20 executions for each of the four learning methods and close to them the standard deviations.

Breast

The best accuracy methods are *QDA* and *LDA*.

The reduction of dimensions is more effective in *QDA*.

According to the value of the overfit indicator, the most flexible methods are *LDA* and *QDA*, but when reducing the dimensions *NBC* goes to the first position

Prostate

We observe that *QDA* performs very poorly, as expected given the high dimensionality of this dataset (more than 12625) and the relatively low number of samples (around 100), which do not ease the accurate computation of the covariance matrices.

This affects all methods, the best ones being *NSC* and *LDA*.

The overfit of *QDA* is huge, and another order of magnitude is also relevant for *NBC*.

We also note that the accuracy of *QDA* varies greatly with the sample (high standard deviation), so we are already seeing that this method is not suitable for this dataset

Through dimensionality reduction by PCA, we have seen that we improve this results.

In fact *QDA* improves significantly and becomes reliable. In another order of magnitude *NBC* and *LDA* improve but not *NSC* because on its own way, it already reduces the complexity of the model.