KNN

September 11, 2024

1 k-Nearest Neighbors (kNN) Algorithm

1.1 Overview

The k-Nearest Neighbors (kNN) algorithm is one of the simplest machine learning algorithms and is based on the idea that similar data points are likely to have similar outcomes. It is a non-parametric, lazy learning algorithm that is used for both classification and regression tasks.

1.1.1 How kNN Works

1. **Training Phase**: The kNN algorithm does not have an explicit training phase. Instead, it memorizes the training dataset.
2. **Prediction Phase**:
    - For a given test data point, the algorithm computes the distance between this test point and all training data points.
    - It then selects the 'k' closest training data points (neighbors).
    - The most common label among these neighbors is assigned as the prediction for the test point.

1.1.2 Key Points

- The choice of 'k' is crucial; a smaller 'k' can be sensitive to noise in the data, while a larger 'k' can make the algorithm computationally expensive.
- Common distance metrics used are Euclidean, Manhattan, and Minkowski.

1.1.3 Implementation Objective

In this notebook, we will implement the kNN algorithm from scratch using Python. We will test our implementation on a dataset and evaluate its performance using metrics such as confusion matrix, accuracy, recall, precision, and F1-score.

[34]:
```
!pip install seaborn
```

```
Requirement already satisfied: seaborn in c:\users\cassi\miniconda3\lib\site-
packages (0.13.2)
Requirement already satisfied: numpy!=1.24.0,>=1.20 in
c:\users\cassi\miniconda3\lib\site-packages (from seaborn) (1.26.4)
Requirement already satisfied: pandas>=1.2 in
c:\users\cassi\miniconda3\lib\site-packages (from seaborn) (2.2.2)
```

```
Requirement already satisfied: matplotlib!=3.6.1,>=3.4 in
c:\users\cassi\miniconda3\lib\site-packages (from seaborn) (3.8.4)
Requirement already satisfied: contourpy>=1.0.1 in
c:\users\cassi\miniconda3\lib\site-packages (from
matplotlib!=3.6.1,>=3.4->seaborn) (1.2.0)
Requirement already satisfied: cycler>=0.10 in
c:\users\cassi\miniconda3\lib\site-packages (from
matplotlib!=3.6.1,>=3.4->seaborn) (0.11.0)
Requirement already satisfied: fonttools>=4.22.0 in
c:\users\cassi\miniconda3\lib\site-packages (from
matplotlib!=3.6.1,>=3.4->seaborn) (4.51.0)
Requirement already satisfied: kiwisolver>=1.3.1 in
c:\users\cassi\miniconda3\lib\site-packages (from
matplotlib!=3.6.1,>=3.4->seaborn) (1.4.4)
Requirement already satisfied: packaging>=20.0 in
c:\users\cassi\miniconda3\lib\site-packages (from
matplotlib!=3.6.1,>=3.4->seaborn) (23.2)
Requirement already satisfied: pillow>=8 in c:\users\cassi\miniconda3\lib\site-
packages (from matplotlib!=3.6.1,>=3.4->seaborn) (10.4.0)
Requirement already satisfied: pyparsing>=2.3.1 in
c:\users\cassi\miniconda3\lib\site-packages (from
matplotlib!=3.6.1,>=3.4->seaborn) (3.0.9)
Requirement already satisfied: python-dateutil>=2.7 in
c:\users\cassi\miniconda3\lib\site-packages (from
matplotlib!=3.6.1,>=3.4->seaborn) (2.9.0.post0)
Requirement already satisfied: pytz>=2020.1 in
c:\users\cassi\miniconda3\lib\site-packages (from pandas>=1.2->seaborn) (2024.1)
Requirement already satisfied: tzdata>=2022.7 in
c:\users\cassi\miniconda3\lib\site-packages (from pandas>=1.2->seaborn) (2023.3)
Requirement already satisfied: six>=1.5 in c:\users\cassi\miniconda3\lib\site-
packages (from python-dateutil>=2.7->matplotlib!=3.6.1,>=3.4->seaborn) (1.16.0)
```

[35]:
```python
import numpy as np
from collections import Counter
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.metrics import precision_score, f1_score, recall_score,␣
↪confusion_matrix, roc_auc_score, roc_curve
```

1.1.4 kNN algorithm implementation

[36]:
```python
def euclidean_distance(x1, x2):
    return np.sqrt(np.sum((x1 - x2) ** 2))

def manhattan_distance(x1, x2):
    return np.sum(np.abs(x1 - x2))
```

```python
def minkowski_distance(x1, x2, p=2):
    return np.sum(np.abs(x1 - x2) ** p) ** (1 / p)

class KNN:
    def __init__(self, k=3, distance_metric='euclidean', weights='uniform',␣
↪p=2):
        """
        Initialize the k-Nearest Neighbors model.

        Parameters:
        - k: Number of neighbors to consider.
        - distance_metric: Metric for distance calculation ('euclidean',␣
↪'manhattan', 'minkowski').
        - weights: Weighting function ('uniform', 'distance').
        - p: Power parameter for Minkowski distance (used if␣
↪distance_metric='minkowski').
        """
        self.k = k
        self.distance_metric = distance_metric
        self.weights = weights
        self.p = p

    def fit(self, X, y):
        """
        Fit the model with the training data.

        Parameters:
        - X: Training data features.
        - y: Training data labels.
        """
        self.X_train = X
        self.y_train = y

    def predict(self, X):
        """
        Predict the class labels for the provided data.

        Parameters:
        - X: Data to predict labels for.

        Returns:
        - y_pred: Predicted labels.
        """
        y_pred = [self._predict(x) for x in X]
        return np.array(y_pred)
```

```
    def _predict(self, x):
        """
        Predict the class label for a single data point.

        Parameters:
        - x: Data point to predict.

        Returns:
        - Most common class label among the nearest neighbors.
        """
        # Compute distances between x and all examples in the training set
        if self.distance_metric == 'euclidean':
            distances = [euclidean_distance(x, x_train) for x_train in self.
↪X_train]
        elif self.distance_metric == 'manhattan':
            distances = [manhattan_distance(x, x_train) for x_train in self.
↪X_train]
        elif self.distance_metric == 'minkowski':
            distances = [minkowski_distance(x, x_train, self.p) for x_train in␣
↪self.X_train]
        else:
            raise ValueError(f"Unsupported distance metric: {self.
↪distance_metric}")

        # Sort by distance and return indices of the first k neighbors
        k_indices = np.argsort(distances)[:self.k]

        # Extract the labels of the k nearest neighbor training samples
        k_nearest_labels = [self.y_train[i] for i in k_indices]

        if self.weights == 'uniform':
            # Return the most common class label
            most_common = Counter(k_nearest_labels).most_common(1)
        elif self.weights == 'distance':
            # Weight by inverse distance
            weight_counts = Counter()
            for idx, label in zip(k_indices, k_nearest_labels):
                weight_counts[label] += 1 / (distances[idx] + 1e-10)  # Adding␣
↪a small constant to avoid division by zero
            most_common = weight_counts.most_common(1)
        else:
            raise ValueError(f"Unsupported weights option: {self.weights}")

        return most_common[0][0]
```

1.1.5 Evaluation function for kNN

[37]:
```
def evaluate_knn(X_train, X_test, y_train, y_test, k=3,␣
↪distance_metric='euclidean', weights='uniform', p=2):
    """
    Evaluate the k-Nearest Neighbors model.

    Parameters:
    - X_train, X_test: Training and test data features.
    - y_train, y_test: Training and test data labels.
    - k: Number of neighbors to consider.
    - distance_metric: Distance metric to use ('euclidean', 'manhattan',␣
↪'minkowski').
    - weights: Weighting function ('uniform', 'distance').
    - p: Power parameter for Minkowski distance (if applicable).
    """
    # Initialize and train the kNN model
    knn = KNN(k=k, distance_metric=distance_metric, weights=weights, p=p)
    knn.fit(X_train, y_train)

    # Predict on the test set
    predictions = knn.predict(X_test)

    # Calculate accuracy
    accuracy = np.sum(predictions == y_test) / len(y_test)
    print(f'Accuracy: {accuracy:.2f}')

    # Calculate precision, recall, and F1-score
    precision = precision_score(y_test, predictions, average='weighted')
    recall = recall_score(y_test, predictions, average='weighted')
    f1 = f1_score(y_test, predictions, average='weighted')

    print(f'Precision: {precision:.2f}')
    print(f'Recall: {recall:.2f}')
    print(f'F1 Score: {f1:.2f}')

    # Compute confusion matrix
    conf_matrix = confusion_matrix(y_test, predictions)
    classes = np.unique(y_test)

    # Plot normalized confusion matrix
    plt.figure(figsize=(8, 6))
    sns.heatmap(conf_matrix, annot=True, fmt="d", cmap="Blues",␣
↪xticklabels=classes, yticklabels=classes)
    plt.title("Confusion Matrix - kNN")
    plt.xlabel("Predicted Label")
    plt.ylabel("True Label")
```

```
    plt.show()

    # Calculate ROC-AUC score for binary classification
    if len(classes) == 2:
        roc_auc = roc_auc_score(y_test, predictions)
        print(f'ROC AUC Score: {roc_auc:.2f}')

        # Plot ROC Curve
        fpr, tpr, _ = roc_curve(y_test, predictions)
        plt.figure()
        plt.plot(fpr, tpr, label=f'ROC Curve (area = {roc_auc:.2f})')
        plt.plot([0, 1], [0, 1], linestyle='--')
        plt.xlabel('False Positive Rate')
        plt.ylabel('True Positive Rate')
        plt.title('Receiver Operating Characteristic (ROC) Curve')
        plt.legend(loc='lower right')
        plt.show()
    else:
        print("ROC AUC Score and ROC Curve are not applicable for multiclass␣
↪classification.")
```

1.1.6 Load and preprocess datasets

Iris Dataset

[38]:
```
iris = pd.read_csv('https://archive.ics.uci.edu/ml/machine-learning-databases/
↪iris/iris.data', header=None)
iris.columns = ['sepal_length', 'sepal_width', 'petal_length', 'petal_width',␣
↪'class']
iris['class'] = iris['class'].astype('category').cat.codes
X_iris = iris.iloc[:, :-1].values
y_iris = iris.iloc[:, -1].values
```

Penguins Dataset

[39]:
```
penguins = sns.load_dataset('penguins').dropna()
penguins['species'] = penguins['species'].astype('category').cat.codes
penguins['island'] = penguins['island'].astype('category').cat.codes
penguins['sex'] = penguins['sex'].astype('category').cat.codes
X_penguins = penguins.drop('species', axis=1).values
y_penguins = penguins['species'].values
```

Titanic Dataset

[40]:
```
# Carregar conjunto de dados Titanic
titanic = sns.load_dataset('titanic')

# Preencher valores faltantes sem usar inplace=True
titanic['age'] = titanic['age'].fillna(titanic['age'].mean())
titanic['embarked'] = titanic['embarked'].fillna(titanic['embarked'].mode()[0])
```

```
titanic = titanic.dropna(subset=['embark_town', 'sex', 'fare', 'class'])

# Transformar características categóricas em numéricas
titanic['sex'] = titanic['sex'].astype('category').cat.codes
titanic['embarked'] = titanic['embarked'].astype('category').cat.codes
titanic['class'] = titanic['class'].astype('category').cat.codes

# Separar características e rótulos
X_titanic = titanic[['pclass', 'sex', 'age', 'sibsp', 'parch', 'fare',␣
↪'embarked']].values
y_titanic = titanic['survived'].values
```

Census Income Dataset

[41]:
```
census = pd.read_csv('https://archive.ics.uci.edu/ml/machine-learning-databases/
↪adult/adult.data', header=None)
census.columns = ['age', 'workclass', 'fnlwgt', 'education', 'education-num',␣
↪'marital-status',
                  'occupation', 'relationship', 'race', 'sex', 'capital-gain',␣
↪'capital-loss',
                  'hours-per-week', 'native-country', 'income']
for column in ['workclass', 'education', 'marital-status', 'occupation',␣
↪'relationship', 'race', 'sex', 'native-country', 'income']:
    census[column] = census[column].astype('category').cat.codes
X_census = census.drop('income', axis=1).values
y_census = census['income'].values
```

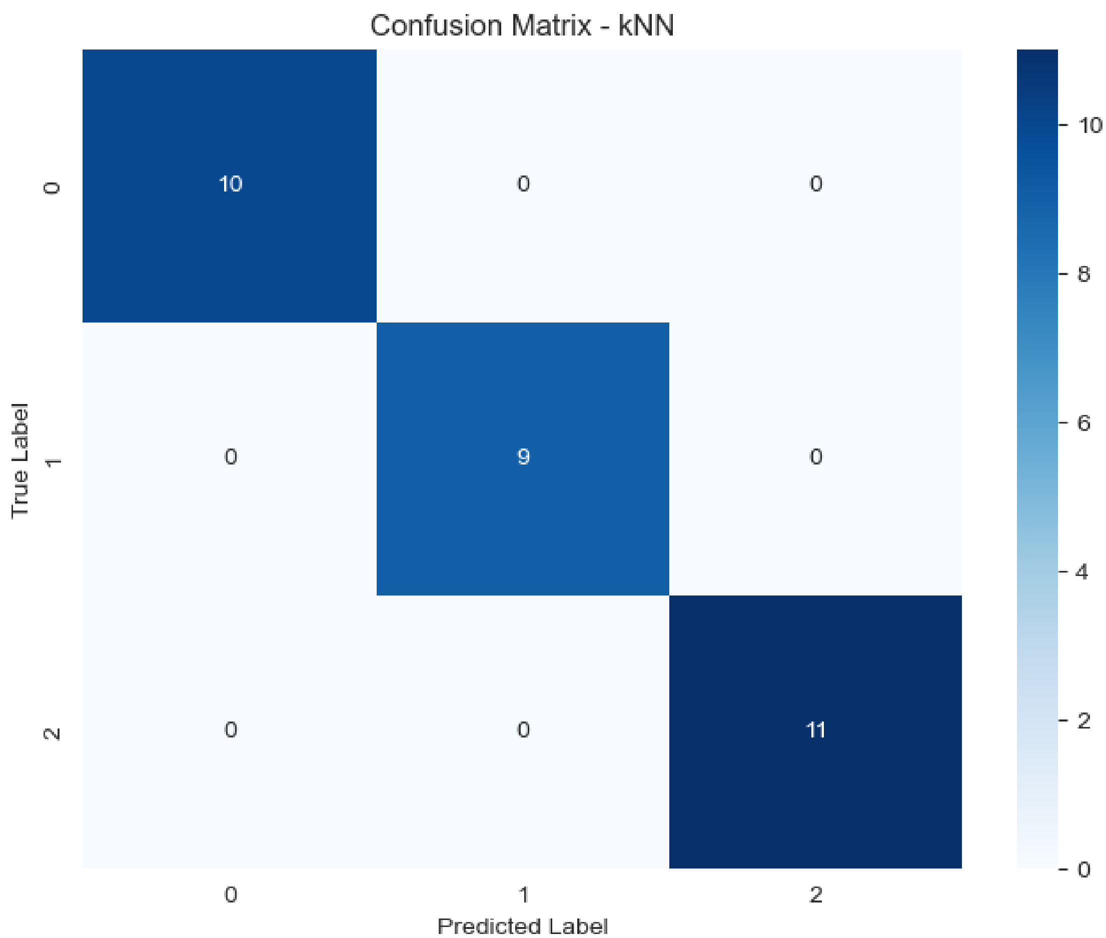
1.1.7 Test kNN on all datasets

[42]:
```
from sklearn.model_selection import train_test_split

datasets = {
    'Iris': {
        'data': (X_iris, y_iris),
        'k': 5,  # A moderate value to balance between overfitting and␣
↪underfitting. Suitable for a small dataset like Iris.
        'distance_metric': 'euclidean',  # Euclidean distance is appropriate␣
↪for continuous numeric features that are comparable.
        'weights': 'uniform',  # Uniform weights work well since the dataset is␣
↪balanced and well-separated.
        'p': 2  # p=2 corresponds to Euclidean distance, which is standard for␣
↪continuous data.
    },
    'Penguins': {
        'data': (X_penguins, y_penguins),
        'k': 7,  # A slightly larger k to reduce sensitivity to noise in a␣
↪moderately sized dataset.
```

```
        'distance_metric': 'euclidean',  # Suitable for continuous physical measurements, ensuring a natural distance measure.
        'weights': 'distance',  # Closer neighbors are more likely to belong to the same species; weighting by distance improves accuracy.
        'p': 2  # p=2 maintains Euclidean distance for continuous features.
    },
    'Titanic': {
        'data': (X_titanic, y_titanic),
        'k': 10,  # A larger k to provide more stability in the presence of class imbalance and mixed feature types.
        'distance_metric': 'manhattan',  # Manhattan distance is effective for datasets with mixed binary and continuous data.
        'weights': 'distance',  # Distance weighting gives more influence to closer neighbors, which can improve performance on noisy data.
        'p': 1  # p=1 corresponds to Manhattan distance, handling mixed feature types effectively.
    },
    'Census': {
        'data': (X_census, y_census),
        'k': 15,  # A higher k for better generalization in a large dataset with diverse categorical and continuous features.
        'distance_metric': 'minkowski',  # Provides flexibility in handling both types of features by adjusting p.
        'weights': 'uniform',  # Uniform weights help balance the influence of different points in a large, diverse dataset.
        'p': 1.5  # A mixed approach between Manhattan (p=1) and Euclidean (p=2) distances, suitable for varied feature types.
    }
}


for name, params in datasets.items():
    print(f"Testing kNN on {name} dataset with k={params['k']}, distance_metric={params['distance_metric']}, weights={params['weights']}, p={params['p']}")

    # Extract data and parameters
    X, y = params['data']
    k = params['k']
    distance_metric = params['distance_metric']
    weights = params['weights']
    p = params['p']

    # Split the data into training and testing sets
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
```

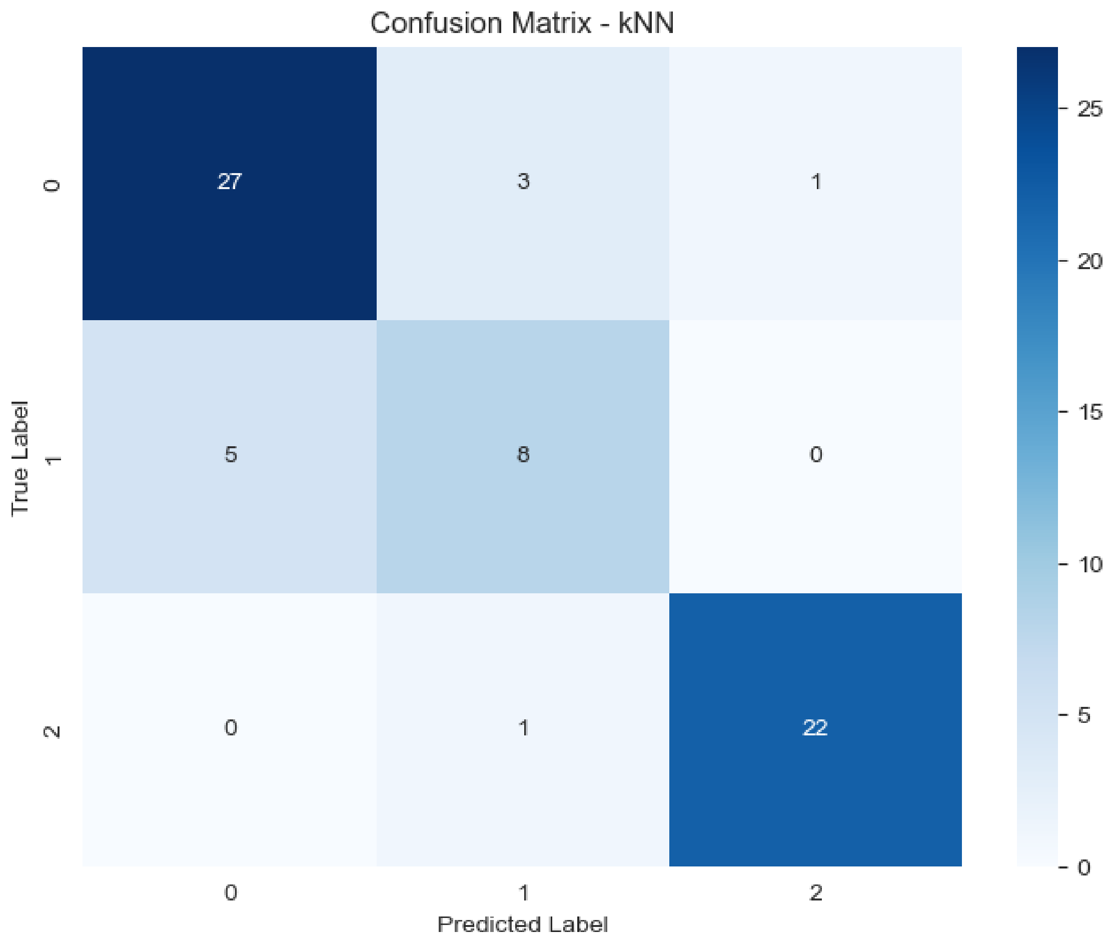
```
# Evaluate kNN with the specific parameters for the current dataset
evaluate_knn(X_train, X_test, y_train, y_test, k=k,␣
↪distance_metric=distance_metric, weights=weights, p=p)
```

```
Testing kNN on Iris dataset with k=5, distance_metric=euclidean,
weights=uniform, p=2
Accuracy: 1.00
Precision: 1.00
Recall: 1.00
F1 Score: 1.00
```

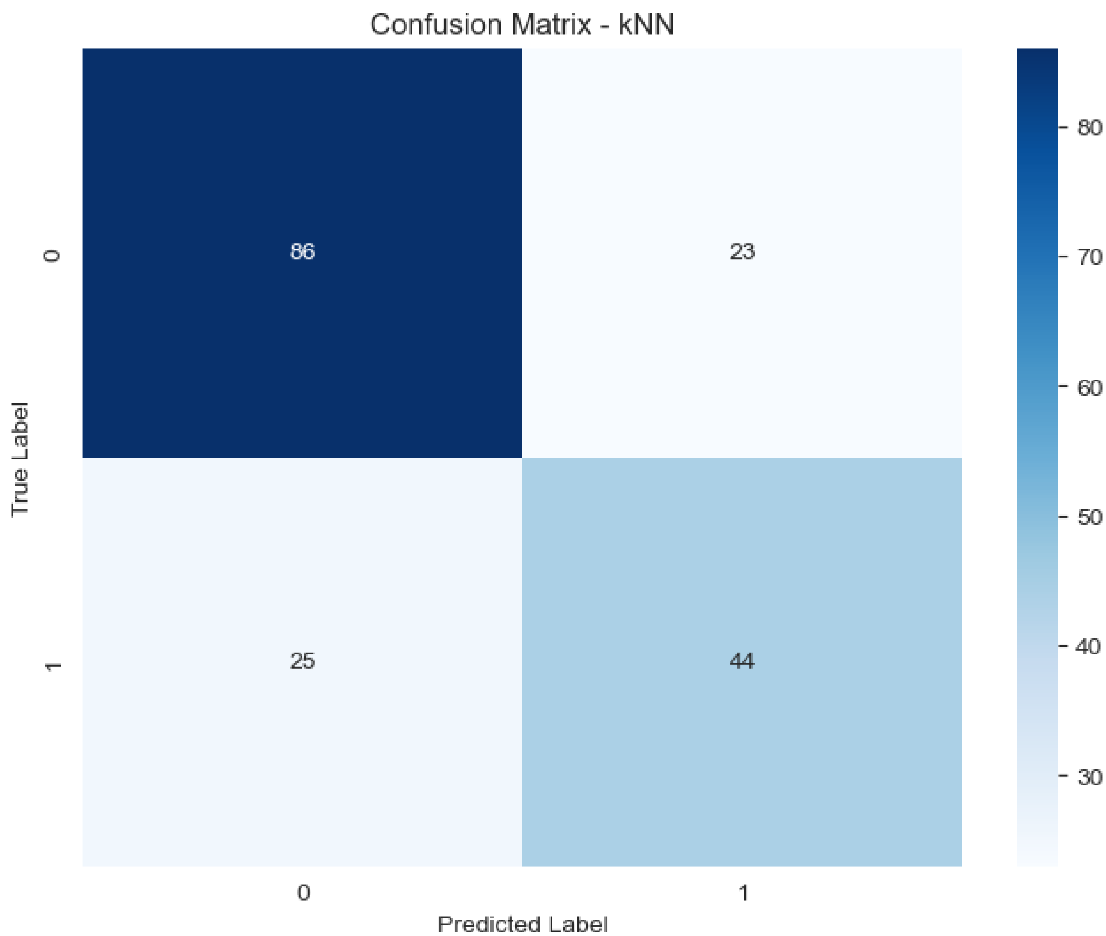



```
ROC AUC Score and ROC Curve are not applicable for multiclass classification.
Testing kNN on Penguins dataset with k=7, distance_metric=euclidean,
weights=distance, p=2
Accuracy: 0.85
Precision: 0.85
Recall: 0.85
```

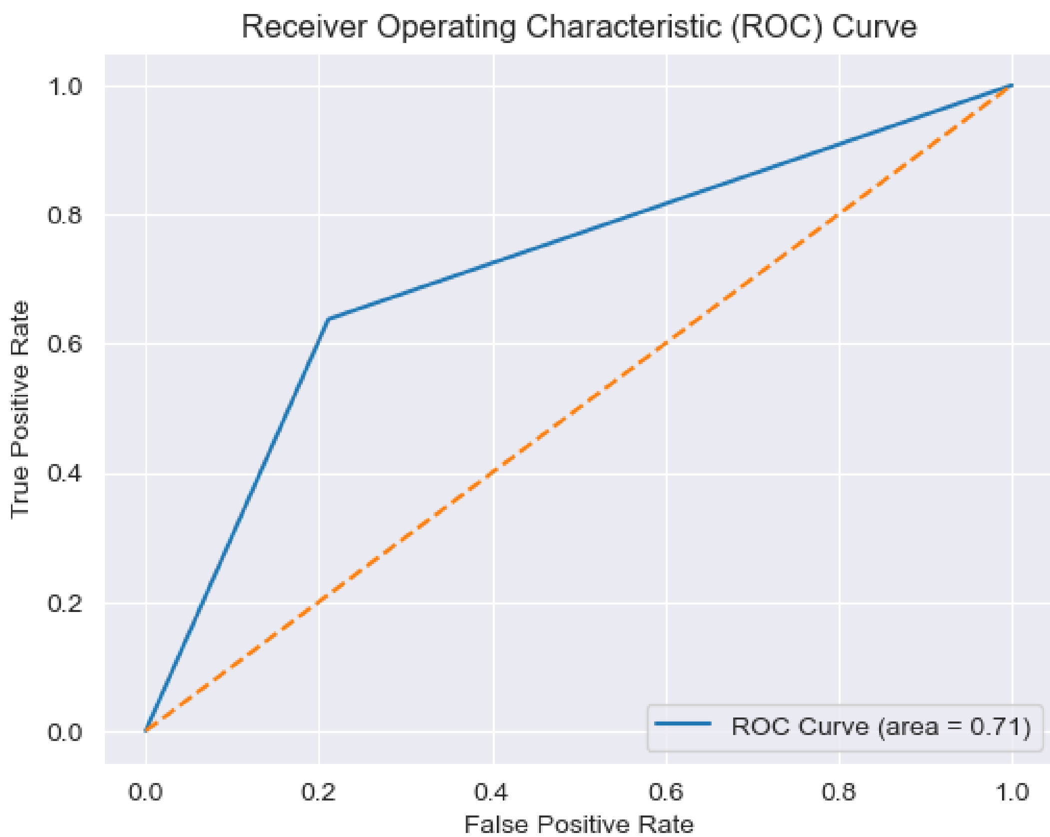
```
F1 Score: 0.85
```



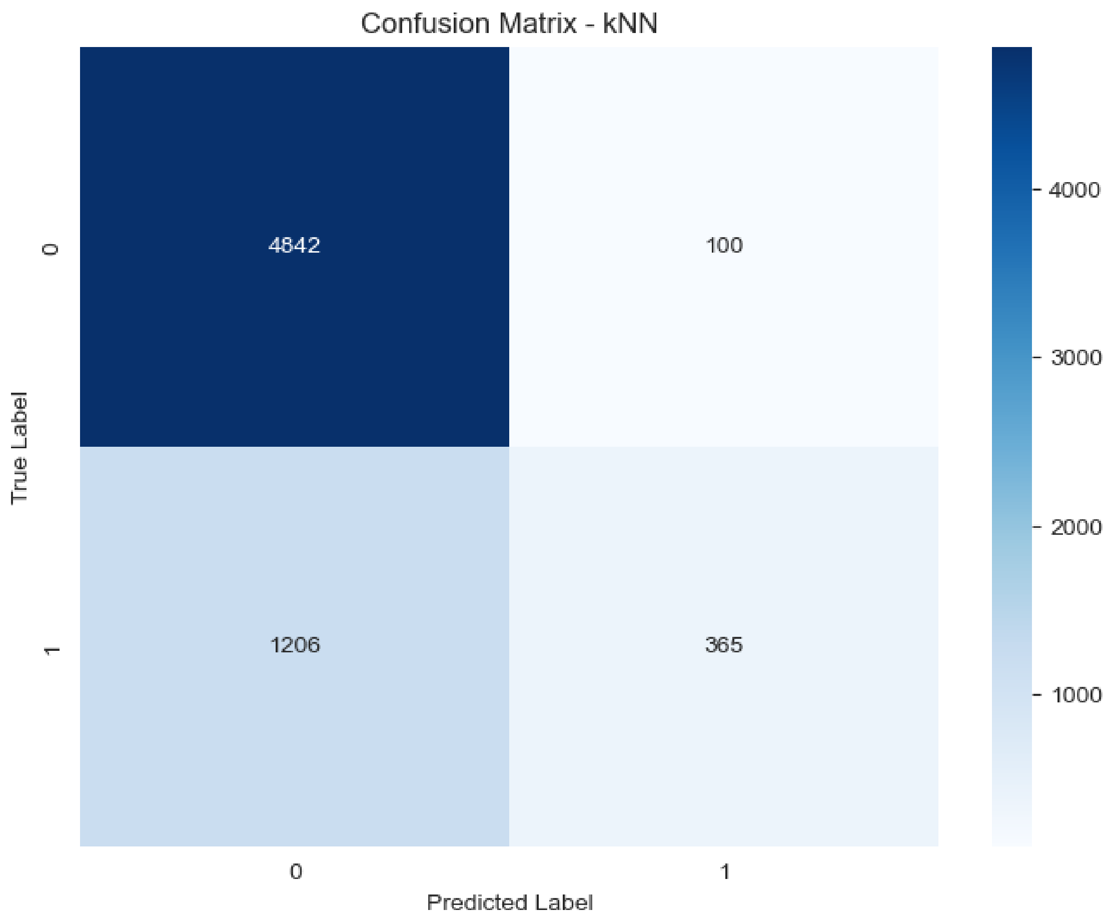

```
ROC AUC Score and ROC Curve are not applicable for multiclass classification.
Testing kNN on Titanic dataset with k=10, distance_metric=manhattan,
weights=distance, p=1
Accuracy: 0.73
Precision: 0.73
Recall: 0.73
F1 Score: 0.73
```



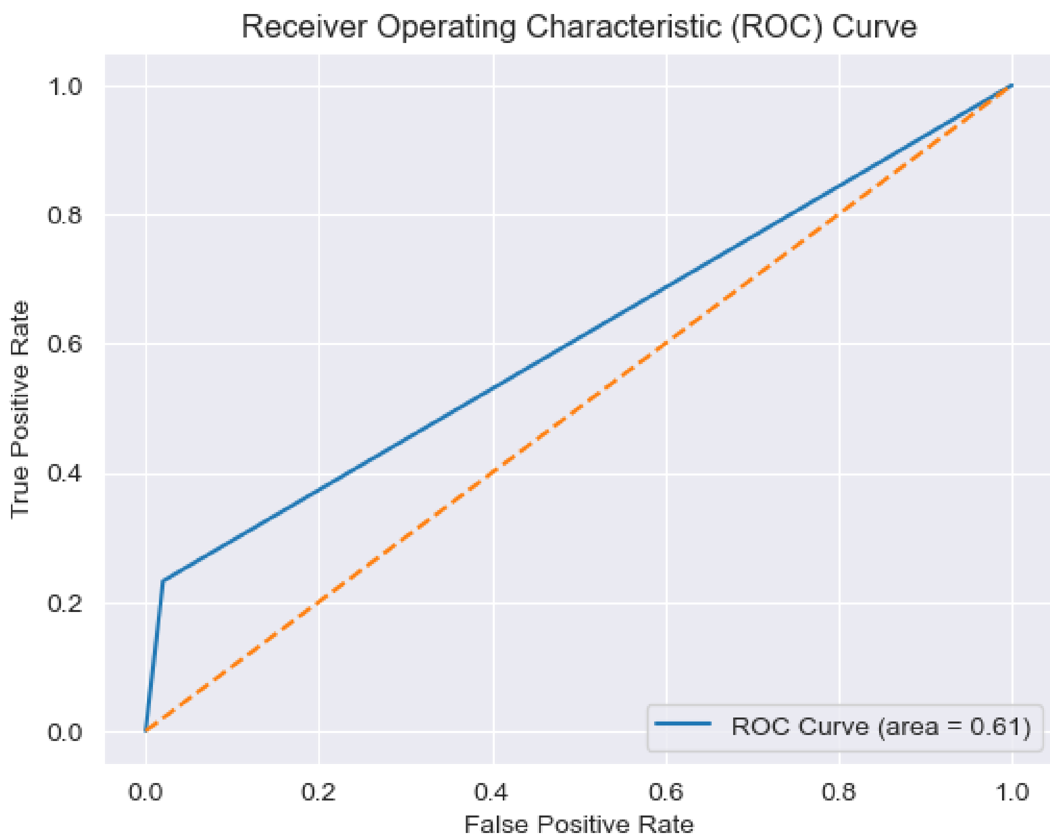

```
ROC AUC Score: 0.71
```




```
Testing kNN on Census dataset with k=15, distance_metric=minkowski,
weights=uniform, p=1.5
Accuracy: 0.80
Precision: 0.80
Recall: 0.80
F1 Score: 0.76
```



ROC AUC Score: 0.61


Receiver Operating Characteristic (ROC) Curve
1.0
0.8
0.6
0.4
0.2
0.0
True Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
False Positive Rate
ROC Curve (area = 0.61)