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Objective

Practice the searching for optimal tuning parameters

You will practice:

- How can K-fold cross-validation be used to search for an optimal tuning parameter?
- How can this process be made more efficient?
- How do you search for multiple tuning parameters at once?
- What do you do with those tuning parameters before making real predictions?
- How can the computational expense of this process be reduced?

First, import the required libraries

```
"""
Import:
- pandas
- sklearn Train-Test split
- sklearn Standard Scaler
- sklearn K Neighbors Classifier
- sklearn Cross val score
- sklearn Grid Search Cross Validation
- matplotlib
"""
import pandas as pd
from sklearn.model_selection import train_test_split, cross_val_score, GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.neighbors import KNeighborsClassifier
import matplotlib.pyplot as plt

# Keep the following lines (you can comment them out to see what happens)
import warnings

# Suppress all warnings
warnings.filterwarnings("ignore")
```

Read the data. For this exercise we are using the 'winequality-white.csv' file

Note: The path in your drive might change

```
from google.colab import drive
drive.mount('/content/drive')
# Read the content in a df DataFrame using Pandas. Be careful with the separators
df = pd.read_csv('/content/drive/My Drive/winequality-white.csv', sep=';')
# show the first 5 instances
df.head()
```

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force_remount=True).
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol	quality
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8	6
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5	6
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1	6
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	6
4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9	6

Next steps: Generate code with df View recommended plots

```
# Show the number of rows and columns
print(df.shape)
```

```
(4898, 12)
```

```
# Show the description of the DataFrame
df.describe()

# Check for missing values
# df.isnull().sum()
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	
count	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	4898.000000	489
mean	6.854788	0.278241	0.334192	6.391415	0.045772	35.308085	138.360657	0.994027	3.188267	0.489847	1
std	0.843868	0.100795	0.121020	5.072058	0.021848	17.007137	42.498065	0.002991	0.151001	0.114126	
min	3.800000	0.080000	0.000000	0.600000	0.009000	2.000000	9.000000	0.987110	2.720000	0.220000	
25%	6.300000	0.210000	0.270000	1.700000	0.036000	23.000000	108.000000	0.991723	3.090000	0.410000	
50%	6.800000	0.260000	0.320000	5.200000	0.043000	34.000000	134.000000	0.993740	3.180000	0.470000	1
75%	7.300000	0.320000	0.390000	9.900000	0.050000	46.000000	167.000000	0.996100	3.280000	0.550000	1
max	14.200000	1.100000	1.660000	65.800000	0.346000	289.000000	440.000000	1.038980	3.820000	1.080000	1

Generate our X and y. y is our column 'quality'

```
# Get X and y
X = df.drop('quality', axis=1)
y = df['quality']
```

```
# Show the first 5 elements of X
X.head()
```

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	pH	sulphates	alcohol
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	3.00	0.45	8.8
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	3.30	0.49	9.5
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	3.26	0.44	10.1
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9
4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	3.19	0.40	9.9

Next steps: Generate code with X View recommended plots

```
# Show the first 5 elements of y
y.head()
```

```
0    6
1    6
2    6
3    6
4    6
Name: quality, dtype: int64
```

Split train and test

```
# Get X_train, X_test, y_train, and y_test.
# Use a 80-20 split, with random state of 42
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
```

```
# Show the sizes for your datasets
print(X_train.shape)
print(X_test.shape)
print(y_train.shape)
print(y_test.shape)
```

```
(3918, 11)
(980, 11)
(3918,)
(980,)
```

Do you think we need to Standardize X?

```
# Standardize your X_train using a StadardScaler
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
```

```
# Show the 5 rows of the scaled dataset
print(X_train_scaled[:5])
```

```
[[ 5.15119310e-01 -1.07623315e+00  2.27730764e-01  3.40419470e-01
  -8.13688488e-01  5.34064605e-01 -6.41932319e-01 -4.47040725e-01
  -3.28261014e-01 -7.02444738e-01  1.54037099e+00]
 [-6.69188091e-01 -2.88776731e-01  8.95831948e-01  1.00207124e+00
  -2.17211567e-01  7.73947112e-01  1.35510550e+00  9.03369755e-01
  -6.18856911e-02  2.66074147e-01 -8.21711966e-01]
 [-1.49820327e+00  4.00247639e-01 -2.28071805e-02  1.84736700e-01
  -4.00742927e-01 -6.05377303e-01 -1.02232048e+00 -4.60280044e-01
   4.04271124e-01  1.93263316e-03  4.81506217e-01]
 [ 4.13963498e-02 -8.79369048e-01  1.44218115e-01 -9.24503038e-01
  -4.46625767e-01 -1.25612289e-01 -8.79674917e-01 -3.04718052e-01
   1.37895801e-01  4.42168490e-01  2.37152807e-01]
 [ 9.88842271e-01  2.03383533e-01 -6.07395717e-01  2.43240669e+00
   3.33382515e-01  5.42995912e-02  8.55846045e-01  1.88307932e+00
   7.13019704e-02  8.99798045e-02 -8.86517384e-02]]
```

Create a KNN classifier considering just 5 neighbors

```
# Define a K Neighbors Classifier with 5 neighbors
knn_classifier = KNeighborsClassifier(n_neighbors=5)
```

To train our model, we will use cross-validation using 5 folds for accuracy

```
# use the cross_val_score() method to train our knn classifier with X_train and y_train
#, and 5 folds. Use accuracy as metric.
# Save the result in a variable scores
scores = cross_val_score(knn_classifier, X_train_scaled, y_train, cv=5, scoring='accuracy')
```

```
# print the scores obtained
scores
```

```
array([0.55357143, 0.54591837, 0.5497449 , 0.53128991, 0.54916986])
```

```
# get the average accuracy as an estimate of out-of-sample accuracy
scores.mean()
```

```
0.5459388927984987
```

This is the accuracy of our model using 5 neighbors! Can we improve it?

Let's now search for the optimal value of neighgbors (k)

Let's use a more efficient parameter tuning using `GridSearchCV`

Allows you to define a grid of parameters that will be searched using K-fold cross-validation

```
# define the parameter values that should be searched
# We are going to use the same range, from 1 to 31 (inclusive)
# Define a variable to store a list with the range values
param_range = list(range(1, 32))
```

```
# Show the list of values
print("List of parameter values:", param_range)
```

```
List of parameter values: [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30
```

Let's create a parameter grid. In other words, let's map the the parameter names to the values that should be searched

```
# Define a variable to store the dictionary of parameters
# The parameter is the number of neighbors mapped to the list of
#values we obtained previously
param_grid = {'n_neighbors': param_range}
# show your dictionary of parameters
print("Dictionary of parameters:", param_grid)
```

```
Dictionary of parameters: {'n_neighbors': [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26
```

```
# Instantiate a new KNN model WITHOUT any parameters
knn_model = KNeighborsClassifier()
```

Instantiate a GridSearchCV object

```
# Use as parameters the following:
# knn model,
# the dictionary of parameters,
# the number of folds (5),
# 'accuracy' as the metric
# In addition, you can use the parameter n_jobs=-1 to run the computations in parallel (if supported by your OS)
grid_search = GridSearchCV(estimator=knn_model, param_grid=param_grid, cv=5, scoring='accuracy', n_jobs=-1)
```

```
# show the object created
grid_search
```

```
▸ GridSearchCV
▸ estimator: KNeighborsClassifier
    ▸ KNeighborsClassifier
```

Let's train the grid with our X_train and y_train data

```
# use the object to train with X_train and y_train
grid_search.fit(X_train_scaled, y_train)
```

```
▸ GridSearchCV
▸ estimator: KNeighborsClassifier
    ▸ KNeighborsClassifier
```

Let's view the results.

We can create a Pandas DataFrame using the output of the cv_results_ as input for our DataFrame

```
# view the results (cv_results) as a pandas DataFrame
results_subset = pd.DataFrame(grid_search.cv_results_)[['mean_test_score', 'std_test_score', 'params']]
results_subset
```

	mean_test_score	std_test_score	params
0	0.607451	0.009383	{'n_neighbors': 1}
1	0.557168	0.006918	{'n_neighbors': 2}
2	0.545939	0.005701	{'n_neighbors': 3}
3	0.551295	0.010879	{'n_neighbors': 4}
4	0.545939	0.007717	{'n_neighbors': 5}
5	0.543390	0.004105	{'n_neighbors': 6}
6	0.550028	0.011898	{'n_neighbors': 7}
7	0.544918	0.007160	{'n_neighbors': 8}
8	0.542873	0.015039	{'n_neighbors': 9}
9	0.541602	0.008034	{'n_neighbors': 10}
10	0.540588	0.012345	{'n_neighbors': 11}
11	0.543391	0.005674	{'n_neighbors': 12}
12	0.548496	0.008029	{'n_neighbors': 13}
13	0.549008	0.007187	{'n_neighbors': 14}
14	0.551303	0.004481	{'n_neighbors': 15}
15	0.553343	0.009877	{'n_neighbors': 16}
16	0.555895	0.012417	{'n_neighbors': 17}
17	0.556661	0.015029	{'n_neighbors': 18}
18	0.559471	0.016320	{'n_neighbors': 19}
19	0.559985	0.013793	{'n_neighbors': 20}
20	0.555387	0.009105	{'n_neighbors': 21}
21	0.552837	0.009365	{'n_neighbors': 22}
22	0.550286	0.010638	{'n_neighbors': 23}
23	0.551305	0.009179	{'n_neighbors': 24}
24	0.552581	0.008260	{'n_neighbors': 25}
25	0.553093	0.009246	{'n_neighbors': 26}
26	0.554115	0.011207	{'n_neighbors': 27}
27	0.556924	0.013606	{'n_neighbors': 28}
28	0.555394	0.014468	{'n_neighbors': 29}
29	0.555647	0.011809	{'n_neighbors': 30}
30	0.549775	0.008936	{'n_neighbors': 31}

Next steps: Generate code with `results_subset` View recommended plots

```
# We can also print the array of mean scores only (mean_test_score)
# Store the results in a separate variable
mean_scores = grid_search.cv_results_['mean_test_score']

# print the variable
print(mean_scores)
```

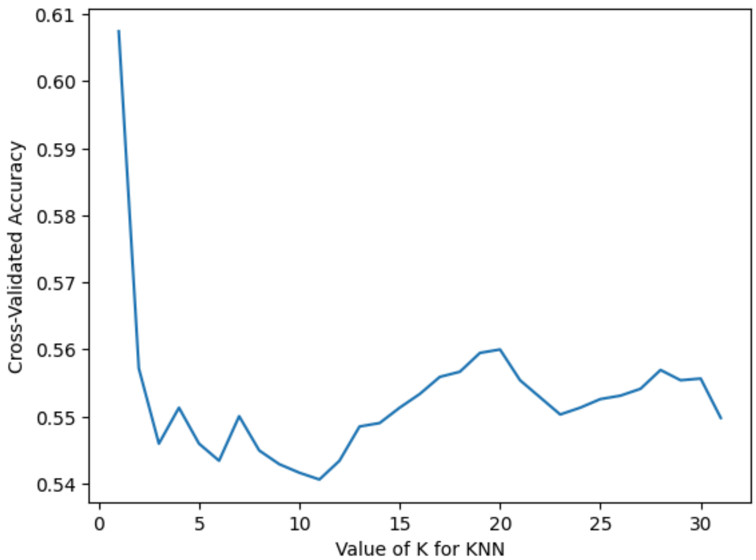
```
[0.60745139 0.55716794 0.54593922 0.55129506 0.54593889 0.54339048
 0.55002802 0.54491783 0.54287278 0.54160151 0.54058827 0.5433908
 0.54849578 0.54900761 0.55130288 0.55334304 0.55589471 0.556661
 0.55947136 0.55998514 0.55538712 0.5528374  0.55028573 0.55130548
 0.55258132 0.55309348 0.55411486 0.55692359 0.55539363 0.55564743
 0.5497752 ]
```

Let's visualize the scores

```
k_range = list(range(1, 32))
grid_mean_scores = grid_search.cv_results_['mean_test_score']

# plot the results
plt.plot(k_range, grid_mean_scores)
plt.xlabel('Value of K for KNN')
plt.ylabel('Cross-Validated Accuracy')
```

```
Text(0, 0.5, 'Cross-Validated Accuracy')
```



Finally, get the parameter for the best model

```
# Print the best score
print(grid_search.best_score_)

# Print the best parameters
print(grid_search.best_params_)

# Print the best estimator
print(grid_search.best_estimator_)
```

```
0.6074513905178931
{'n_neighbors': 1}
KNeighborsClassifier(n_neighbors=1)
```

We improved our model by searching the best k for the neighbors!

But, what would happen if our model has more parameters? Let's see how we can search the best combination of parameters

Searching multiple parameters simultaneously

First, let's define the parameter values that should be searched

```
# define the parameter values that should be searched
# As before, define a list for the range of neighbors, from 1 to 31 (inclusive)
param_range_neighbors = list(range(1, 32))


# define a list for the weight options ('uniform' and 'distance')
param_weights = ['uniform', 'distance']
```

Create a parameter grid. For that, we need to map the parameter names to the values that should be searched

```
# Create a dictionary mapping the parameters to a key
# You can see the parameter here:
# https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html
param_grid = {'n_neighbors': param_range_neighbors, 'weights': param_weights}


# print the content of the grid dictionary
print(param_grid)
```

```
{'n_neighbors': [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31], 'we
```

Instantiate and train the grid

```
# As before, we use a vanilla knn model, the dictionay of parameters, 5 folds, and accuracy as the score
knn_model = KNeighborsClassifier()
param_grid = {'n_neighbors': param_range_neighbors, 'weights': param_weights}
grid_search.fit(X_train_scaled, y_train)
```

```
▸ GridSearchCV
▸ estimator: KNeighborsClassifier
  ▸ KNeighborsClassifier
```

As before, let's create a pandas dataframe to see the results

```
# view the results
results_df = pd.DataFrame(grid_search.cv_results_)[['mean_test_score', 'std_test_score', 'params']]

results_df
```

	mean_test_score	std_test_score	params
0	0.607451	0.009383	{'n_neighbors': 1}
1	0.557168	0.006918	{'n_neighbors': 2}
2	0.545939	0.005701	{'n_neighbors': 3}
3	0.551295	0.010879	{'n_neighbors': 4}
4	0.545939	0.007717	{'n_neighbors': 5}
5	0.543390	0.004105	{'n_neighbors': 6}
6	0.550028	0.011898	{'n_neighbors': 7}
7	0.544918	0.007160	{'n_neighbors': 8}
8	0.542873	0.015039	{'n_neighbors': 9}
9	0.541602	0.008034	{'n_neighbors': 10}
10	0.540588	0.012345	{'n_neighbors': 11}
11	0.543391	0.005674	{'n_neighbors': 12}
12	0.548496	0.008029	{'n_neighbors': 13}
13	0.549008	0.007187	{'n_neighbors': 14}
14	0.551303	0.004481	{'n_neighbors': 15}
15	0.553343	0.009877	{'n_neighbors': 16}
16	0.555895	0.012417	{'n_neighbors': 17}
17	0.556661	0.015029	{'n_neighbors': 18}
18	0.559471	0.016320	{'n_neighbors': 19}
19	0.559985	0.013793	{'n_neighbors': 20}
20	0.555387	0.009105	{'n_neighbors': 21}
21	0.552837	0.009365	{'n_neighbors': 22}
22	0.550286	0.010638	{'n_neighbors': 23}
23	0.551305	0.009179	{'n_neighbors': 24}
24	0.552581	0.008260	{'n_neighbors': 25}
25	0.553093	0.009246	{'n_neighbors': 26}
26	0.554115	0.011207	{'n_neighbors': 27}
27	0.556924	0.013606	{'n_neighbors': 28}
28	0.555394	0.014468	{'n_neighbors': 29}
29	0.555647	0.011809	{'n_neighbors': 30}
30	0.549775	0.008936	{'n_neighbors': 31}

Next steps: Generate code with `results_df` View recommended plots

Examine the best model

```
# Print the best score
print(grid_search.best_score_)

# Print the best parameters
print(grid_search.best_params_)
```

```
0.6074513905178931
{'n_neighbors': 1}
```

Wow! We have improved more our model!

Now you can use those parameters to train a model for predictions using the test dataset

What is the accuracy of your final model using the test dataset?

Write the code for getting that result and answer the following questions

- Does the model prsents overfitting?

- What could you test to improve your model?