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K Nearest Neighbor

Estimated time needed: **30** minutes

In this lab, you will learn about and practice the K Nearest Neighbor (KNN) model. KNN is a straightforward but very effective model that can be used for both classification and regression tasks. If the feature space is not very large, KNN can be a high-interpretable model because you can explain and understand how a prediction is made by looking at its nearest neighbors.

We will be using a tumor sample dataset containing lab test results about tumor samples. The objective is to classify whether a tumor is malicious (cancer) or benign. As such, it is a typical binary classification task.

Objectives

After completing this lab, you will be able to:

- Train KNN models with different neighbor hyper-parameters
- Evaluate KNN models on classification tasks
- Tune the number of neighbors and find the optimized one for a specific task

First, let's install `seaborn` for visualization tasks and import required libraries for this lab.

In [1]:

```
# All Libraries required for this Lab are listed below. The Libraries pre-installed on S
# !mamba install -qy pandas==1.3.3 numpy==1.21.2 ipywidgets==7.4.2 scipy==7.4.2 tqdm==4.
# Note: If your environment doesn't support "!mamba install", use "!pip install".
```

In [2]:

```
import pandas as pd
import numpy as np
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import train_test_split
from sklearn import metrics
# Evaluation metrics related methods
from sklearn.metrics import classification_report, accuracy_score, f1_score, confusion_m
import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline
```

In [3]:

```
# Define a random seed to reproduce any random process
rs = 123
```

In [4]:

```
# Ignore any deprecation warnings
import warnings
warnings.filterwarnings("ignore", category=DeprecationWarning)
```

Load and explore the tumor sample dataset

We first load the dataset `tumor.csv` as a Pandas dataframe:

In [5]:

```
# Read dataset in csv format
dataset_url = "https://cf-courses-data.s3.us.cloud-object-storage.appdomain.cloud/IBM-ML"
tumor_df = pd.read_csv(dataset_url)
```

Then, let's quickly take a look at the head of the dataframe.

In [6]:

```
tumor_df.head()
```

Out[6]:

	Clump	UnifSize	UnifShape	MargAdh	SingEpiSize	BareNuc	BlandChrom	NormNucl	Mi
0	5	1	1	1	2	1	3	1	·
1	5	4	4	5	7	10	3	2	·
2	3	1	1	1	2	2	3	1	·
3	6	8	8	1	3	4	3	7	·
4	4	1	1	3	2	1	3	1	·

And, display its columns.

In [7]:

```
tumor_df.columns
```

Out[7]:

```
Index(['Clump', 'UnifSize', 'UnifShape', 'MargAdh', 'SingEpiSize', 'BareNuc',  
      'BlandChrom', 'NormNuc1', 'Mit', 'Class'],  
      dtype='object')
```

Each observation in this dataset contains lab test results about a tumor sample, such as clump or shapes. Based on these lab test results or features, we want to build a classification model to predict if this tumor sample is malicious (cancer) or benign. The target variable `y` is specified in the `Class` column.

Then, let's split the dataset into input `X` and output `y` :

In [8]:

```
X = tumor_df.iloc[:, :-1]  
y = tumor_df.iloc[:, -1:]
```

And, we first check the statistics summary of features in `X` :

In [9]:

```
X.describe()
```

Out[9]:

	Clump	UnifSize	UnifShape	MargAdh	SingEpiSize	BareNuc	BlandChrom
count	683.000000	683.000000	683.000000	683.000000	683.000000	683.000000	683.000000
mean	4.442167	3.150805	3.215227	2.830161	3.234261	3.544656	3.445095
std	2.820761	3.065145	2.988581	2.864562	2.223085	3.643857	2.449697
min	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
25%	2.000000	1.000000	1.000000	1.000000	2.000000	1.000000	2.000000
50%	4.000000	1.000000	1.000000	1.000000	2.000000	1.000000	3.000000
75%	6.000000	5.000000	5.000000	4.000000	4.000000	6.000000	5.000000
max	10.000000	10.000000	10.000000	10.000000	10.000000	10.000000	10.000000

As we can see from the above cell output, all features are numeric and ranged between 1 to 10. This is very convenient as we do not need to scale the feature values as they are already in the same range.

Next, let's check the class distribution of output `y` :

In [10]:

```
y.value_counts(normalize=True)
```

Out[10]:

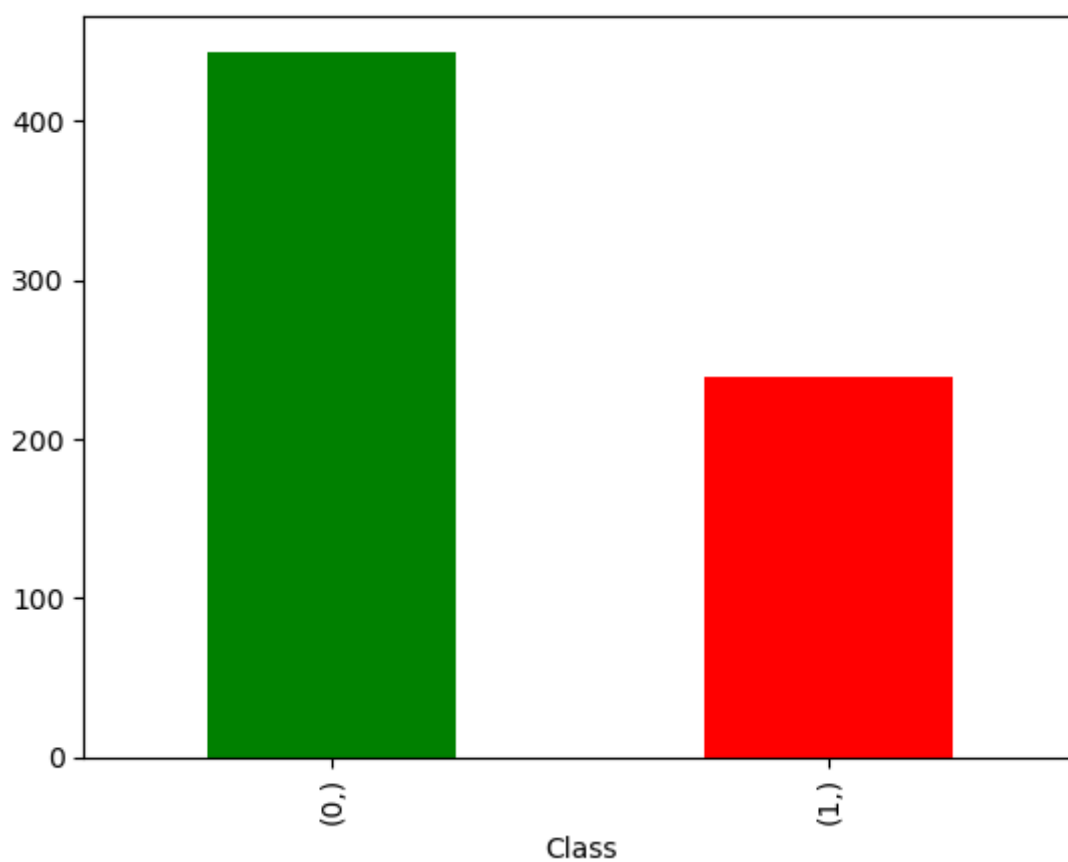
```
Class
0      0.650073
1      0.349927
dtype: float64
```

In [11]:

```
y.value_counts().plot.bar(color=['green', 'red'])
```

Out[11]:

<Axes: xlabel='Class'>



We have about 65% benign tumors (Class = 0) and 35% cancerous tumors (Class = 1), which is not a very imbalanced class distribution.

Process and split training and testing datasets

In [12]:

```
# Split 80% as training dataset  
# and 20% as testing dataset  
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, stratify=y, ran
```

Train and evaluate a KNN classifier with the number of neighbors set to 2

Training a KNN classifier is very similar to training other classifiers in `sklearn`, we first need to define a `KNeighborsClassifier` object. Here we use `n_neighbors=2` argument to specify how many neighbors will be used for prediction, and we keep other arguments to be their default values.

In [13]:

```
# Define a KNN classifier with `n_neighbors=2`  
knn_model = KNeighborsClassifier(n_neighbors=2)
```

Then we can train the model with `X_train` and `y_train`, and we use `ravel()` method to convert the data frame `y_train` to a vector.

In [14]:

```
knn_model.fit(X_train, y_train.values.ravel())
```

Out[14]:

```
▼      KNeighborsClassifier  
KNeighborsClassifier(n_neighbors=2)
```

And, we can make predictions on the `X_test` dataframe.

In [15]:

```
preds = knn_model.predict(X_test)
```

To evaluate the KNN classifier, we provide a pre-defined method to return the commonly used evaluation metrics such as accuracy, recall, precision, f1score, and so on, based on the true classes in the 'y_test' and model predictions.

In [16]:

```
def evaluate_metrics(yt, yp):
    results_pos = {}
    results_pos['accuracy'] = accuracy_score(yt, yp)
    precision, recall, f_beta, _ = precision_recall_fscore_support(yt, yp, average='bina
    results_pos['recall'] = recall
    results_pos['precision'] = precision
    results_pos['f1score'] = f_beta
    return results_pos
```

In [17]:

```
evaluate_metrics(y_test, preds)
```

Out[17]:

```
{'accuracy': 0.9416058394160584,
 'recall': 0.875,
 'precision': 0.9545454545454546,
 'f1score': 0.9130434782608695}
```

We can see that there is a great classification performance on the tumor sample dataset. This means the KNN model can effectively recognize cancerous tumors. Next, it's your turn to try a different number of neighbors to see if we could get even better performance.

Coding exercise: Train and evaluate a KNN classifier with number of neighbors set to 5

First, define a KNN classifier with KNeighborsClassifier class:

In [18]:

```
# Type your code here
knn_model = KNeighborsClassifier(n_neighbors=5)
```

Then train the model with `X_train` and `y_train`:

In [19]:

```
# Type your code here
knn_model.fit(X_train, y_train.values.ravel())
```

Out[19]:

```
▼ KNeighborsClassifier
KNeighborsClassifier()
```

And, make predictions on `X_test` dataframe:

In [20]:

```
# Type your code here
model = KNeighborsClassifier(n_neighbors=5)
model.fit(X_train, y_train.values.ravel())
preds = model.predict(X_test)
evaluate_metrics(y_test, preds)
```

Out[20]:

```
{'accuracy': 0.9781021897810219,
 'recall': 0.9791666666666666,
 'precision': 0.9591836734693877,
 'f1score': 0.9690721649484536}
```

At last, you can evaluate your KNN model with provided `evaluate_metrics()` method.

[Click here for a sample solution](#)

Tune the number of neighbors to find the optimized one

OK, you may wonder which `n_neighbors` argument may give you the best classification performance. We can try different `n_neighbors` (the K value) and check which K gives the best classification performance.

Here we could try K from 1 to 50, and store the aggregated `f1score` for each k into a list.

In [21]:

```
# Try K from 1 to 50
max_k = 50
# Create an empty list to store f1score for each k
f1_scores = []
```

Then we will train 50 KNN classifiers with K ranged from 1 to 50.

In [22]:

```
for k in range(1, max_k + 1):
    # Create a KNN classifier
    knn = KNeighborsClassifier(n_neighbors=k)
    # Train the classifier
    knn = knn.fit(X_train, y_train.values.ravel())
    preds = knn.predict(X_test)
    # Evaluate the classifier with f1score
    f1 = f1_score(preds, y_test)
    f1_scores.append((k, round(f1_score(y_test, preds), 4)))
# Convert the f1score list to a dataframe
f1_results = pd.DataFrame(f1_scores, columns=['K', 'F1 Score'])
f1_results.set_index('K')
```


Out[22]:

F1 Score	
K	
1	0.9485
2	0.9130
3	0.9485
4	0.9583
5	0.9691
6	0.9583
7	0.9583
8	0.9474
9	0.9474
10	0.9474
11	0.9474
12	0.9474
13	0.9474
14	0.9474
15	0.9583
16	0.9583
17	0.9583
18	0.9583
19	0.9583
20	0.9583
21	0.9583
22	0.9583
23	0.9583
24	0.9583
25	0.9583
26	0.9583
27	0.9583
28	0.9474
29	0.9474
30	0.9474
31	0.9474
32	0.9474
33	0.9474
34	0.9362
35	0.9362
36	0.9362

F1 Score	
K	
37	0.9362
38	0.9362
39	0.9362
40	0.9362
41	0.9362
42	0.9362
43	0.9362
44	0.9362
45	0.9362
46	0.9362
47	0.9362
48	0.9362
49	0.9362
50	0.9362

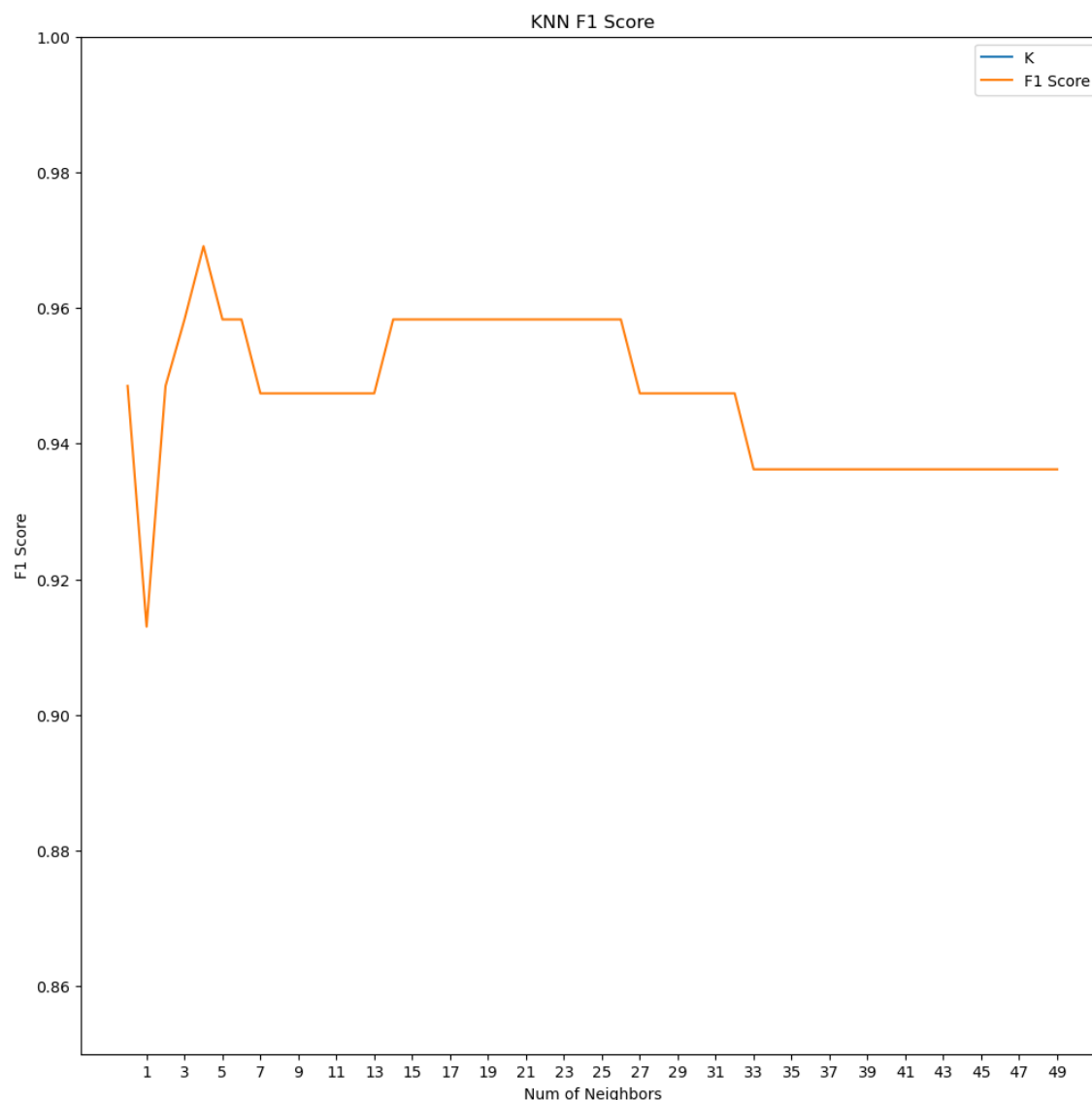
This is a long list and different to analysis, so let's visualize the list using a linechart.

In [23]:

```
# Plot F1 results
ax = f1_results.plot(figsize=(12, 12))
ax.set(xlabel='Num of Neighbors', ylabel='F1 Score')
ax.set_xticks(range(1, max_k, 2));
plt.ylim((0.85, 1))
plt.title('KNN F1 Score')
```

Out[23]:

Text(0.5, 1.0, 'KNN F1 Score')



As we can see from the F1 score linechart, the best K value is 5 with about 0.9691 f1score.

Next steps

Great! Now you have learned about and applied the KNN model to solve a real-world tumor type classification problem. You also tuned the KNN to find the best K value. Later, you will continue learning other popular classification models with different structures, assumptions, cost functions, and application scenarios.

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Other Contributors

Change Log

Date (YYYY-MM-DD)	Version	Changed By	Change Description
2021-11-9	1.0	Yan	Created the initial version
2022-3-29	1.1	Steve Hord	QA Pass

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