





# Dados e Aprendizagem Automática

Support Vector Machine:

Hyperparameter Tuning with GridSearchCV

DAA @ MEI-1º/MiEI-4º — 1º Semestre Bruno Fernandes, César Analide, Dalila Alves, Filipa Ferraz, Victor Alves

### Contents

2

- Support Vector Machine
- Hyperparameter Tuning with GridSearchCV
- Hands On

#### Exercise:

- Problem: Development of a Machine Learning Model able to classify if a patient has breast cancer
- Classification Approach: Support Vector Machine approach to solve this problem
- Dataset: table with information regarding the patient ID, diagnosis and real-valued features computed for each cell nucleus, including:
  - Radius (mean of distances from center to points on the perimeter)
  - Texture (standard deviation of gray-scale values)
  - Perimeter
  - Area
  - Smoothness (local variation in radius lengths)
  - Compactness (perimeter^2 / area 1.0)
  - Concavity (severity of concave portions of the contour)
  - Concave points (number of concave portions of the contour)
  - Symmetry
  - Fractal dimension ("coastline approximation" 1)

5

#### **Import libraries**

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline
```

#### Get the data

We'll use the built in breast cancer dataset from Scikit Learn. We can get with the *load* function:

```
from sklearn.datasets import load_breast_cancer

cancer = load_breast_cancer()
```

The data set is presented in the form of a dictionary:

```
cancer.keys()
dict_keys(['data', 'target', 'frame', 'target_names', 'DESCR', 'feature_names', 'filename', 'data_module'])
```

We can obtain information and arrays from this dictionary to set up our data frame and understand the features:

```
cancer['feature names']
array(['mean radius', 'mean texture', 'mean perimeter', 'mean area',
       'mean smoothness', 'mean compactness', 'mean concavity',
       'mean concave points', 'mean symmetry', 'mean fractal dimension',
       'radius error', 'texture error', 'perimeter error', 'area error',
       'smoothness error', 'compactness error', 'concavity error',
       'concave points error', 'symmetry error',
       'fractal dimension error', 'worst radius', 'worst texture',
       'worst perimeter', 'worst area', 'worst smoothness',
       'worst compactness', 'worst concavity', 'worst concave points',
       'worst symmetry', 'worst fractal dimension'], dtype='<U23')
print(cancer['DESCR'])
.. _breast_cancer_dataset:
Breast cancer wisconsin (diagnostic) dataset
**Data Set Characteristics:**
    :Number of Instances: 569
    :Number of Attributes: 30 numeric, predictive attributes and the class
    :Attribute Information:
        - radius (mean of distances from center to points on the perimeter)
        - texture (standard deviation of gray-scale values)
```

•••

#### Set up the dataframe

```
df_feat = pd.DataFrame(cancer['data'],columns=cancer['feature_names'])
df_feat.info()
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 569 entries, 0 to 568
Data columns (total 30 columns):
                              Non-Null Count Dtype
     Column
                              569 non-null
     mean radius
                                              float64
     mean texture
                              569 non-null
                                              float64
     mean perimeter
                              569 non-null
                                              float64
 3
                              569 non-null
                                              float64
     mean area
     mean smoothness
                              569 non-null
                                              float64
                              569 non-null
                                              float64
     mean compactness
                              569 non-null
                                              float64
     mean concavity
     mean concave points
                              569 non-null
                                              float64
     mean symmetry
                              569 non-null
                                              float64
     mean fractal dimension
                              569 non-null
                                              float64
     radius error
                              569 non-null
                                              float64
                                              float64
     texture error
                              569 non-null
                                              float64
     perimeter error
                              569 non-null
     area error
                              569 non-null
                                              float64
     smoothness error
                              569 non-null
                                              float64
     compactness error
                              569 non-null
                                              float64
     concavity error
                              569 non-null
                                              float64
     concave points error
                              569 non-null
                                              float64
     symmetry error
                              569 non-null
                                              float64
     fractal dimension error 569 non-null
                                              float64
     rco --- -..11
                                              £1 - - ± C A
```

```
cancer['target']
0, 0, 1, 0, 1, 1, 1, 1, 1, 0, 0, 1, 0, 0, 1, 1, 1, 1, 0, 1, 0, 0,
     1, 1, 1, 1, 0, 1, 0, 0, 1, 0, 1, 0, 0, 1, 1, 1, 0, 0, 1, 0, 0, 0,
     1, 1, 1, 0, 1, 1, 0, 0, 1, 1, 1, 0, 0, 1, 1, 1, 1, 0, 1, 1, 0, 1,
     1, 1, 1, 1, 1, 1, 0, 0, 0, 1, 0, 0, 1, 1, 1, 0, 0, 1, 0, 1, 0,
      0, 1, 0, 0, 1, 1, 0, 1, 1, 0, 1, 1, 1, 1, 0, 1, 1, 1, 1, 1, 1, 1, 1,
     1, 1, 0, 1, 1, 1, 1, 0, 0, 1, 0, 1, 1, 0, 0, 1, 1, 0, 0, 1, 1, 1,
     1, 0, 1, 1, 0, 0, 0, 1, 0, 1, 0, 1, 1, 1, 0, 1, 1, 0, 0, 1, 0, 0,
     0, 0, 1, 0, 0, 0, 1, 0, 1, 0, 1, 1, 0, 1, 0, 0, 0, 0, 1, 1, 0, 0,
     1, 1, 1, 0, 1, 1, 1, 1, 1, 0, 0, 1, 1, 0, 1, 1, 0, 0, 1, 0, 1, 1,
     1, 1, 0, 1, 1, 1, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
     0, 0, 1, 1, 1, 1, 1, 1, 0, 1, 0, 1, 1, 0, 1, 1, 0, 1, 0, 0, 1, 1,
     1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 1, 1, 0, 1, 0, 1, 1, 1, 1, 1,
     1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 1, 1, 0, 1, 0, 1, 1, 1, 1, 0, 0,
      0, 1, 1, 1, 1, 0, 1, 0, 1, 0, 1, 1, 1, 0, 1, 1, 1, 1, 1, 1, 1, 0,
     0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 0, 1, 0, 0, 0, 1, 0, 0,
     1, 1, 1, 1, 1, 0, 1, 1, 1, 1, 1, 0, 1, 1, 0, 1, 1, 0, 0, 1, 1,
      1, 1, 1, 1, 0, 1, 1, 1, 1, 1, 1, 0, 1, 1, 1, 1, 1, 0, 1, 1, 0,
     1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 1, 0, 0, 1, 0, 1, 1, 1, 1,
     1, 0, 1, 1, 0, 1, 0, 1, 1, 0, 1, 0, 1, 1, 1, 1, 1, 1, 1, 1, 0, 0,
     1, 1, 1, 1, 1, 1, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 1, 1, 1, 1,
     1, 1, 1, 0, 1, 0, 1, 1, 0, 1, 1, 1, 1, 1, 0, 0, 1, 0, 1, 0, 1, 1,
     1, 1, 1, 0, 1, 1, 0, 1, 0, 1, 0, 0, 1, 1, 1, 0, 1, 1, 1, 1, 1, 1,
     1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 1])
```

```
df_target = pd.DataFrame(cancer['target'],columns=['Cancer'])

Now let's check the dataframe:

df_target.head()

Cancer
0      0
1      0
2      0
3      0
4      0
```

### **Exploratory Data Analysis**

#### Train Test Split

```
from sklearn.model selection import train test_split
X_train, X_test, y_train, y_test = train_test_split(df_feat, np.ravel(df_target), test_size=0.30, random_state=2021)
sns.set_style('whitegrid')
sns.countplot(x='Cancer', data = pd.DataFrame(y train,columns=['Cancer']) ,palette='RdBu r')
<AxesSubplot:xlabel='Cancer', ylabel='count'>
                                                                             sns.set_style('whitegrid')
                                                                             sns.countplot(x='Cancer', data = pd.DataFrame(y_test,columns=['Cancer']) ,palette='RdBu_r')
  250
                                                                             <AxesSubplot:xlabel='Cancer', ylabel='count'>
  200
                                                                                100
  150
count
  100
                                                                              count
   50
                                                                                 40
                                                                                 20
                              Cancer
```

Cancer

### Concepts

- Model Parameters: a model's (internal) configuration variable whose value is estimated from the training data, i.e., the value is not set manually. Examples include:
  - Weights in Artificial Neural Networks
  - Support vectors in Support Vector Machines

- Model Hyperparameters: a model's (external) configuration variable whose value can be set manually. It is difficult to know the best value for each hyperparameter in advance. Tuning a model consists of finding the best (or at least a good) configuration of the hyperparameters. Examples include:
  - Optimizer and learning rate in Artificial Neural Networks
  - C and gamma in Support Vector Machines
  - Quality measure and Pruning method in Decision Trees

### **Train the Support Vector Classifier**

#### 10-Fold Cross Validation

Let's try the Cross Validation technique with 10 folds:

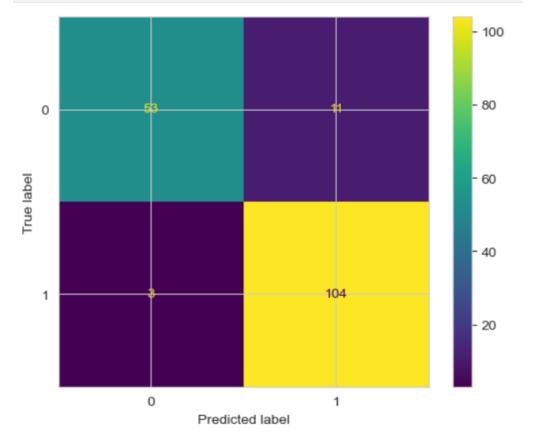
```
from sklearn.model selection import cross val score
from sklearn.svm import SVC
cross valid model = SVC(random state=2021)
scores = cross val score(cross valid model, df feat, np.ravel(df target), cv=10)
scores
array([0.89473684, 0.84210526, 0.89473684, 0.92982456, 0.92982456,
       0.92982456, 0.94736842, 0.92982456, 0.92982456, 0.91071429])
print("%0.2f accuracy with a standard deviation of %0.2f" % (scores.mean(), scores.std()))
0.91 accuracy with a standard deviation of 0.03
And now without Cross Validation:
from sklearn.svm import SVC
model = SVC(random_state=2021)
model.fit(X_train,y_train)
           SVC
SVC(random_state=2021)
```

#### **Predictions and evaluations**

Let's predict using the trained model:

```
predictions = model.predict(X test)
from sklearn.metrics import classification_report, ConfusionMatrixDisplay, accuracy_score
print("%0.2f accuracy" % (accuracy_score(y_test, predictions)))
0.92 accuracy
print(classification_report(y_test,predictions))
              precision
                           recall f1-score
                   0.95
                             0.83
                                       0.88
                                                   64
                   0.90
                            0.97
                                       0.94
                                                  107
                                       0.92
                                                  171
    accuracy
                                       0.91
   macro avg
                   0.93
                             0.90
                                                  171
weighted avg
                   0.92
                             0.92
                                       0.92
                                                  171
```

ConfusionMatrixDisplay.from\_predictions(y\_test, predictions)
plt.show()



#### GridSearch

- Finding the right parameters (such as the values of C or gamma to use) is a complicated task
- The idea of creating a "grid" of parameters and trying out all the possible combinations is called GridSearch
  - This method is common enough for Scikit-learnto have this functionality incorporated with GridSearchCV (CV stands for Cross-Validation)
  - GridSearchCV receives a dictionary describing the parameters to be tried and the model to be trained
  - The parameter grid is defined as a dictionary in which the keys are the parameters and the values are the settings to be tested

```
param_grid = {'C': [0.1, 1, 10, 100, 1000], 'gamma': [1, 0.1, 0.01, 0.001, 0.0001], 'kernel': ['rbf']}
from sklearn.model_selection import GridSearchCV
```

- GridSearchCV is a meta-estimator
- It takes an estimator like SVC and creates a new estimator that behaves in exactly the same way in this case, like a classifier

Add refit=True and choose verbose for the number you want (verbose means the text output that describes the process)

#### Train a model with GridSearchCV

Now its time to train a Support Vector Machine Classifier

Call the SVC() model from sklearn and fit the model to the training data:

```
grid = GridSearchCV(SVC(random_state=2021), param_grid, refit=True, verbose=3)
```

#### What does fit do:

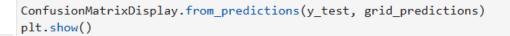
- Runs the same loop with cross-validation to find the best parameter combination
- Once it has the best combination, it runs fit again on all data passed to fit (without cross-validation) to built a single new model using the best parameter setting

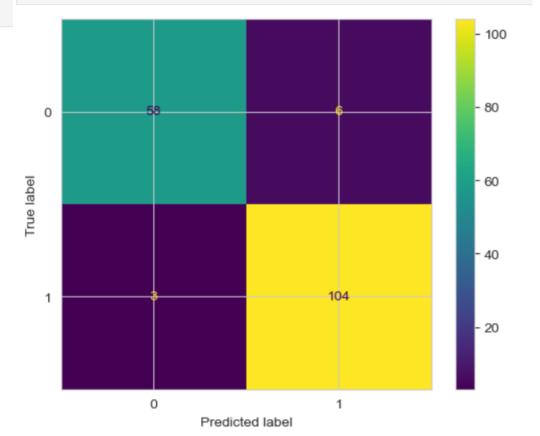
```
grid.fit(X train,y train)
Fitting 5 folds for each of 25 candidates, totalling 125 fits
[CV 1/5] END ......C=0.1, gamma=1, kernel=rbf;, score=0.625 total time=
[CV 2/5] END ......C=0.1, gamma=1, kernel=rbf;, score=0.625 total time=
                                                                           0.0s
[CV 3/5] END ......C=0.1, gamma=1, kernel=rbf;, score=0.625 total time=
                                                                           0.0s
[CV 4/5] END ......C=0.1, gamma=1, kernel=rbf;, score=0.633 total time=
                                                                           0.05
[CV 5/5] END ......C=0.1, gamma=1, kernel=rbf;, score=0.633 total time=
                                                                           0.05
[CV 3/5] END ..C=1000, gamma=0.0001, kernel=rbf;, score=0.912 total time=
[CV 4/5] END ..C=1000, gamma=0.0001, kernel=rbf;, score=0.937 total time=
                                                                          0.05
[CV 5/5] END ..C=1000, gamma=0.0001, kernel=rbf;, score=0.911 total time=
▶ GridSearchCV
▶ estimator: SVC
      ► SVC
```

You can inspect the best parameters found by GridSearchCV in the best\_params\_ attribute and the best estimator in the best\_estimator\_ attribute:

Then you can re-run predictions on this grid object just as you would with a normal model:

```
grid_predictions = grid.predict(X_test)
print(classification_report(y_test,grid_predictions))
             precision
                          recall f1-score support
                   0.95
                            0.91
                                       0.93
                                                  64
           1
                            0.97
                                      0.96
                   0.95
                                                 107
                                       0.95
                                                 171
    accuracy
                                      0.94
                                                 171
                   0.95
                            0.94
   macro avg
weighted avg
                  0.95
                            0.95
                                      0.95
                                                 171
```



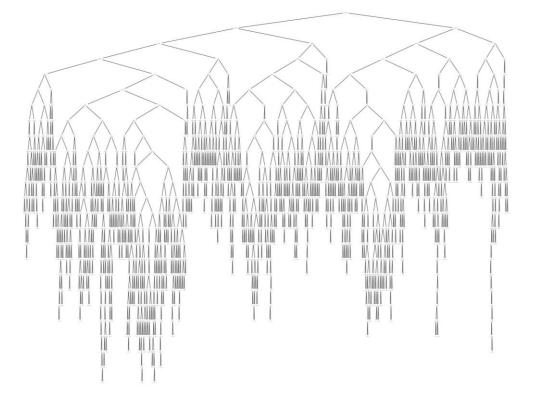


### Hands On



1. Plot the resultant tree (plot\_tree) and save it as figure (.png)

```
fig = plt.figure(figsize=(25,20))
tree.plot_tree(dt_model)
plt.show()
fig.savefig("dt_plot.png")
```



2. Using export\_text to represent the tree. Save it in a log file

```
text representation = tree.export text(dt model)
print(text representation)
with open("dt_text.log", "w") as fout:
   fout.write(text representation)
--- feature 1 <= 25.00
    --- feature 4 <= 1020.50
        --- feature_5 <= 91.50
            --- feature_4 <= 1011.50
                --- feature 3 <= 15.50
                    --- feature_3 <= 11.50
                        --- feature_6 <= 1.50
                            --- feature 4 <= 1002.00
                                --- class: 1
                               feature 4 > 1002.00
                                   feature 3 <= 10.50
                                    --- feature 2 <= 1.50
                                        --- feature 7 <= 1.50
                                           |--- truncated branch of depth 6
                                        --- feature 7 > 1.50
                                           |--- truncated branch of depth 3
                                    --- feature 2 > 1.50
                                        --- class: 1
                                    feature 3 > 10.50
```

179

313

175

1500

1500

1500

0.73

#### Model evaluation

3

**Decision Tree** 

support	f1-score	recall	precision	
632	0.74	0.74	0.75	1
201	0.56	0.55	0.58	2

0.73

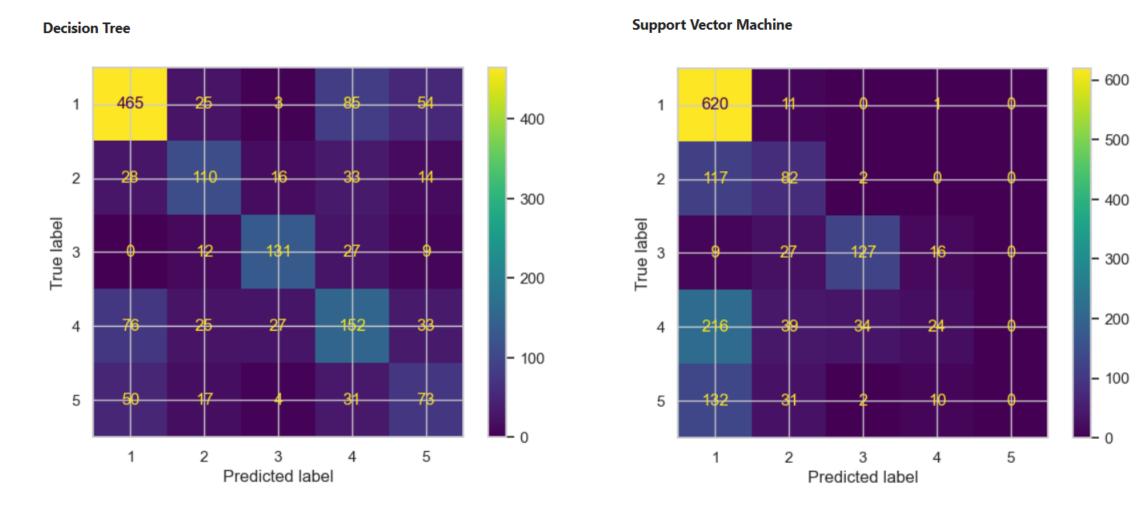
0.46 0.49 0.47 0.40 0.42 0.41 0.62 accuracy 0.58 0.58 macro avg 0.58 weighted avg 0.62 0.62 0.62

0.72

#### **Support Vector Machine**

	precision	recall	f1-score	support
1	0.57	0.98	0.72	632
2	0.43	0.41	0.42	201
3	0.77	0.71	0.74	179
4	0.47	0.08	0.13	313
5	0.00	0.00	0.00	175
accuracy		1	0.57	1500
macro avg	0.45	0.44	0.40	1500
weighted avg	0.49	0.57	0.47	1500

#### Model evaluation



GridSearch

#### **Decision Tree**

```
print(dt model.get depth())
print(dt model.get n leaves())
24
1189
param grid dt = {'criterion': ['gini', 'entropy'], 'max depth': [1,2,3,4,5,6,7,8,9,10]}
estimator_dt = DecisionTreeClassifier(random_state=2022)
grid dt = GridSearchCV(estimator dt, param grid_dt, refit=True, verbose=2)
grid dt.fit(X train,y train)
Fitting 5 folds for each of 20 candidates, totalling 100 fits
[CV] END ......criterion=gini, max depth=1; total time=
[CV] END ......criterion=gini, max depth=1; total time=
[CV] END ......criterion=gini, max depth=1; total time=
                                                                    0.05
[CV] END ......criterion=gini, max depth=1; total time=
                                                                    0.0s
[CV] END ......criterion=gini, max_depth=1; total time=
                                                                    0.0s
             GridSearchCV
  estimator: DecisionTreeClassifier
       ▶ DecisionTreeClassifier
```

#### **Support Vector Machine**

```
param_grid_svc = {'C': [0.1,1, 10, 100], 'gamma': [1,0.1,0.01,0.001], 'kernel': ['rbf']}
estimator svc = SVC(random state=2022)
grid svc = GridSearchCV(estimator svc, param grid svc, refit=True, verbose=2)
grid svc.fit(X train,y train)
Fitting 5 folds for each of 16 candidates, totalling 80 fits
1.4s
1.5s
1.3s
1.3s
1.0s
1.0s
1.0s
1.1s
GridSearchCV
 ▶ estimator: SVC
   ► SVC
```

### GridSearch

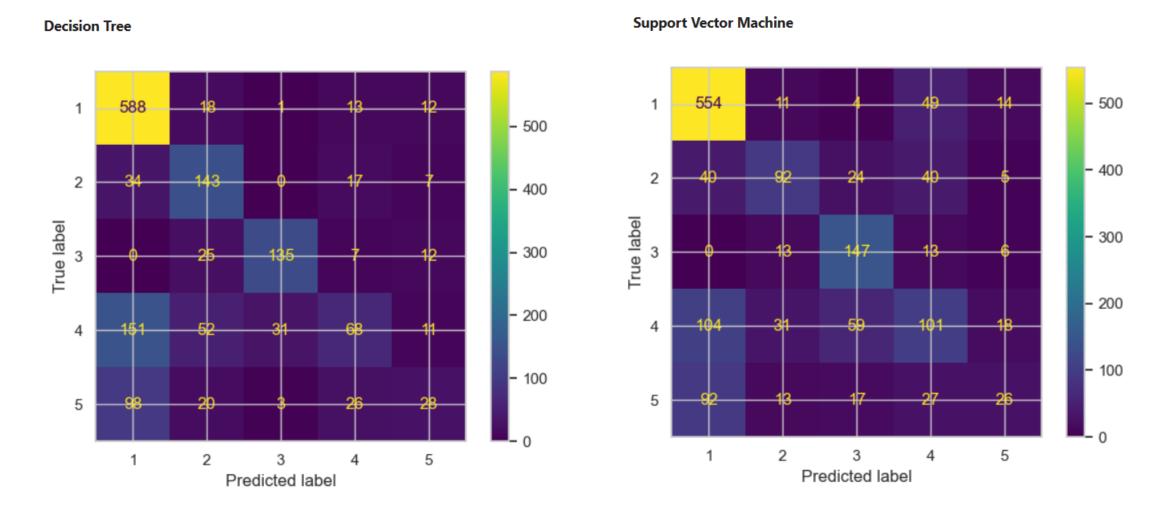
#### **Decision Tree**

	precision	recall	f1-score	support
1	0.68	0.93	0.78	632
2	0.55	0.71	0.62	201
3	0.79	0.75	0.77	179
4	0.52	0.22	0.31	313
5	0.40	0.16	0.23	175
accuracy			0.64	1500
macro avg	0.59	0.55	0.54	1500
weighted avg	0.61	0.64	0.60	1500

#### **Support Vector Machine**

	precision	recall	f1-score	support
1 2	0.70 0.57	0.88 0.46	0.78 0.51	632 201
3	0.59	0.82	0.68	179
4 5	0.44 0.38	0.32 0.15	0.37 0.21	313 175
accuracy			0.61	1500
macro avg	0.54	0.53	0.51	1500
weighted avg	0.58	0.61	0.58	1500

### GridSearch



A Decision Tree is pruned by replacing an entire subtree with a leaf node. If the expected error rate in the subtree is higher than that of a single leaf, it is replaced.

```
print(dt_model.get_depth())
print(dt_model.get_n_leaves())
24
1189
```

▶ DecisionTreeClassifier

#### **Best Depth Tree**

```
max_depth = dt_model.get_depth()
max_depth

24

param_grid = {'max_depth': [max_depth for max_depth in range(1, max_depth + 1)]}
estimator = DecisionTreeClassifier(random_state=42)

max_depth_grid_search = GridSearchCV(estimator, param_grid)

max_depth_grid_search.fit(X_train, y_train)

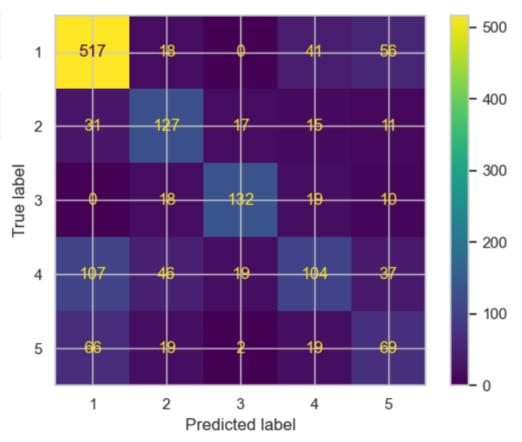
ForidSearchCV
Festimator: DecisionTreeClassifier
```

You can inspect the best parameters found by GridSearchCV in the best params attribute and the best estimator in the best estimator attribute:

```
max depth grid search.best params
{'ccp_alpha': 0.0008316875137151618}
max_depth_tree = max_depth_grid_search.best_estimator_
print(max_depth_tree)
DecisionTreeClassifier(ccp_alpha=0.0008316875137151618, random_state=42)
best_max_depth = max_depth_tree.get_depth()
print(best_max_depth)
17
```

#### Model evaluation

	precision	recall	f1-score	support
1	0.72	0.82	0.76	632
2	0.56	0.63	0.59	201
3	0.78	0.74	0.76	179
4	0.53	0.33	0.41	313
5	0.38	0.39	0.39	175
accuracy			0.63	1500
macro avg	0.59	0.58	0.58	1500
weighted avg	0.62	0.63	0.62	1500



#### **Cost Complexity Pruning**

Another pruning technique

```
ccp alphas = dt model.cost complexity pruning path(X train, y train)["ccp alphas"]
ccp alphas
array([0.00000000e+00, 1.90476190e-05, 2.38095238e-05, 3.78151261e-05,
       4.76190476e-05, 6.66666667e-05, 7.14285714e-05, 7.14285714e-05,
       7.61904762e-05, 7.61904762e-05, 8.57142857e-05, 9.52380952e-05,
       9.52380952e-05, 9.52380952e-05, 9.52380952e-05, 9.52380952e-05,
       1.08843537e-04, 1.14285714e-04, 1.22448980e-04, 1.36645963e-04,
       1.39097744e-04, 1.40394089e-04, 1.42857143e-04, 1.58730159e-04,
       1.59663866e-04, 1.61904762e-04, 1.63265306e-04, 1.70068027e-04,
       1.71428571e-04, 1.71428571e-04, 1.71428571e-04, 1.72397220e-04,
       1.74603175e-04, 1.74603175e-04, 1.75824176e-04, 1.77777778e-04,
       1.79271709e-04, 1.80952381e-04, 1.82539683e-04, 1.82857143e-04,
       1.90476190e-04, 1.90476190e-04, 1.90476190e-04, 1.90476190e-04,
       1.90476190e-04, 1.90476190e-04, 1.90476190e-04, 1.90476190e-04,
       1.90476190e-04, 1.90476190e-04, 1.90476190e-04, 1.90476190e-04,
       2.11640212e-04, 2.11640212e-04, 2.11764706e-04, 2.14285714e-04,
       2.14285714e-04, 2.14285714e-04, 2.14285714e-04, 2.14285714e-04,
       2.14285714e-04, 2.14285714e-04, 2.14285714e-04, 2.14285714e-04,
       2.14285714e-04, 2.14285714e-04, 2.14285714e-04, 2.14285714e-04,
       2.14285714e-04, 2.14285714e-04, 2.15873016e-04, 2.27106227e-04,
       2.27891156e-04, 2.28571429e-04, 2.28571429e-04, 2.28571429e-04,
       2.28571429e-04, 2.28571429e-04, 2.28571429e-04, 2.28571429e-04,
       2.28571429e-04, 2.28571429e-04, 2.28571429e-04, 2.33333333e-04,
       2.33486943e-04, 2.38095238e-04, 2.38095238e-04, 2.38095238e-04,
        •••
```

```
estimator.get params().keys()
dict_keys(['ccp_alpha', 'class_weight', 'criterion', 'max_depth', 'max_feature
s', 'max_leaf_nodes', 'min_impurity_decrease', 'min_samples_leaf', 'min_sample
s_split', 'min_weight_fraction_leaf', 'random_state', 'splitter'])
param_grid = {'ccp_alpha': [alpha for alpha in ccp_alphas]}
estimator_dt = DecisionTreeClassifier(random_state=42)
ccp_alpha_grid_search = GridSearchCV(estimator_dt, param_grid)
ccp alpha grid search.fit(X train,y train)
             GridSearchCV
 Pestimator: DecisionTreeClassifier
       ▶ DecisionTreeClassifier
ccp_alpha_grid_search.best_params_
{'ccp alpha': 0.0008316875137151618}
best_ccp_alpha_tree = ccp_alpha_grid_search.best_estimator
print(best ccp alpha tree)
DecisionTreeClassifier(ccp alpha=0.0008316875137151618, random state=42)
```

#### Model evaluation

	precision	recall	f1-score	support
1	0.72	0.82	0.76	632
2	0.56	0.63	0.59	201
3	0.78	0.74	0.76	179
4	0.53	0.33	0.41	313
5	0.38	0.39	0.39	175
accuracy			0.63	1500
macro avg	0.59	0.58	0.58	1500
weighted avg	0.62	0.63	0.62	1500

