Wine classification using Scikit-learn's Multi-layer Perceptron Classifier

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1 Importing modules

```
[1]: import pandas as pd
     import numpy as np
     import seaborn as sns
     import matplotlib.pyplot as plt
     plt.rcParams['figure.dpi'] = 200

     from sklearn.preprocessing import StandardScaler, LabelEncoder, MinMaxScaler
     from sklearn.model_selection import train_test_split
     from sklearn.neural_network import MLPClassifier
     from sklearn.inspection import DecisionBoundaryDisplay
     from sklearn.metrics import confusion_matrix, classification_report
```

2 Import Data Frame

```
[2]: columnsWine = ["WineID", "Alcohol", "MalicAcid", "Ash", "AlcalinityOfAsh",␣
      ↪"Magnesium", "TotalPhenols",
                    "Flavanoids", "NonflavanoidPhenols","Proanthocyanins",␣
      ↪"ColorIntensity", "Hue", "OD280/OD315", "Proline"]

     df = pd.read_csv(r"C:\Users\Cristofer Becerra S\Documents\Tec de Monterrey\7mo␣
      ↪Semestre\Datasets\wine.data",
                      names = columnsWine)
```

```
[3]: df.head()
```

```
[3]:    WineID  Alcohol  MalicAcid   Ash  AlcalinityOfAsh  Magnesium  TotalPhenols  \
     0       1    14.23       1.71  2.43             15.6        127          2.80
     1       1    13.20       1.78  2.14             11.2        100          2.65
     2       1    13.16       2.36  2.67             18.6        101          2.80
     3       1    14.37       1.95  2.50             16.8        113          3.85
     4       1    13.24       2.59  2.87             21.0        118          2.80

        Flavanoids  NonflavanoidPhenols  Proanthocyanins  ColorIntensity   Hue  \
0         3.06                    0.28               2.29              5.64  1.04
1         2.76                    0.26               1.28              4.38  1.05
2         3.24                    0.30               2.81              5.68  1.03
3         3.49                    0.24               2.18              7.80  0.86
4         2.69                    0.39               1.82              4.32  1.04

   OD280/OD315  Proline
0         3.92     1065
1         3.40     1050
2         3.17     1185
3         3.45     1480
4         2.93      735
```

3 Preprocessing data for the Neural Network

We wish to standardize the input of the neural network to align with the Multi-layer Perceptron Classifier's output. We apply a Min-Max scaling to our feature data and a Label Encoder to our wine categories.

[4]:
```
le = LabelEncoder()
# scaler = StandardScaler()
minmax = MinMaxScaler()
```

[5]:
```
x = minmax.fit_transform(df.drop(columns = "WineID"))
y = le.fit_transform(df.WineID)
```

4 Train-validate-test split

We divide the dataset into 3 subsets: **train** (56%), **validate** (24%), and **test** (20%). We will also work with the same random state (0) for all Sklearn's functions for reproducibility.

[6]:
```
rs, rsData = 0, 0
x1, x_test, y1, y_test = train_test_split(x, y, train_size = 0.8, random_state␣
  ↪= rsData)
x_train, x_validate, y_train, y_validate = train_test_split(x1, y1, train_size␣
  ↪= 0.7, random_state = rsData)
```

5 Neural Network Comparison

We will compare the performance of two neural networks with a fixed set of epochs (50). The goal is to obtain the best score without overfitting witht the given restraint (epochs).

[7]:
```
epochs = 50
```

5.1 Simple NN

First we build a simple neural network. Let a simple neural network have 1 hidden layer with 2 neurons, optimized by *optimized* Stochastic Gradient Descent (Adaptive Moment Estimation, Adam) using a ReLu activation function, an adaptive learning rate starting at 0.01.

[8]:
```
simpleNN = MLPClassifier(random_state = rs, hidden_layer_sizes = (2,),␣
 ↪learning_rate = "adaptive",
                                learning_rate_init = 0.01, max_iter = epochs)
```

We can train and overview its performance by a simple mean accuracy score for both training and test datasets.

[9]:
```
simpleNN.fit(x_train, y_train)
print("Training score: ", round(simpleNN.score(x_train, y_train), 4))
print("Validate score: ", round(simpleNN.score(x_validate, y_validate), 4))
print("Test score: ", round(simpleNN.score(x_test, y_test), 4))
```

```
Training score:  0.7778
Validate score:  0.814
Test score:  0.8056
```

```
C:\Users\Cristofer Becerra S\pyproject\Jupyter\lib\site-
packages\sklearn\neural_network\_multilayer_perceptron.py:702:
ConvergenceWarning: Stochastic Optimizer: Maximum iterations (50) reached and
the optimization hasn't converged yet.
  warnings.warn(
```

It appears that the optimization does not converge with the iterations constraint, but it yields decent results without overfitting. Given more iterations the loss function will indeed minimize and yield better scores, and hopefully it doesn't fall into overfitting territory.

[10]:
```
del simpleNN
```

5.2 Optimized NN

Now, we can perform a *rudimentary* optimization of the parameters of the network. This can be done using Scikit-learn's GridSearch algorithm for exhaustive search of the best model using different combinations passed to it.

5.2.1 Simple Grid Search Optimization

[11]:
```
from sklearn.model_selection import GridSearchCV
```

Since Adam is an optimizer of the simple SGD, we can reduce the combinations by only employing this version of SGD. Also, given the functionality of Scikit-learn and the fact that adaptive learning rate is more practical than constant (generally yielding better results for rudimentary implementations such as this one), we will also reduce the parameters by only using adaptive learning rates. We will focus the grid search on the structure of the layers, the learning rate and the regularization parameter.

```
[12]: hyperparameters = {'activation': ['relu'],
                         'hidden_layer_sizes': [(2,), (4,), (8,), (16,), (64,),
                                                (2,2,), (4,2), (2,4), (8,2), (2,8),␣
       ↪(8,4), (4,8),
                                               (2,2,2), (4,2,2), (2,4,2), (4,2,4),␣
       ↪(4,8,2), (4,8,4), (8,8,8)],
                         'alpha': [0.0001, 0.0005, 0.001, 0.01],
                         'learning_rate_init': [0.001, 0.01, 0.1],
                         'learning_rate': ['adaptive'],
                         'solver': ['adam']}
```

DANGER: this is an intensive CPU cell. Do not run this cell if your computer isn't very capable or if you're running it in Google Colab (it'll truly take forever). You've been warned.

```
[13]: nn = MLPClassifier(random_state = rs, max_iter = epochs)

      hps = GridSearchCV(nn, hyperparameters, n_jobs = -1, cv = 5) # hyper-parameter␣
       ↪search

      hps.fit(x_train, y_train);

      bestH = hps.best_params_

      SearchResults = pd.DataFrame(hps.cv_results_)
      SearchResults = SearchResults.sort_values("rank_test_score", ascending = True)
      SearchResults.head()
```

```
[13]:      mean_fit_time  std_fit_time  mean_score_time  std_score_time  \
      170       0.187684      0.034293         0.001395        0.001857
      113       0.115902      0.008395         0.001432        0.001070
      65        0.061001      0.002577         0.001225        0.001631
      68        0.062889      0.005991         0.000942        0.001162
      70        0.076852      0.004012         0.002548        0.002399

          param_activation param_alpha param_hidden_layer_sizes param_learning_rate  \
      170             relu       0.001                (8, 8, 8)            adaptive
      113             relu      0.0005                (8, 8, 8)            adaptive
      65              relu      0.0005                     (8,)            adaptive
      68              relu      0.0005                    (16,)            adaptive
      70              relu      0.0005                    (64,)            adaptive

          param_learning_rate_init param_solver  \
      170                      0.1         adam
      113                      0.1         adam
      65                       0.1         adam
      68                       0.1         adam
      70                      0.01         adam
```

```
                                                params  split0_test_score  \
170  {'activation': 'relu', 'alpha': 0.001, 'hidden…               0.95
113  {'activation': 'relu', 'alpha': 0.0005, 'hidde…               0.95
65   {'activation': 'relu', 'alpha': 0.0005, 'hidde…               0.95
68   {'activation': 'relu', 'alpha': 0.0005, 'hidde…               0.95
70   {'activation': 'relu', 'alpha': 0.0005, 'hidde…               0.95

     split1_test_score  split2_test_score  split3_test_score  \
170                1.0               1.00               0.95
113                1.0               1.00               0.90
65                 1.0               0.95               0.95
68                 1.0               0.95               0.95
70                 1.0               0.95               0.95

     split4_test_score  mean_test_score  std_test_score  rank_test_score
170                1.0             0.98        0.024495                1
113                1.0             0.97        0.040000                2
65                 1.0             0.97        0.024495                2
68                 1.0             0.97        0.024495                2
70                 1.0             0.97        0.024495                2
```

5.3 Performance Comparison

Once we have obtained our "optimized" parameters, we proceed to define them in order to compare their performance.

[14]:
```
simpleNN = MLPClassifier(random_state = rs, hidden_layer_sizes = (2,),␣
 ↪learning_rate = "adaptive",
                         learning_rate_init = 0.01, max_iter = epochs)

# Best model so far - 1.0 train, validate, test; convergence in 110 iterations
# optimizedNN = MLPClassifier(random_state = rs, hidden_layer_sizes = (8,8,16),␣
 ↪learning_rate = "adaptive",
#                              alpha = 0.01, learning_rate_init = 0.01, max_iter␣
 ↪= 110)

optimizedNN = MLPClassifier(random_state = rs, hidden_layer_sizes = (8,8,8),␣
 ↪learning_rate = "adaptive",
                            alpha = 0.001, learning_rate_init = 0.01, max_iter␣
 ↪= epochs)
```

We run a partial fit with the set number of epochs and storing their respective scores each iteration.

[15]:
```
simpleTrainScore, simpleValidateScore, optimizedTrainScore,␣
 ↪optimizedValidateScore = [], [], [], []
simpleTestScore, optimizedTestScore = [], []
```

```
for i in range(0, epochs):

    simpleNN.partial_fit(x_train, y_train, np.unique(y_train))

    simpleTrainScore.append(simpleNN.score(x_train, y_train))
    simpleValidateScore.append(simpleNN.score(x_validate, y_validate))
    simpleTestScore.append(simpleNN.score(x_test, y_test))

    optimizedNN.partial_fit(x_train, y_train, np.unique(y_train))

    optimizedTrainScore.append(optimizedNN.score(x_train, y_train))
    optimizedValidateScore.append(optimizedNN.score(x_validate, y_validate))
    optimizedTestScore.append(optimizedNN.score(x_test, y_test))
```

Peeking into the overall performance of our “optimized” NN:

[16]:
```
print("Training score: ", optimizedNN.score(x_train, y_train))
print("Validate score: ", optimizedNN.score(x_validate, y_validate))
print("Testing score: ", optimizedNN.score(x_test, y_test))
```

```
Training score:  0.98989898989899
Validate score:  1.0
Testing score:  1.0
```

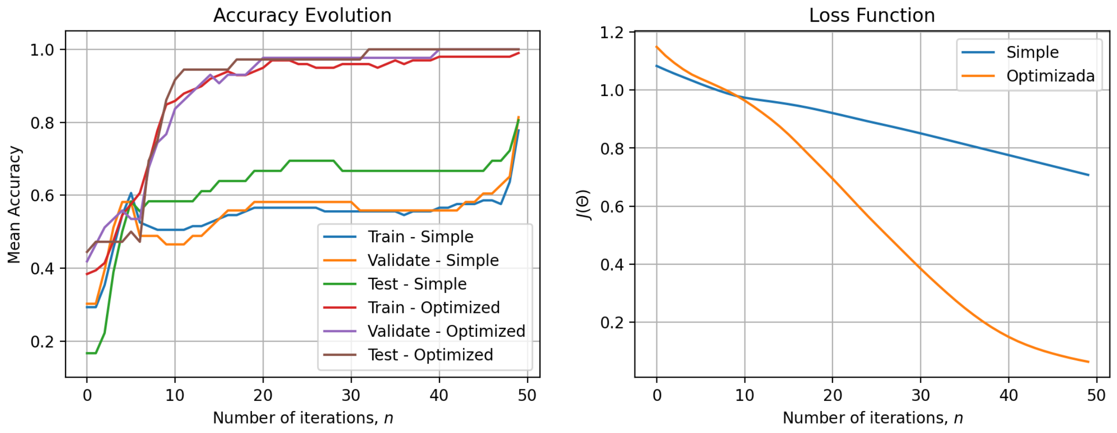
We can see that the NN performs extremely well in comparison with the simple NN, and is also not in overfitting territory; on the contrary, the NN performs better in the validate and test sets.

5.4 Accuracy & Loss

Plotting the evolution of the accuracy on all sets and the loss function

[17]:
```
fig, axes = plt.subplots(1,2, figsize = (12,4))

axes[0].plot(simpleTrainScore, label = "Train - Simple ")
axes[0].plot(simpleValidateScore, label = "Validate - Simple")
axes[0].plot(simpleTestScore, label = "Test - Simple")

axes[0].plot(optimizedTrainScore, label = "Train - Optimized ")
axes[0].plot(optimizedValidateScore, label = "Validate - Optimized")
axes[0].plot(optimizedTestScore, label = "Test - Optimized")

axes[0].set_title("Accuracy Evolution")
axes[0].set_xlabel(r"Number of iterations, $n$")
axes[0].set_ylabel("Mean Accuracy")
axes[0].set_ylim([0.1, 1.05])
#axes[0].set_xlim([20, 80])
axes[0].grid(True)
axes[0].legend()
```

```
axes[1].plot(simpleNN.loss_curve_, label = "Simple")
axes[1].plot(optimizedNN.loss_curve_, label = "Optimizada")
axes[1].set_title("Loss Function")
axes[1].set_xlabel(r"Number of iterations, $n$")
axes[1].set_ylabel(r"$J(\Theta)$")
axes[1].legend()
axes[1].grid(True)

plt.show()
```



5.5 Classification Metrics

We can also inspect the metrics of classification with a prediction on the subsets:

5.5.1 Train

[18]:
```
print(classification_report(y_train, optimizedNN.predict(x_train),␣
↪target_names=["Wine A", "Wine B", "Wine C"]))
```

```
              precision    recall  f1-score   support

      Wine A       1.00      0.97      0.98        33
      Wine B       0.97      1.00      0.99        37
      Wine C       1.00      1.00      1.00        29

    accuracy                           0.99        99
   macro avg       0.99      0.99      0.99        99
weighted avg       0.99      0.99      0.99        99
```

5.5.2 Validate

[19]:
```
print(classification_report(y_validate, optimizedNN.predict(x_validate),␣
  ↪target_names=["Wine A", "Wine B", "Wine C"]))
```

```
              precision    recall  f1-score   support

      Wine A       1.00      1.00      1.00        12
      Wine B       1.00      1.00      1.00        18
      Wine C       1.00      1.00      1.00        13

    accuracy                           1.00        43
   macro avg       1.00      1.00      1.00        43
weighted avg       1.00      1.00      1.00        43
```

5.5.3 Test

[20]:
```
print(classification_report(y_test, optimizedNN.predict(x_test),␣
  ↪target_names=["Wine A", "Wine B", "Wine C"]))
```

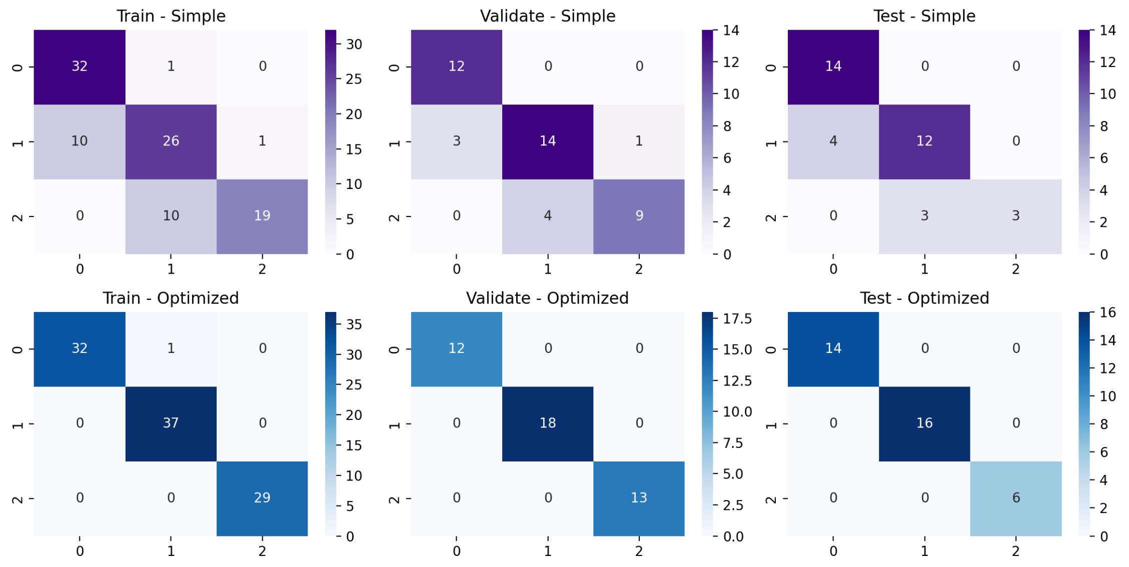
```
              precision    recall  f1-score   support

      Wine A       1.00      1.00      1.00        14
      Wine B       1.00      1.00      1.00        16
      Wine C       1.00      1.00      1.00         6

    accuracy                           1.00        36
   macro avg       1.00      1.00      1.00        36
weighted avg       1.00      1.00      1.00        36
```

5.6 Confusion Matrices

Plotting the confusion matrices for both neural networks in the 3 subsets

[21]:
```
fig, axes = plt.subplots(2, 3, figsize = (12, 6))

sns.heatmap(confusion_matrix(y_train, simpleNN.predict(x_train)), annot = True,␣
  ↪cmap = "Purples", ax = axes[0,0])
axes[0,0].set_title("Train - Simple")

sns.heatmap(confusion_matrix(y_validate, simpleNN.predict(x_validate)), annot =␣
  ↪True, cmap = "Purples", ax = axes[0,1])
axes[0,1].set_title("Validate - Simple")

sns.heatmap(confusion_matrix(y_test, simpleNN.predict(x_test)), annot = True,␣
  ↪cmap = "Purples", ax = axes[0,2])
axes[0,2].set_title("Test - Simple")
```

```
sns.heatmap(confusion_matrix(y_train, optimizedNN.predict(x_train)), annot =␣
↪True, cmap = "Blues", ax = axes[1,0])
axes[1,0].set_title("Train - Optimized")

sns.heatmap(confusion_matrix(y_validate, optimizedNN.predict(x_validate)),␣
↪annot = True, cmap = "Blues", ax = axes[1,1])
axes[1,1].set_title("Validate - Optimized")

sns.heatmap(confusion_matrix(y_test, optimizedNN.predict(x_test)), annot =␣
↪True, cmap = "Blues", ax = axes[1,2])
axes[1,2].set_title("Test - Optimized")

plt.tight_layout()
plt.show()
```



Train - Simple	0	1	2
0	32	1	0
1	10	26	1
2	0	10	19

Validate - Simple	0	1	2
0	12	0	0
1	3	14	1
2	0	4	9

Test - Simple	0	1	2
0	14	0	0
1	4	12	0
2	0	3	3

Train - Optimized	0	1	2
0	32	1	0
1	0	37	0
2	0	0	29

Validate - Optimized	0	1	2
0	12	0	0
1	0	18	0
2	0	0	13

Test - Optimized	0	1	2
0	14	0	0
1	0	16	0
2	0	0	6

5.7 Performance as a function of Train-Test split

We can inspect the beahavior of our "optimized" NN as a train-test split changes proportions.

```
[ ]: train_score, test_score = [], []

PS = np.linspace(0.01, 0.99, epochs)

for ps in PS:

    x1, x_test, y1, y_test = train_test_split(x, y, train_size = ps,␣
↪random_state = rsData)
```

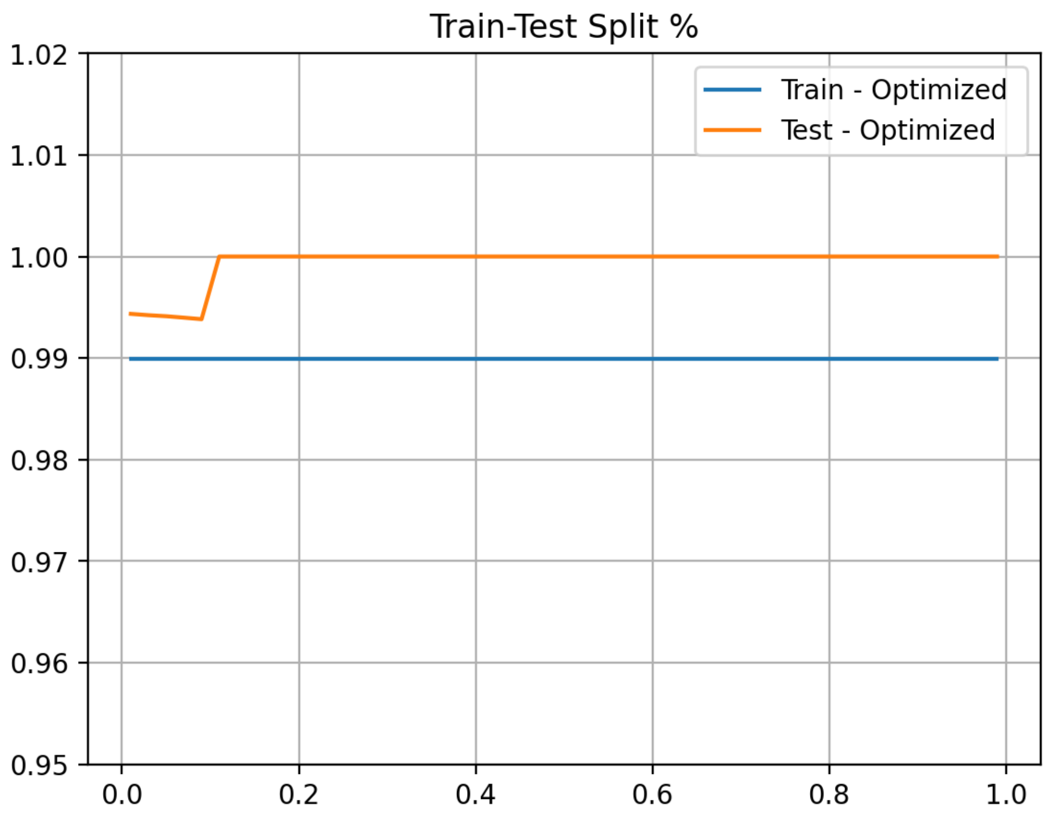
```
    optimizedNN.fit(x_train, y_train);

    train_score.append(optimizedNN.score(x_train, y_train))
    test_score.append(optimizedNN.score(x_test, y_test))
```

[23]:
```
print("Training score: ", np.array(train_score).mean())
print("Testing score: ", np.array(test_score).mean())
```

```
Training score:  0.98989898989899
Testing score:  0.9994098129366435
```

The mean score for both subsets suggests that the NN is very stable with different proportions of training and testing data. We can plot this variation as a function of the split percentage.

[24]:
```
plt.plot(PS, train_score, label = "Train - Optimized ")
plt.plot(PS, test_score, label = "Test - Optimized")
plt.title("Train-Test Split %")
plt.ylim([0.95, 1.02])
plt.grid(True)
plt.legend()
plt.show()
```



5.8 Performance as a function of Random State

Another important factor that can impact performance is the random state of the data split. We can test this in a similar fashion as the last evolution (train-test split)

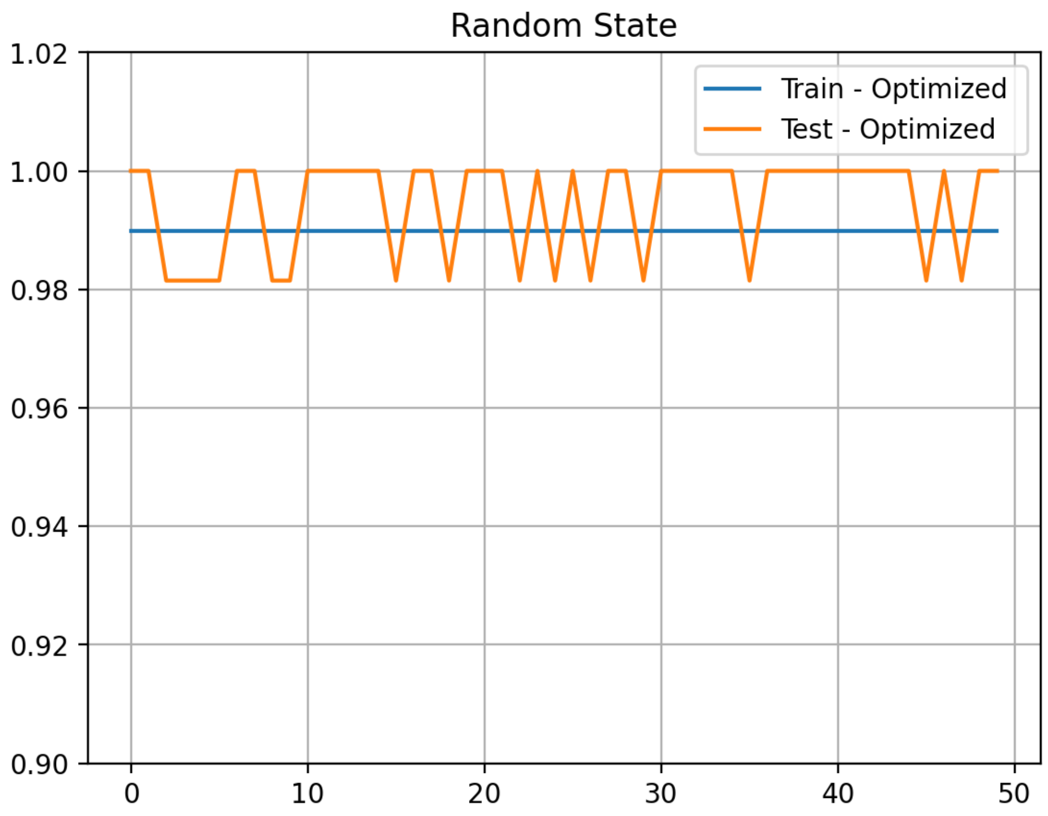
```
[ ]: train_score_rs, test_score_rs = [], []

     for i in range(epochs):

         x1, x_test, y1, y_test = train_test_split(x, y, train_size = 0.7,␣
      ↪random_state = i)

         optimizedNN.fit(x_train, y_train);

         train_score_rs.append(optimizedNN.score(x_train, y_train))
         test_score_rs.append(optimizedNN.score(x_test, y_test))
```

```
[26]: print("Training score: ", np.array(train_score_rs).mean())
      print("Testing score: ", np.array(test_score_rs).mean())
```

```
Training score:  0.98989898989899
Testing score:  0.9944444444444442
```

Once again, the NN performs extremely well in a very stable manner. We can also plot the evolution

```
[27]: plt.plot(train_score_rs, label = "Train - Optimized ")
      plt.plot(test_score_rs, label = "Test - Optimized")
      plt.title("Random State")
      plt.ylim([0.9, 1.02])
      plt.grid(True)
      plt.legend()
      plt.show()
```



In this case we can see that testing performance oscillates between 0.98 and 1. This indicates that our NN is sensible to overfitting with different random samples of the data. This makes sense since the optimization with grid search was performed with a fixed random state of data.

6 Model Predictions

Finally, we can make specific predictions with our model. We extract the first five observations of the test dataset and make a Pandas DataFrame for visualization purposes.

[28]:
```
x_predictions = pd.DataFrame(x_test[0:5], columns = columnsWine[1:])
x_predictions.head()
```

[28]:
```
    Alcohol  MalicAcid       Ash  AlcalinityOfAsh  Magnesium  TotalPhenols  \
0  0.531579   0.616601  0.513369         0.613402   0.163043      0.231034
1  0.365789   0.357708  0.486631         0.587629   0.217391      0.241379
2  0.500000   0.604743  0.689840         0.412371   0.347826      0.493103
3  0.160526   0.260870  0.588235         0.567010   0.152174      0.334483
4  0.444737   0.199605  0.491979         0.613402   0.152174      0.137931

   Flavanoids  NonflavanoidPhenols  Proanthocyanins  ColorIntensity       Hue  \
0    0.263713             0.905660         0.381703        0.300341  0.292683
```

```
1    0.316456                 1.000000          0.318612          0.121160   0.308943
2    0.436709                 0.226415          0.495268          0.274744   0.447154
3    0.284810                 0.660377          0.296530          0.129693   0.422764
4    0.299578                 0.660377          0.384858          0.172355   0.325203

   OD280/OD315   Proline
0     0.271062  0.169044
1     0.743590  0.026391
2     0.824176  0.350927
3     0.542125  0.286733
4     0.421245  0.149786
```

Then we can create another Data Frame to store the real category of wine, and then add the column of the predictions yielded by our optimized neural network.

```
[29]: y_prediction = pd.DataFrame(y_test[0:5], columns = ["Real"])
      y_prediction["Prediction"] = optimizedNN.predict(x_test[0:5])
      y_prediction
```

```
[29]:    Real  Prediction
      0     1           1
      1     1           1
      2     0           0
      3     1           1
      4     1           1
```

We get an expected result: our neural network aced the five predictions.