main

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Aufteilung: Import, Regression Models: Matr. Nr 9452857 Hyperparameter Tuning, Comments: Matr. Nr 1113800

Before doing anything installing all needed dependencies

[ ]:
```
!pip3 install -U pandas
!pip3 install -U scikit-learn
!pip3 install -U matplotlib
```

1 Aufgabe 1

[2]:
```
import os
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn import set_config
set_config(transform_output="pandas")
```

Import data

[3]:
```
white_raw = pd.read_csv(os.getcwd() + "/dataset/winequality-white.csv",␣
↪delimiter=";")
red_raw = pd.read_csv(os.getcwd() + "/dataset/winequality-red.csv", delimiter=";
↪")
```

Split wine in Test and Training Data (75% / 25%)

[4]:
```
red_raw
```

[4]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	\
0	7.4	0.700	0.00	1.9	0.076	
1	7.8	0.880	0.00	2.6	0.098	
2	7.8	0.760	0.04	2.3	0.092	
3	11.2	0.280	0.56	1.9	0.075	
4	7.4	0.700	0.00	1.9	0.076	
…	…	…	…	…	…	
1594	6.2	0.600	0.08	2.0	0.090	
1595	5.9	0.550	0.10	2.2	0.062	

```
1596            6.3             0.510         0.13             2.3      0.076
1597            5.9             0.645         0.12             2.0      0.075
1598            6.0             0.310         0.47             3.6      0.067

      free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
0                    11.0                  34.0  0.99780  3.51       0.56
1                    25.0                  67.0  0.99680  3.20       0.68
2                    15.0                  54.0  0.99700  3.26       0.65
3                    17.0                  60.0  0.99800  3.16       0.58
4                    11.0                  34.0  0.99780  3.51       0.56
…                     …                     …        …     …          …
1594                 32.0                  44.0  0.99490  3.45       0.58
1595                 39.0                  51.0  0.99512  3.52       0.76
1596                 29.0                  40.0  0.99574  3.42       0.75
1597                 32.0                  44.0  0.99547  3.57       0.71
1598                 18.0                  42.0  0.99549  3.39       0.66

      alcohol  quality
0         9.4        5
1         9.8        5
2         9.8        5
3         9.8        6
4         9.4        5
…         …          …
1594     10.5        5
1595     11.2        6
1596     11.0        6
1597     10.2        5
1598     11.0        6

[1599 rows x 12 columns]
```

[5]:
```
white_training_Data, white_test_data, white_training_scores, white_test_scores␣
↪= (train_test_split(white_raw.drop("quality", axis=1),␣
↪white_raw['quality'],test_size=0.25, random_state=39))

red_training_Data, red_test_data, red_training_scores, red_test_scores =␣
↪(train_test_split(red_raw.drop("quality", axis=1),␣
↪red_raw['quality'],test_size=0.25, random_state=39))
```

[6]:
```
white_training_Data
```

[6]:
```
      fixed acidity  volatile acidity  citric acid  residual sugar  chlorides  \
3965            7.3             0.380         0.23            6.50      0.050
3954            6.3             0.330         0.20           17.90      0.066
580             7.4             0.410         0.66           10.80      0.051
1637            8.1             0.120         0.49            1.20      0.042
```

```
1310            5.2             0.365         0.08           13.50      0.041
…             …               …             …              …          …
3195            7.0             0.210         0.42            5.30      0.037
2275            7.5             0.290         0.26           14.95      0.067
1088            7.4             0.200         0.37           16.95      0.048
105             7.3             0.130         0.32           14.40      0.051
3465            6.8             0.190         0.34            1.90      0.040

      free sulfur dioxide  total sulfur dioxide  density    pH  sulphates  \
3965                 18.0                 102.0  0.99304  3.10       0.55
3954                 36.0                 161.0  0.99910  3.14       0.51
580                  77.0                 194.0  0.99760  3.05       0.46
1637                 43.0                 160.0  0.99340  3.13       0.48
1310                 37.0                 142.0  0.99700  3.46       0.39
…                   …                    …      …   …        …
3195                 36.0                 123.0  0.99321  3.14       0.52
2275                 47.0                 178.0  0.99838  3.04       0.49
1088                 43.0                 190.0  0.99950  3.03       0.42
105                  34.0                 109.0  0.99740  3.20       0.35
3465                 41.0                 108.0  0.99000  3.25       0.45

      alcohol
3965     11.2
3954      8.8
580       8.7
1637      9.7
1310      9.9
…        …
3195     10.9
2275      9.2
1088      9.2
105       9.2
3465     12.9

[3673 rows x 11 columns]
```

2 Aufgabe 2

Performing a Principal Component Analysis

we need to standardize features with StandardScaler(). We do this to make sure that different features have the same impact on the result

[7]:
```
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()

white_training_Data_scaled = scaler.fit_transform(white_training_Data)
```

```
white_test_data_scaled = scaler.transform(white_test_data)

red_training_Data_scaled = scaler.fit_transform(red_training_Data)
red_test_data_scaled = scaler.transform (red_test_data)
```

[8]:
```
from sklearn.decomposition import PCA
```

[9]:
```
pcaWhite = PCA(n_components='mle')
white_training_Data_pca = pcaWhite.fit_transform(white_training_Data_scaled)
white_test_data_pca = pcaWhite.transform(white_test_data_scaled)
```

[10]:
```
pcaRed = PCA(n_components='mle')
red_training_Data_pca = pcaRed.fit_transform(red_training_Data)
red_test_data_pca = pcaRed.transform(red_test_data)
```

3 Aufgabe 3

[11]:
```
from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay


def plot_metrics(test_scores, test_predictions):
    cm = confusion_matrix(test_scores, test_predictions.round(), labels=[0,␣
 ↪1,2,3,4,5,6,7,8,9,10])
    cm_disp = ConfusionMatrixDisplay(cm)
    cm_disp.plot()
```

[12]:
```
import numpy as np
from math import sqrt

from sklearn.neighbors import KNeighborsRegressor
from sklearn.svm import SVR
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import mean_absolute_error, mean_squared_error
from sklearn.metrics import r2_score, mean_absolute_percentage_error


# Function to calculate model and print Bewertungsmetriken
def model_regressor_grid_calculator(estimator: any, param_grid: dict | list,
                                    training_data: any, valid_data: any,␣
 ↪training_scores: any, valid_scores: any):
    #select the best HyperParameters while using cross-validation for it (cv=3)
    random_search = GridSearchCV(estimator, param_grid=param_grid, cv=3,␣
 ↪n_jobs=-1, scoring='r2')
    random_search.fit(training_data, training_scores)

    print("Beste Hyperparameter: " + str(random_search.best_params_))
```

```
    # Select the best model from Grid Search
    optimal_model = random_search.best_estimator_

    # Selected Params
    cv_results = pd.DataFrame(random_search.cv_results_).loc[random_search.
↪best_index_]

    r2_score_cv = [cv_results['split0_test_score'],
                   cv_results['split1_test_score'],
                   cv_results['split2_test_score'],
                   ]
    r2_score_cv_mean = cv_results['mean_test_score']
    r2_score_cv_std = cv_results['std_test_score']

    print('Cross Validation')
    print(f'- R^2: {r2_score_cv}')
    print(f'- R^2 Durchschnittlicher: {r2_score_cv_mean:.4f}')
    print(f'- R^2 Standardabweichung: {r2_score_cv_std:.4f}')
    print('\r\n')


    predicted_test_scores = optimal_model.predict(valid_data)

    r2_score_test = r2_score(valid_scores, predicted_test_scores)
    rmse_test = sqrt(mean_squared_error(valid_scores, predicted_test_scores))
    mape_test = mean_absolute_percentage_error(valid_scores,␣
↪predicted_test_scores)

    print('Test:')
    print(f'- R^2: {r2_score_test:.4f}')
    print(f'- RMSE: {rmse_test:.2f}')
    print(f'- MAPE: {mape_test:.2%}')

    plot_metrics(valid_scores, predicted_test_scores)

    return cv_results, optimal_model
```

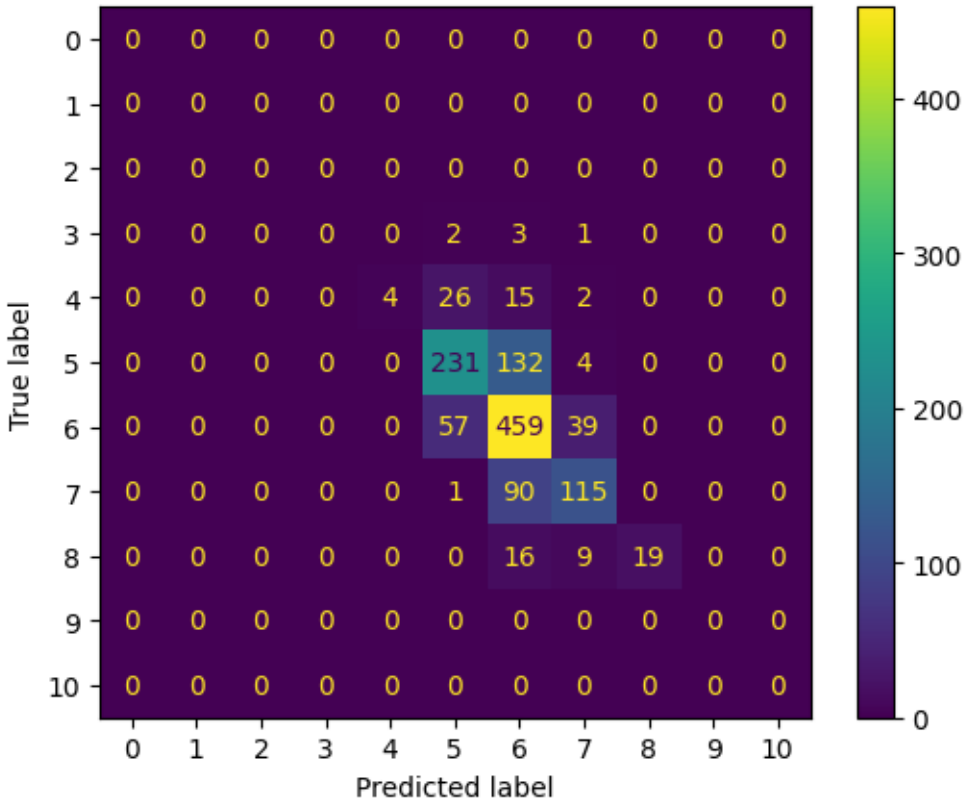
Implementing two Regression methods: Nearest Neighbor Regression and Support Vector Regression. Comparing the performance of both regression models at both datasets.

3.1 White

3.1.1 Nearest Neighbor Regression

[13]:
```
parameters = {
    'n_neighbors': np.arange(1, 70, 1),
    'leaf_size' : np.arange(1, 50, 1),
    'weights': ['uniform', 'distance']
}
final_parameters = {
    'n_neighbors': [23],
    'leaf_size' : [1],
    'weights': ['distance']
}
knn_regressor = KNeighborsRegressor()
cv_results, optimal_model =␣
 ↪model_regressor_grid_calculator(estimator=knn_regressor,␣
 ↪param_grid=final_parameters, training_data=white_training_Data_pca,␣
 ↪valid_data=white_test_data_pca, training_scores=white_training_scores,␣
 ↪valid_scores=white_test_scores)
```

```
Beste Hyperparameter: {'leaf_size': 1, 'n_neighbors': 23, 'weights': 'distance'}
Cross Validation
- R^2: [0.4439410001966234, 0.4578456890889915, 0.46936491337660613]
- R^2 Durchschnittlicher: 0.4571
- R^2 Standardabweichung: 0.0104


Test:
- R^2: 0.4862
- RMSE: 0.64
- MAPE: 7.66%
```



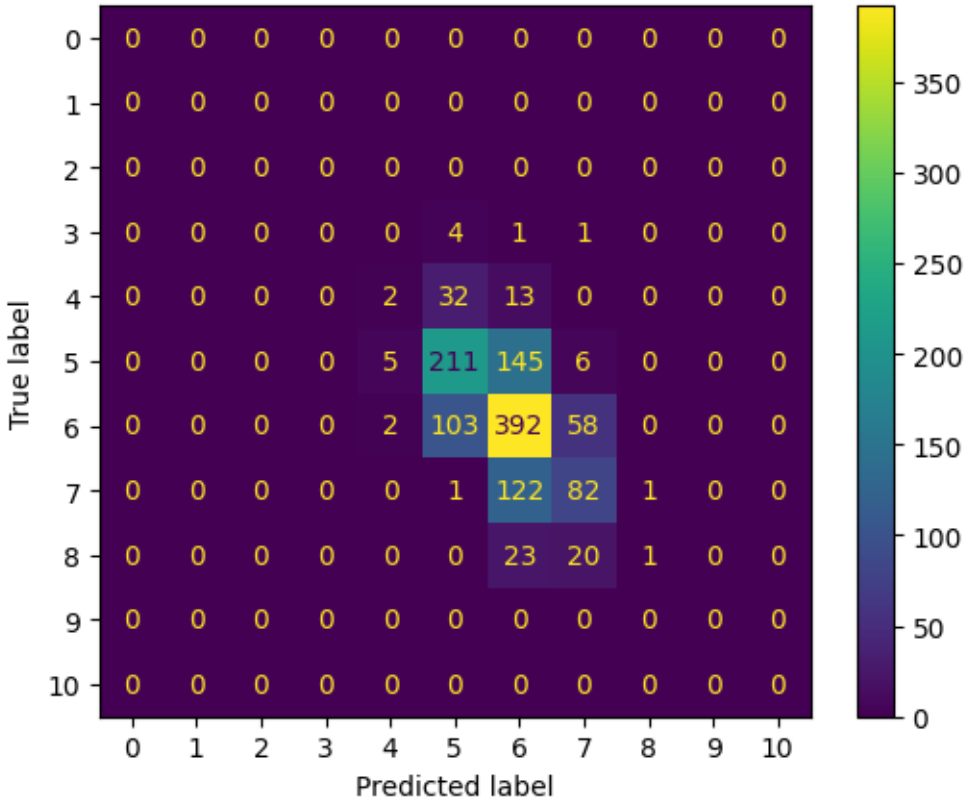
3.1.2 Support Vektor Regression

[14]:
```
parameters = {
    'kernel': ['rbf'],
    'epsilon': np.linspace(0.2, 0.4, 10),
    'C': np.linspace(1, 5, 20),
}
final_parameters = {'C': [1.631578947368421], 'epsilon': [0.3111111111111111],␣
 ↪'kernel': ['rbf']}

svm_regressor = SVR()
cv_results, optimal_model =␣
 ↪model_regressor_grid_calculator(estimator=svm_regressor,␣
 ↪param_grid=final_parameters, training_data=white_training_Data_pca,␣
 ↪valid_data=white_test_data_pca, training_scores=white_training_scores,␣
 ↪valid_scores=white_test_scores)
```

```
Beste Hyperparameter: {'C': 1.631578947368421, 'epsilon': 0.3111111111111111,
'kernel': 'rbf'}
Cross Validation
- R^2: [0.35387360216597596, 0.4023140411195696, 0.4207932174740727]
```

- R^2 Durchschnittlicher: 0.3923
- R^2 Standardabweichung: 0.0282

Test:
- R^2: 0.3616
- RMSE: 0.71
- MAPE: 9.86%



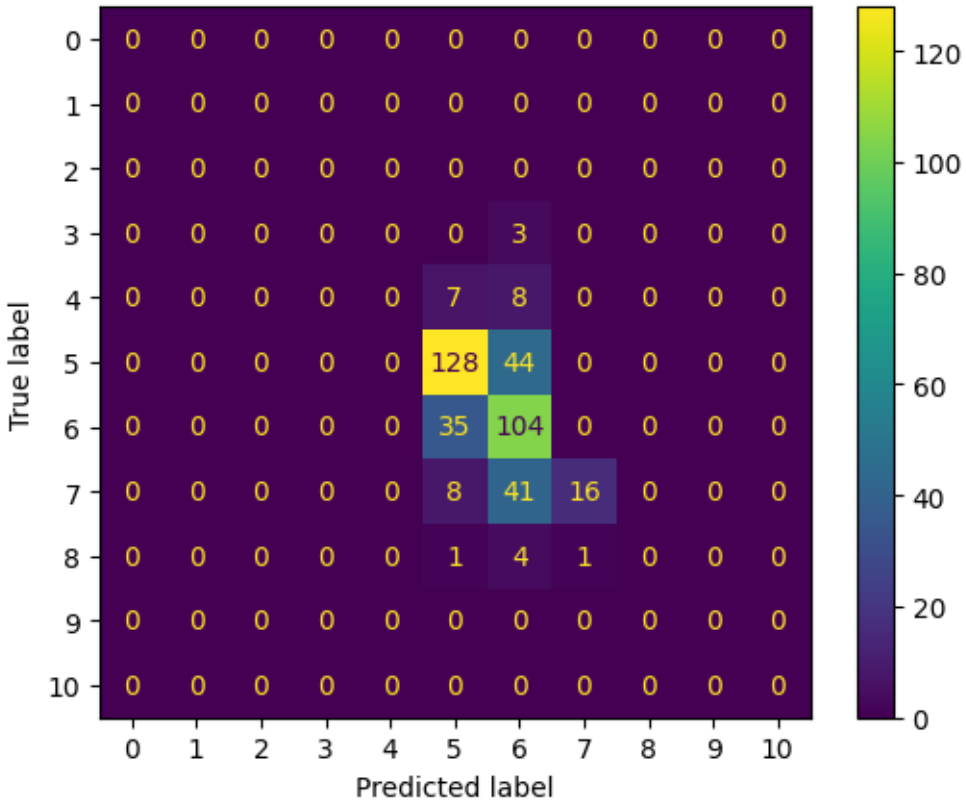
The Nearest Neighbor Regression analysis for white wine provided a R^2 value of 0,4862, where as the SVR analysis delivered a R^2 value of 0,3616. The decreased value indicates a weaker explanatory power compared to the Nearest Neighbor Regression. Also, the RMSE value rose from 0,64 at Nearest Neighbor Regression to 0,71 in the Support Vector Regression. Therefore, the value shows a higher deviation between the predicted and actual values. Furthermore, the MAPE value rose from 7,66% to 9,86%, indicating a higher percentage average deviation. In conclusion, the Nearest Neighbor Regression provides a better performance in comparison to the Support Vector Regression.

3.2 Red

3.2.1 Nearest Neighbor Regression

[15]:
```
parameters = {
    'n_neighbors': np.arange(1, 70, 1),
    'leaf_size' : np.arange(1, 50, 1),
    'weights': ['uniform', 'distance']
}
final_parameters = {
    'n_neighbors': [19],
    'leaf_size' : [1],
    'weights': ['distance']
}
knn_regressor = KNeighborsRegressor()
cv_results, optimal_model =␣
 ↪model_regressor_grid_calculator(estimator=knn_regressor,␣
 ↪param_grid=final_parameters, training_data=red_training_Data_pca,␣
 ↪valid_data=red_test_data_pca, training_scores=red_training_scores,␣
 ↪valid_scores=red_test_scores)
```

```
Beste Hyperparameter: {'leaf_size': 1, 'n_neighbors': 19, 'weights': 'distance'}
Cross Validation
- R^2: [0.2569778231764722, 0.28101540049050555, 0.21336805786223734]
- R^2 Durchschnittlicher: 0.2505
- R^2 Standardabweichung: 0.0280


Test:
- R^2: 0.2810
- RMSE: 0.74
- MAPE: 9.36%
```

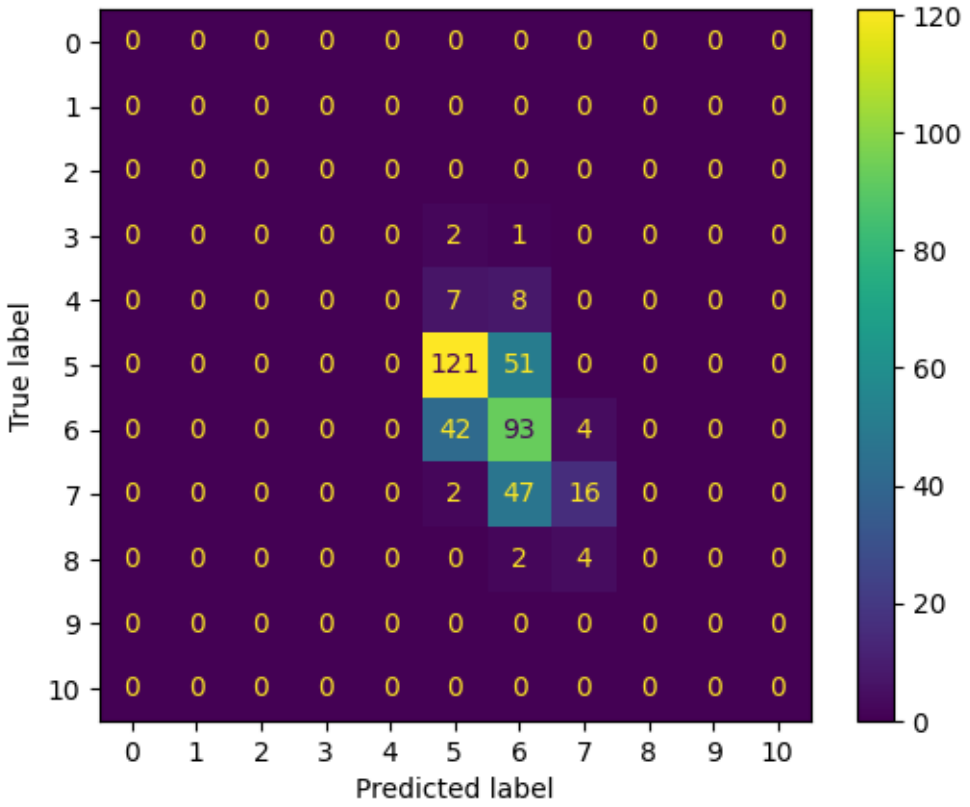


3.2.2 Support Vektor Regression

[16]:
```
parameters = {
    'kernel': ['rbf'],
    #'gamma' : ['scale', 'auto'],
    'epsilon': np.arange(0.1, 0.30, 0.01),
    'C': np.linspace(60, 70, 10),
}

final_parameters = {'C': [67.77777777777777], 'epsilon': [0.2899999999999999],␣
 ↪'kernel': ['rbf']}

svm_regressor = SVR()
cv_results, optimal_model =␣
 ↪model_regressor_grid_calculator(estimator=svm_regressor,␣
 ↪param_grid=final_parameters, training_data=red_training_Data_pca,␣
 ↪valid_data=red_test_data_pca, training_scores=red_training_scores,␣
 ↪valid_scores=red_test_scores)
```

```
Beste Hyperparameter: {'C': 67.77777777777777, 'epsilon': 0.2899999999999999,
'kernel': 'rbf'}
```

```
Cross Validation
- R^2: [0.29053634264358497, 0.3103429817566672, 0.2715251995718748]
- R^2 Durchschnittlicher: 0.2908
- R^2 Standardabweichung: 0.0158


Test:
- R^2: 0.3914
- RMSE: 0.68
- MAPE: 9.77%
```



For the red wine, the Support Vector Regression outperforms the Nearest Neighbor-Regression. The higher R^2 value (0,3914 vs 0,2810) indicates that the model explains a larger proportion of variance in the dataset. The other metrics also achieve better results, like a slightly higher MAPE value.

3.3 Conclusion

The Nearest Neighbor Regression based on the dataset for the white wine outperforms both its counterparts for the red wine, by relying on a larger dataset (~3 times larger). Despite that, the Support Vector Regression model for red wine outperforms the white wine SVR with its R^2 and MAPE, which indicates a better fit to the red wine dataset.

In conclusion, the Nearest Neighbor Regression model seems to perform better for white wine, while the Support Vector Regression model seems to deliver better results for the red wine.