Air_Quality_Assessment_Project / index.ipynb

EngBrian refined the notebook 5b20a79 · 7 minutes ago

2768 lines (2768 loc) · 656 KB

Preview Code Blame Raw

Project Title: **Predicting Air Quality Using Machine Learning**

Name: Brian Kipyegon

Course: DSFT-12

Facilitator: Nikita Njoroge

Business Problem

Air pollution is a growing concern worldwide, impacting both the environment and human health. To support proactive decision-making, it is essential to develop models that can accurately classify air quality based on measurable environmental and demographic factors.

This project aims to create a machine learning model that classifies air quality levels (Good, Moderate, Poor, or Hazardous) with a target performance of over 0.8 recall_score. Such a model can assist policymakers, environmental agencies, and communities in monitoring pollution and mitigating its effects.

Project Objectives

1. Preprocess and Clean the Dataset Handle missing values, outliers, and ensure the dataset is well-formatted for modeling.
2. Explore and Analyze Feature Relationships Understand the impact of environmental and demographic variables on air quality levels through visualizations and correlation analysis.
3. Train Classification Models and Evaluate Performance Apply classification algorithms (Logistic Regression, Decision Trees, Random Tress, XGBoost) and optimize them to achieve at least 0.8 recall_score or equivalent performance.
4. Select the Best Model and Interpret Results Pick the model that works best and use it to draw recommendations

Dataset Overview

The dataset contains 5,000 records, each representing air quality observations in a

The dataset contains 5,000 records, each representing air quality observations in a specific region. The key features include:

- Temperature (°C)
- Humidity (%)
- PM2.5, PM10 (µg/m^3)
- NO2, SO2 (ppb)
- CO (ppm)
- Proximity to Industrial Areas (km)
- Population Density (people/km^2)
- Target: Air Quality Level (Good, Moderate, Poor, Hazardous)

Tools Used

Python (Pandas, NumPy, Matplotlib, Seaborn, Scikit-learn)

Jupyter Notebook

Classification Models (Logistic Regression, Decision Tress, Random Forest, Decision Trees)

Step 1: Load Data, Inspect and Preprocess

In [103…

```
# import necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
import seaborn as sns
import statsmodels.api as sm
from sklearn.model_selection import train_test_split, cross_val_score
from sklearn.preprocessing import MinMaxScaler,label_binarize
from sklearn.linear_model import LogisticRegression
from sklearn.tree import DecisionTreeClassifier,plot_tree
from imblearn.over_sampling import SMOTE
from sklearn.metrics import accuracy_score, precision_score, f1_score, recall
from sklearn.preprocessing import LabelEncoder
from sklearn.ensemble import RandomForestClassifier
from xgboost import XGBClassifier
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay
from sklearn.metrics import roc_curve, auc
import joblib
```

In [2]:
```
# Load the data
df = pd.read_csv('updated_pollution_dataset.csv')
df.head()
```

Out[2]:

	Temperature	Humidity	PM2.5	PM10	NO2	SO2	CO	Proximity_to_Industrial_Ar
0	29.8	59.1	5.2	17.9	18.9	9.2	1.72	
1	28.3	75.6	2.3	12.2	30.8	9.7	1.64	
2	23.1	74.7	26.7	33.8	24.4	12.6	1.63	
3	27.1	39.1	6.1	6.3	13.5	5.3	1.15	
4	26.5	70.7	6.9	16.0	21.9	5.6	1.01	

In [3]:
```
# check for the info
print(df.info())
print(f'The dataset has {df.shape[1]} columns and {df.shape[0]} rows')
# for column in df.columns:
#     print(f'The column "{column}" is of type {df[column].dtype}')
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 5000 entries, 0 to 4999
Data columns (total 10 columns):
 #   Column                        Non-Null Count  Dtype
---  ------                        --------------  -----
 0   Temperature                   5000 non-null   float64
 1   Humidity                      5000 non-null   float64
 2   PM2.5                         5000 non-null   float64
 3   PM10                          5000 non-null   float64
 4   NO2                           5000 non-null   float64
 5   SO2                           5000 non-null   float64
 6   CO                            5000 non-null   float64
 7   Proximity_to_Industrial_Areas 5000 non-null   float64
 8   Population_Density            5000 non-null   int64
 9   Air Quality                   5000 non-null   object
dtypes: float64(8), int64(1), object(1)
memory usage: 390.8+ KB
None
The dataset has 10 columns and 5000 rows
```

In [4]:
```
# check for duplicates
duplicates = df.duplicated()
print(f' Number of duplicates: {sum(duplicates)}')
```

```
Number of duplicates: 0
```

There are no duplicates in the dataset

In [5]:
```
# check for missing values
df.isna().sum()
```

Out[5]:
```
Temperature                    0
Humidity                       0
PM2.5                          0
PM10                           0
NO2                            0
SO2                            0
CO                             0
Proximity_to_Industrial_Areas  0
Population_Density             0
Air Quality                    0
dtype: int64
```

The dataset is clean as it has no missing values

In [6]:
```
# check for outliers in numerical columns

# Select only numerical columns
numeric_cols = df.select_dtypes(include='number')

# Calculate IQR for each numeric column
Q1 = numeric_cols.quantile(0.25)
Q3 = numeric_cols.quantile(0.75)
IQR = Q3 - Q1

# Identify rows with outliers
outlier_mask = (numeric_cols < (Q1 - 1.5 * IQR)) | (numeric_cols > (Q3 + 1.5
df_outliers = df[outlier_mask.any(axis=1)]

print(f"Number of rows with outliers: {df_outliers.shape[0]}")
```

```
Number of rows with outliers: 593
```

In [7]:
```
# replace outliers with median

df_imputed = numeric_cols.copy()

for col in numeric_cols.columns:
    lower = Q1[col] - 1.5 * IQR[col]
    upper = Q3[col] + 1.5 * IQR[col]
    median = df_imputed[col].median()
    df_imputed[col] = df_imputed[col].apply(
        lambda x: median if x < lower or x > upper else x
    )

# Replace in original DataFrame
df[numeric_cols.columns] = df_imputed
df_imputed
```

Out[7]:

	Temperature	Humidity	PM2.5	PM10	NO2	SO2	CO	Proximity_to_Industria
0	29.8	59.1	5.2	17.9	18.9	9.2	1.72	
1	28.3	75.6	2.3	12.2	30.8	9.7	1.64	
2	23.1	74.7	26.7	33.8	24.4	12.6	1.63	
3	27.1	39.1	6.1	6.3	13.5	5.3	1.15	

4	26.5	70.7	6.9	16.0	21.9	5.6	1.01
...	...	...	...	...	...	...	...
4995	40.6	74.1	12.0	21.7	45.5	25.7	2.11
4996	28.1	96.9	6.9	25.0	25.3	10.8	1.54
4997	25.9	78.2	14.2	22.1	34.8	7.8	1.63
4998	25.3	44.4	21.4	29.0	23.7	5.7	0.89
4999	24.1	77.9	12.0	21.7	23.2	10.5	1.38

5000 rows × 9 columns

In [8]:
```
# Rejoin the categorical columns to the imputed dataframe

# Get the categorical columns from the original DataFrame
categorical_cols = df.select_dtypes(exclude='number')

# Concatenate imputed numeric and original categorical columns
df_final = pd.concat([df_imputed, categorical_cols], axis=1)

df_final.head()
```

Out[8]:

	Temperature	Humidity	PM2.5	PM10	NO2	SO2	CO	Proximity_to_Industrial_Ar
0	29.8	59.1	5.2	17.9	18.9	9.2	1.72	
1	28.3	75.6	2.3	12.2	30.8	9.7	1.64	
2	23.1	74.7	26.7	33.8	24.4	12.6	1.63	
3	27.1	39.1	6.1	6.3	13.5	5.3	1.15	
4	26.5	70.7	6.9	16.0	21.9	5.6	1.01	

Step 2: Perform Exploratory Data Analysis (EDA)

In [9]:
```
# check for the decriptive statistics
df_final.describe()
```

Out[9]:

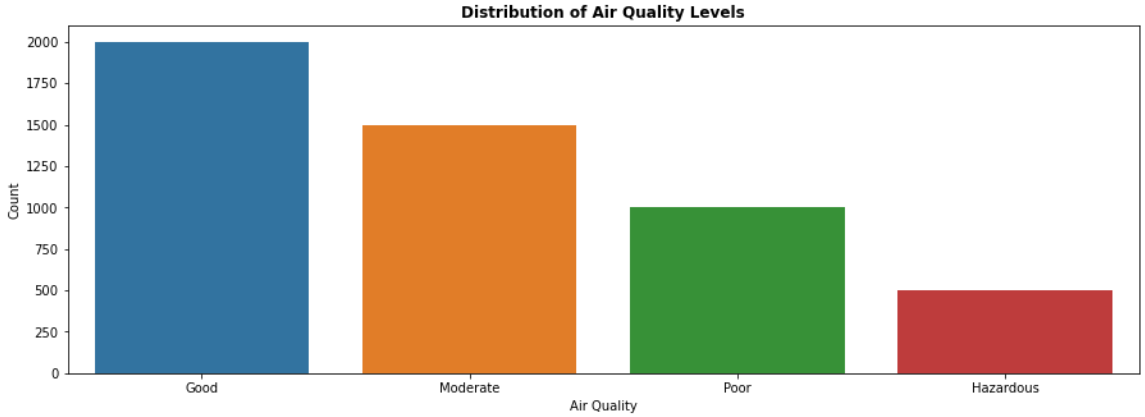
	Temperature	Humidity	PM2.5	PM10	NO2	SO2
count	5000.000000	5000.000000	5000.000000	5000.000000	5000.000000	5000.00000
mean	29.713060	69.870940	14.730400	24.645420	26.009500	9.44880
std	6.218252	15.576654	13.152195	16.169856	8.284051	5.85351

min	13.400000	36.000000	0.000000	-0.200000	7.400000	-6.20000
25%	25.100000	58.300000	4.600000	12.300000	20.100000	5.10000
50%	29.000000	69.800000	12.000000	21.700000	25.300000	8.00000
75%	33.700000	80.200000	20.625000	32.400000	31.325000	12.90000
max	47.300000	113.100000	58.300000	76.800000	49.500000	26.60000

In [10]:
```
# check for target class imbalance
df_final['Air Quality'].value_counts()
```

Out[10]:
```
Air Quality
Good         2000
Moderate     1500
Poor         1000
Hazardous     500
Name: count, dtype: int64
```

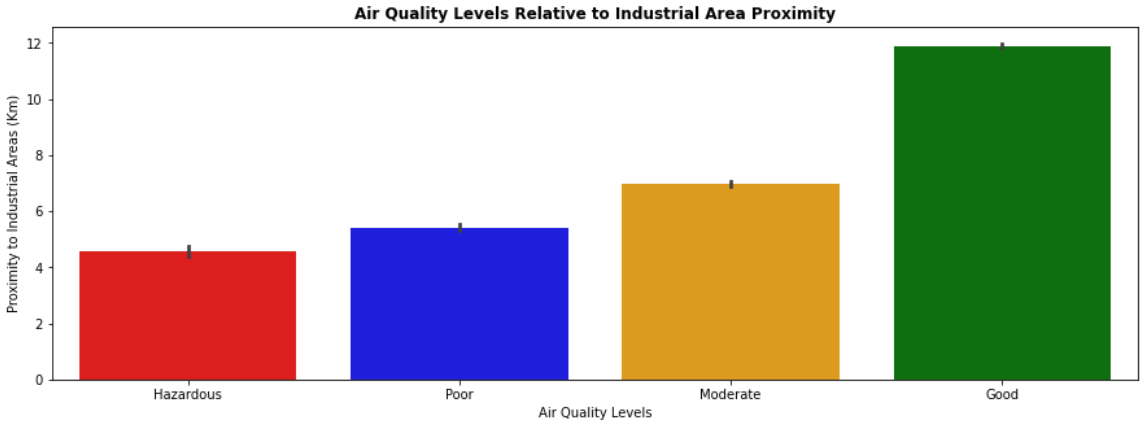
In [11]:
```
# plot a countplot of the target class
plt.figure(figsize=(15, 5))
sns.countplot(x='Air Quality', data=df_final, order=['Good', 'Moderate', 'Poo
plt.title('Distribution of Air Quality Levels', fontweight = 'bold')
plt.ylabel('Count')
plt.xlabel('Air Quality')
plt.show()
```



-> The dataset is imbalanced although not severe, we can impute using Smote

In [ ]:
```
# plot a graph of air quality against Proximity_to_Industrial_Areas

plt.figure(figsize=(15, 5))
custom_palette = {
    'Good': 'green',
    'Moderate': 'orange',
    'Poor': 'blue',
    'Hazardous': 'red'
}

# groupby the columns and sort them out by their index
```

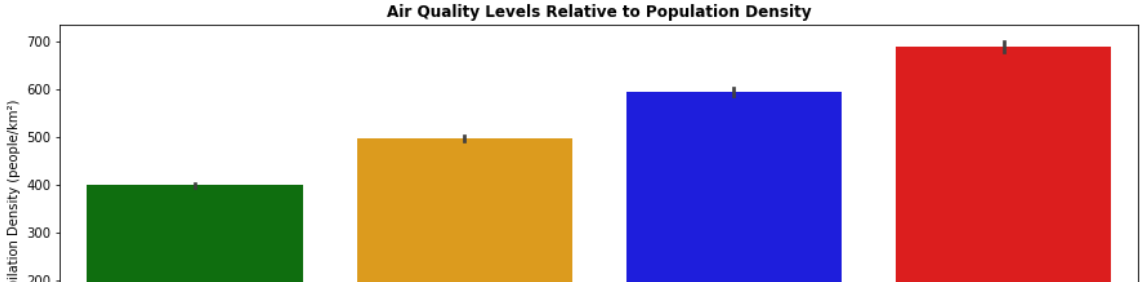
```
# groupby the columns and sort them out by their index
order = df_final.groupby('Air Quality')['Proximity_to_Industrial_Areas'].mean

sns.barplot(x=df_final['Air Quality'], y=df_final['Proximity_to_Industrial_Ar

plt.title('Air Quality Levels Relative to Industrial Area Proximity',fontweig
plt.xlabel('Air Quality Levels')
plt.ylabel('Proximity to Industrial Areas (Km)')
plt.show();
```



-> This graph indicates that the closer an area is to an industrial area, the more polluted the air quality tends to be.

In [13]:

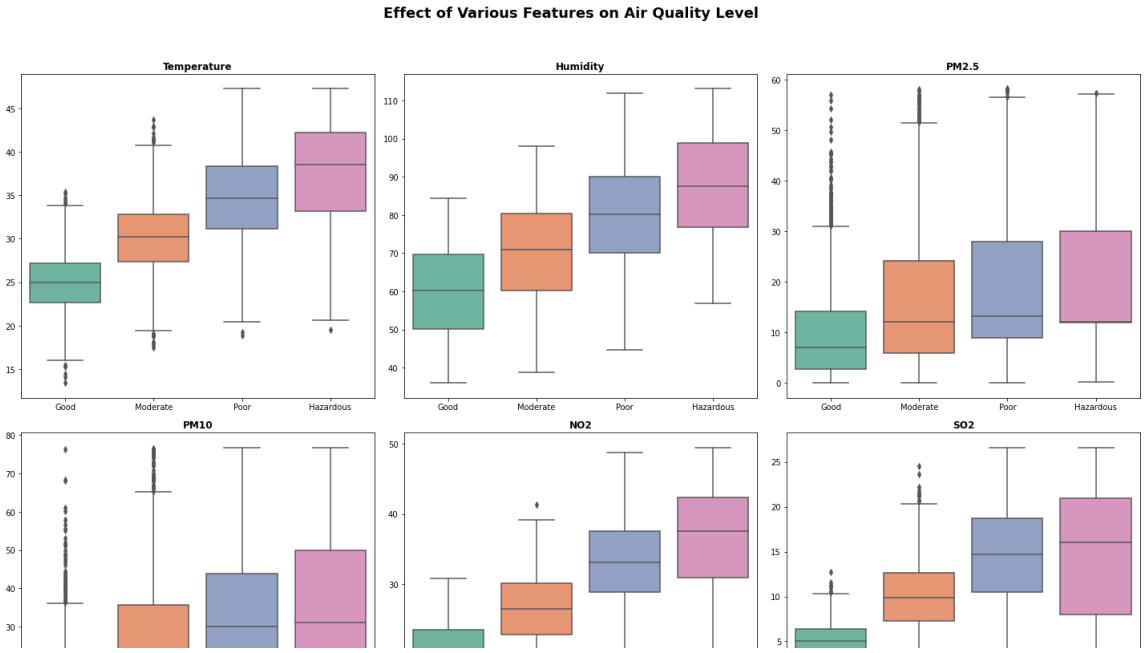
```
# Plot a graph of air quality levels against population density

plt.figure(figsize=(15, 5))
custom_palette = {
    'Good': 'green',
    'Moderate': 'orange',
    'Poor': 'blue',
    'Hazardous': 'red'
}

# groupby the columns and sort them out by their index
order = df_final.groupby('Air Quality')['Population_Density'].mean().sort_val

sns.barplot(x=df_final['Air Quality'], y=df_final['Population_Density'], orde

plt.title('Air Quality Levels Relative to Population Density', fontweight = '
plt.xlabel('Air Quality Levels')
plt.ylabel('Popilation Density (people/km²)')
plt.show();
```

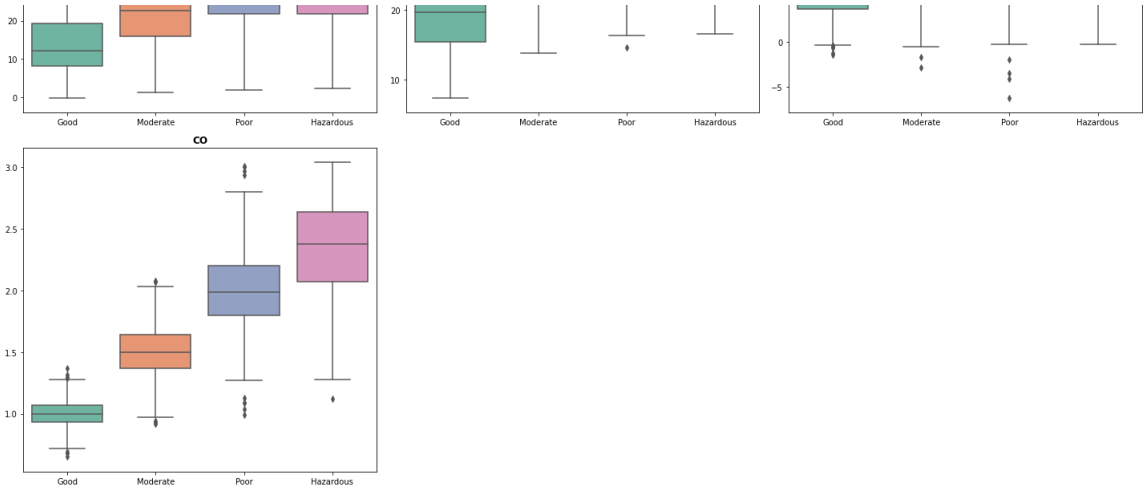


-> This graph indicates that areas with larger populations tend to have more polluted or hazardous air, while less populated areas generally experience better air quality.

In [14]:

```
# Plot a boxplot of the air quality against he other remaining features

# Set plot style and size
plt.figure(figsize=(20, 20))
plt.suptitle('Effect of Various Features on Air Quality Level', fontsize=18,

features = [
    'Temperature',
    'Humidity',
    'PM2.5',
    'PM10',
    'NO2',
    'SO2',
    'CO'
]

order = ['Good', 'Moderate', 'Poor', 'Hazardous']

# Create subplots for each feature
for i, feature in enumerate(features):
    plt.subplot(3, 3, i+1)
    sns.boxplot(x='Air Quality', y=feature, data=df_final, palette='Set2', or
    plt.title(feature, fontsize=12, fontweight='bold')
    plt.xlabel('')
    plt.ylabel('')

plt.tight_layout(rect=[0, 0, 1, 0.96])
plt.show()
```

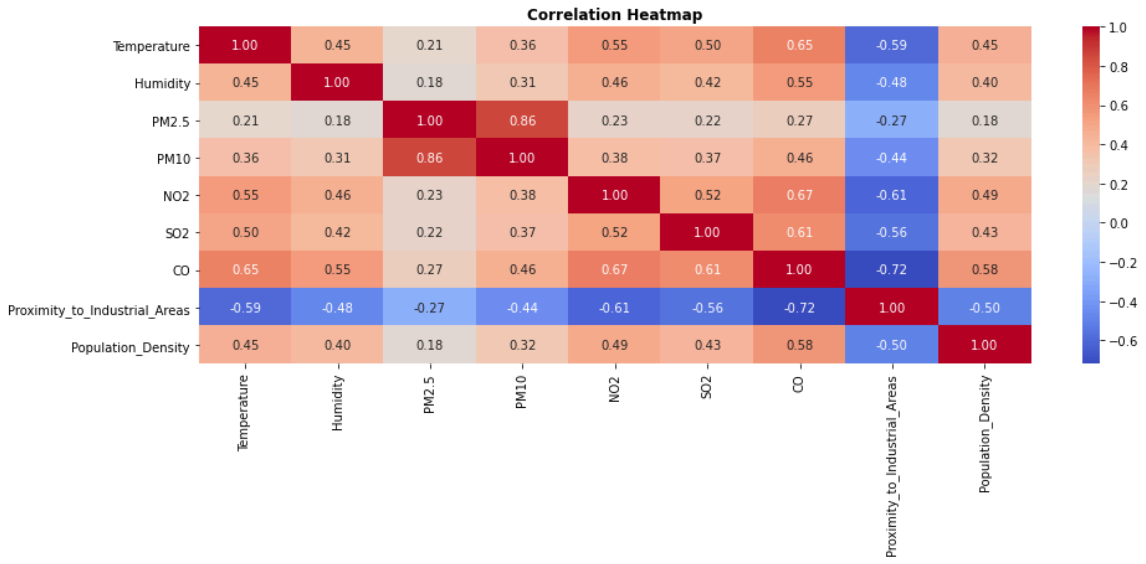




- From the boxplots, it's clear that PM2.5 and PM10 levels go up as the air quality gets worse, from Good to Hazardous. This means they play a big role in how bad the air is.
- CO also rises with poor air quality, so it's another important factor.
- NO2 and SO2 change a bit across the different air quality levels, but not as much. They still have some effect, just not as strong.
- Humidity and Temperature don't seem to change much between the categories, so they probably don't affect air quality that much.

In [15]:

```
# Plot a correlation for the numeric columns only

plt.figure(figsize=(15,5))
sns.heatmap(df_final.corr(numeric_only=True), annot=True, cmap='coolwarm', fm
plt.title('Correlation Heatmap', fontweight = 'bold')
plt.show();
```



- PM2.5 and PM10 are strongly related and both increase when air quality gets worse.
- PM2.5, PM10, NO2, and CO have a strong positive correlation with the Air Quality Index (AQI), meaning they are major contributors to air pollution.
- SO2 and Temperature have a weaker impact on AQI compared to other pollutants.
- Proximity to industrial areas shows a negative correlation with AQI, meaning the farther a place is from industrial zones, the better its air quality. This is expected since factories often release pollutants, so areas closer to them tend to have worse air quality.
- Population density is most strongly linked to CO levels because many everyday human activities release carbon (II) oxide.
- Humidity is negatively related to pollution - higher humidity usually means better air quality because moisture helps settle dust and pollutants.

Step 3: Modelling

(i) Modelling Preprocessing

Since the target variable is multiclass, it needs to be label encoded before being used in modeling.

In [16]:
```
# Encode the target variable

le = LabelEncoder()
df_final['Air Quality Encoded'] = le.fit_transform(df_final['Air Quality'])

# Convert encoded values to float
df_final['Air Quality Encoded'] = df_final['Air Quality Encoded'].astype(floa

# Check mapping
label_mapping = dict(zip(le.classes_, le.transform(le.classes_)))
print("Label Mapping:", label_mapping)
```

```
Label Mapping: {'Good': 0, 'Hazardous': 1, 'Moderate': 2, 'Poor': 3}
```

In [17]:
```
# perfom a train test split

X = df_final.drop(columns=['Air Quality', 'Air Quality Encoded'])
y = df_final['Air Quality Encoded']

X_train, X_test, y_train, y_test = train_test_split(X,y, test_size=0.2, rando
X_train
```

Out[17]:

	Temperature	Humidity	PM2.5	PM10	NO2	SO2	CO	Proximity_to_Industria
4227	38.8	92.5	8.3	29.0	32.8	8.3	2.19	
4676	26.3	54.1	0.9	10.3	25.1	4.5	0.95	
800	37.2	111.3	0.2	8.8	31.9	18.5	2.12	
3671	17.5	57.2	8.7	13.6	25.6	3.1	1.03	
4193	26.7	54.8	5.8	11.3	15.8	4.5	1.25	
...	...	...	...	...	...	...	...	
4426	30.0	59.7	12.0	68.8	22.1	7.4	1.39	
466	27.7	54.0	17.6	23.2	24.6	11.1	1.27	
3092	24.2	67.6	19.4	35.1	24.2	9.6	1.91	
3772	21.4	76.4	15.3	22.1	12.4	3.4	0.96	
860	34.4	103.1	29.2	42.2	25.3	23.6	1.41	

4000 rows × 9 columns

In [18]:

```
# Scale the X values using MinMaxScaler

scaler = MinMaxScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)

# Create DataFrame for scaled training data
X_train_df = pd.DataFrame(X_train_scaled, columns=X_train.columns, index=X_tr
X_train_df
X_test_scaled_df = pd.DataFrame(X_test_scaled, columns=X_test.columns, index=
X_test_scaled_df
```

Out[18]:

	Temperature	Humidity	PM2.5	PM10	NO2	SO2	CO	Prox
1501	0.528024	0.485084	0.205832	0.284416	0.425178	0.710366	0.790795	
2586	0.312684	0.425422	0.013722	0.114286	0.320665	0.262195	0.213389	
2653	0.353982	0.552529	0.070326	0.089610	0.330166	0.466463	0.313808	
1055	0.510324	0.856031	0.135506	0.341558	0.812352	0.984756	0.694561	
705	0.386431	0.234760	0.210978	0.201299	0.306413	0.350610	0.142259	
...	...	...	...	...	...	...	...	
4711	0.601770	0.412451	0.090909	0.088312	0.332542	0.490854	0.246862	
2313	0.271386	0.324254	0.322470	0.336364	0.180523	0.256098	0.154812	
3214	0.516224	0.732815	0.416810	0.388312	0.653207	0.737805	0.414226	

2732	0.424779	0.617380	0.406518	0.487013	0.444181	0.439024	0.238494
1926	0.507375	0.926070	0.607204	0.696104	0.565321	0.902439	0.451883

1000 rows × 9 columns

In [31]:
```
# Use SMOTE to oversample and solve the imbalance

smt = SMOTE()
X_train_resampled, y_train_resampled = smt.fit_resample(X_train_df,y_train)

# Create DataFrame for X_train_resampled
X_train_resampled_df = pd.DataFrame(X_train_resampled, columns=X_train_df.col

# Create DataFrame for y_train_resampled
y_train_resampled_df = y_train_resampled.to_frame(name='Target')

# check the shapes and balancing
print(X_train_resampled_df.shape)
print(y_train_resampled_df.shape)
X_train_resampled_df.head(), y_train_resampled_df.head()

y_train_resampled.value_counts()
```

```
(6364, 9)
(6364, 1)
```

Out[31]:
```
Air Quality Encoded
1.0    1591
0.0    1591
3.0    1591
2.0    1591
Name: count, dtype: int64
```

(ii) Build a logistic regression model using statsmodels

In [30]:
```
# Add constant
X_train_const = sm.add_constant(X_train_resampled_df)

# Fit Multinomial Logistic Regression
model = sm.MNLogit(y_train_resampled_df, X_train_const).fit()
print(model.summary())
```

```
Optimization terminated successfully.
         Current function value: 0.282815
         Iterations 14
                          MNLogit Regression Results
==============================================================================
Dep. Variable:                 Target   No. Observations:                 6364
Model:                        MNLogit   Df Residuals:                     6334
Method:                           MLE   Df Model:                           27
Date:                Mon, 02 Jun 2025   Pseudo R-squ.:                  0.7960
Time:                        13:19:52   Log-Likelihood:                -1799.8
```

```
converged:                       True   LL-Null:                       -8822.4
Covariance Type:            nonrobust   LLR p-value:                     0.000
================================================================================
==================
                     Target=1       coef    std err          z      P>|z|
[0.025      0.975]
--------------------------------------------------------------------------------
------------------
const                           -71.0188      3.913    -18.151      0.000     -
78.688     -63.350
Temperature                      27.8031      3.493      7.960      0.000
20.957      34.649
Humidity                         13.4254      1.947      6.895      0.000
9.609      17.242
PM2.5                            -8.6746      3.829     -2.265      0.023     -
16.180      -1.169
PM10                             14.6435      4.771      3.069      0.002
5.292      23.995
NO2                              29.3403      3.345      8.771      0.000
22.784      35.897
SO2                              25.8680      4.245      6.094      0.000
17.549      34.187
CO                               77.5313      6.184     12.537      0.000
65.411      89.652
Proximity_to_Industrial_Areas   -31.7910      2.643    -12.029      0.000     -
36.971     -26.611
Population_Density               17.2661      2.127      8.118      0.000
13.098      21.434
--------------------------------------------------------------------------------
------------------
                     Target=2       coef    std err          z      P>|z|
[0.025      0.975]
--------------------------------------------------------------------------------
------------------
const                           -27.8678      3.640     -7.657      0.000     -
35.002     -20.734
Temperature                      17.4551      3.393      5.144      0.000
10.804      24.106
Humidity                          3.2285      1.822      1.772      0.076
-0.343       6.800
PM2.5                            -6.3008      3.758     -1.677      0.094     -
13.667       1.065
PM10                             10.0093      4.697      2.131      0.033
0.803      19.216
NO2                              15.2468      3.245      4.698      0.000
8.886      21.607
SO2                              17.3210      4.191      4.133      0.000
9.108      25.534
CO                               48.8915      6.062      8.065      0.000
37.010      60.773
Proximity_to_Industrial_Areas   -17.2409      2.453     -7.029      0.000     -
22.048     -12.433
Population_Density                6.2949      2.013      3.127      0.002
2.349      10.241
--------------------------------------------------------------------------------
------------------
                     Target=3       coef    std err          z      P>|z|
[0.025      0.975]
--------------------------------------------------------------------------------
------------------
```

```
const                           -55.4338      3.863    -14.351      0.000     -
63.005     -47.863
Temperature                      24.9228      3.479      7.164      0.000
18.104      31.741
Humidity                          9.4481      1.922      4.916      0.000
5.681      13.215
PM2.5                            -7.8607      3.811     -2.063      0.039     -
15.330      -0.391
PM10                             13.0637      4.752      2.749      0.006
3.750      22.378
NO2                              25.4564      3.329      7.646      0.000
18.931      31.982
SO2                              24.1124      4.236      5.693      0.000
15.811      32.414
CO                               70.2198      6.173     11.375      0.000
58.121      82.319
Proximity_to_Industrial_Areas   -25.2976      2.589     -9.770      0.000     -
30.373     -20.223
Population_Density               11.8634      2.100      5.649      0.000
7.748      15.979
==============================================================================
=================
```

Model Interpretation

- Pseudo R-squares = 0.7960; The model explains 79.6% of the variability in air quality categories.
- LLR p-value = 0.000; The model is statistically significant

Below is a breakdown of the predictors and how they influence the air quality

→ CO (Carbon (II) Oxide) – Coefficient: 77.53

- The strongest positive predictor. A one-unit increase in CO greatly increases the likelihood of poor air quality.

→ NO2 (Nitrogen (IV) Oxide) – Coefficient: 29.34

- A strong positive contributor. Higher NO2 levels significantly raise the chance of poor air quality

→ SO2 (Sulfur (IV) Oxide) – Coefficient: 25.87

- Significantly increases the likelihood of poor air quality.

→ Proximity to Industrial Areas – Coefficient: -31.79

- Strong negative effect. As distance from industrial areas decreases, the risk of poor air quality increases sharply.

→ Temperature – Coefficient: 27.80

- Higher temperatures are associated with worse air quality, possibly due to

- Higher temperatures are associated with worse air quality, possibly due to enhanced chemical reactions or trapped pollutants.

→ Population Density – Coefficient: 17.26

- Densely populated areas are more likely to have poor air quality due to more pollution from human activities.

→ Humidity – Coefficient: 13.43

- Moderately increases the likelihood of poor air quality, possibly due to its effect on particle suspension and chemical interactions.

→ PM10 (Coarse Particulate Matter) – Coefficient: 14.64

- Has a mild positive effect. Higher PM10 slightly increases the chance of poor air quality.

→ PM2.5 (Fine Particulate Matter) – Coefficient: -8.67

- Although statistically significant, PM2.5 shows a negative effect, suggesting that higher levels are associated with better air quality, which may warrant further investigation.

Conclusion

- The strongest predictors of poor air quality are CO, NO_2, SO_2, temperature, population density, and proximity to industrial areas.
- Humidity and PM10 show moderate influence on air quality.
- While PM2.5 is often used as a key pollution metric, it showed a weak negative relationship in this model and may not be a strong standalone predictor in this case.
- The model highlights key areas to target for pollution control, such as industrial zones and densely populated areas. Further refinement could explore non-linear patterns or interactions between variables.

Why PM2.5 and PM10 May Seem Important, But Don't Stand Out in Regression Models

Even though PM2.5 and PM10 levels rise as air quality worsens as clearly shown in boxplots and correlation matrices, they don't emerge as strong predictors in logistic regression models. This is likely due to multicollinearity, where PM2.5 and PM10 are highly correlated with each other and with other pollutants like CO, NO_2, and SO_2. Such overlap makes it challenging for the regression model to determine the unique impact of each pollutant, leading to inflated standard errors and less reliable coefficient estimates. Therefore, despite their apparent importance, PM2.5 and PM10

may not appear statistically significant in the regression analysis.

For building a predictive model I will use the strongest predictors as stated in our conclusion above.

(iii) Build a predictive model

I will begin by performing cross-validation with each model and use recall_macro as the scoring metric

In [102…

```
# Define function
def cv_models(X, y):
    # Flatten y to avoid DataConversionWarning
    y = y.values.ravel() if hasattr(y, 'values') else y.ravel()

    # Instantiate models
    logreg = LogisticRegression()
    dt = DecisionTreeClassifier()
    rf = RandomForestClassifier()
    xgb = XGBClassifier()

    models = {
        'Logistic Regression': logreg,
        'Decision Tree': dt,
        'Random Forest': rf,
        'XGBoost': xgb
    }

    results = {}
    for name, model in models.items():
        scores = cross_val_score(model, X, y, scoring='recall_macro',cv=10)
        results[name] = scores.mean()

    return results

# Call the function
X_train_resampled_ref = X_train_resampled_df[['CO', 'NO2', 'SO2', 'Population
cv_scores = cv_models(X_train_resampled_ref, y_train_resampled_df)

# Print the results
for model, score in cv_scores.items():
    print(f'Average Recall Score for {model} = {score}')
```

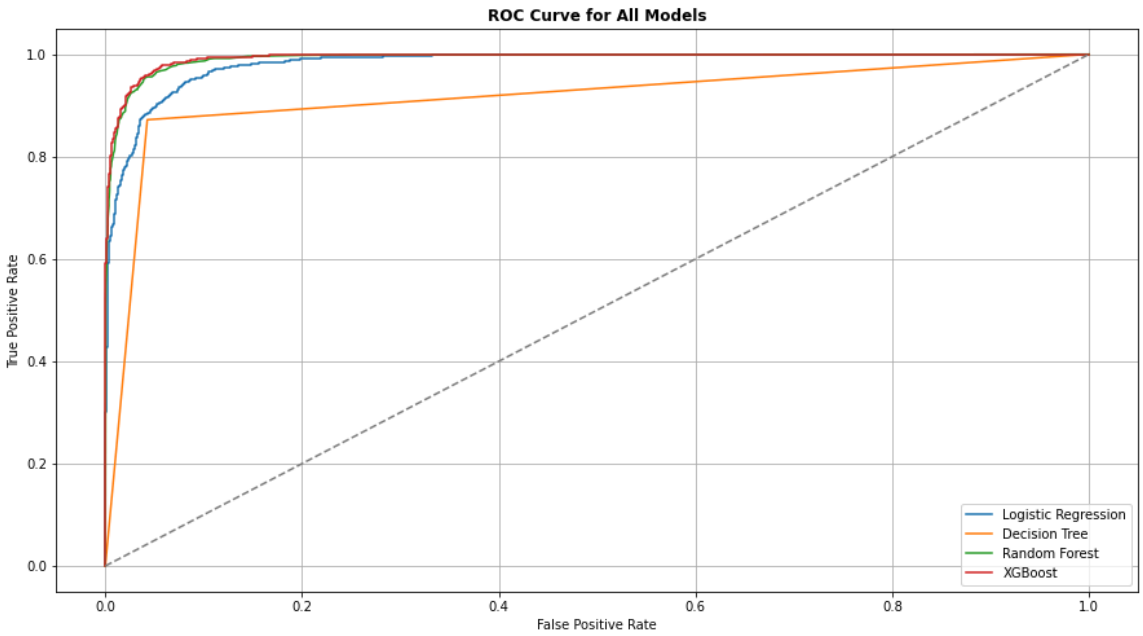
```
Average Recall Score for Logistic Regression = 0.8474331761006291
Average Recall Score for Decision Tree = 0.8925216194968553
Average Recall Score for Random Forest = 0.9321216588050314
Average Recall Score for XGBoost = 0.9277230738993711
```

Plot ROC Curves to compare all the models

In [60]:

```
# Binarize the y_test for ROC curve (assuming 4 classes: 0 to 3)
y_test_bin = label_binarize(y_test.values.ravel() if hasattr(y_test, 'values'
```

```
# Define models in a dictionary
models = {
    'Logistic Regression': LogisticRegression(),
    'Decision Tree': DecisionTreeClassifier(),
    'Random Forest': RandomForestClassifier(),
    'XGBoost': XGBClassifier()
}

# Select features
X_test_scaled_ref = X_test_scaled_df[['CO', 'NO2', 'SO2', 'Population_Density
X_train_ref = X_train_resampled_ref
y_train_ref = y_train_resampled_df.values.ravel() if hasattr(y_train_resample

# Plotting ROC curves
plt.figure(figsize=(15, 8))

for name, model in models.items():
    model.fit(X_train_ref, y_train_ref)
    y_prob = model.predict_proba(X_test_scaled_ref)

    # Compute ROC curve
    fpr, tpr, _ = roc_curve(y_test_bin.ravel(), y_prob.ravel())

    plt.plot(fpr, tpr, label=f'{name}')

plt.plot([0, 1], [0, 1], linestyle='--', color='grey')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Curve for All Models', fontweight='bold')
plt.legend()
plt.grid(True)
plt.show()
```



Print out the AUC for each model

In [95]:

```
# Dictionary to store AUC scores
```

```
# Dictionary to store AUC scores
auc_scores = {}

# Flatten the target
y_train_flat = y_train_resampled_df.values.ravel() if hasattr(y_train_resampl

# Fit models and compute AUC
for name, model in models.items():
    model.fit(X_train_resampled_ref, y_train_flat)
    y_prob = model.predict_proba(X_test_scaled_ref)

    # Compute ROC curve and AUC
    fpr, tpr, threshold = roc_curve(y_test_bin.ravel(), y_prob.ravel())
    auc_score = auc(fpr, tpr)

    # Store and print AUC
    auc_scores[name] = auc_score
    print(f'{name} AUC score: {auc_score}')
```

```
Logistic Regression AUC score: 0.982286
Decision Tree AUC score: 0.9186666666666667
Random Forest AUC score: 0.9916551666666668
XGBoost AUC score: 0.9934746666666667
```

Model Selection Justification

- Given the multiclass nature of the Air Quality target (Good, Moderate, Poor, Hazardous), macro recall is the most suitable metric. It emphasizes correctly identifying all classes, especially reducing false negatives, which is crucial since misclassifying Poor or Hazardous air as safer levels can pose serious health risks.
- While XGBoost slightly outperformed Random Forest in AUC, Random Forest had a marginally better recall score (0.005 higher), indicating it's more effective at capturing all true cases, especially the dangerous ones.
- Since false positives (predicting worse air quality than actual) are less risky than false negatives in this context, Random Forest is preferred for its better recall and reliability in detecting harmful air quality.
- Decision Tree will be used as the baseline model due to its interpretability and simplicity, allowing for straightforward comparison and performance benchmarking against more complex models.

Baseline Model: Decision Trees Model

In [83]:

```
# fit the Decision Trees classifier and use it to predict the test data
dt = DecisionTreeClassifier(class_weight='balanced',random_state=42)
dt.fit(X_train_resampled_ref, y_train_resampled)

y_dt_train_pred = dt.predict(X_train_resampled_ref)
y_dt_test_pred = dt.predict(X_test_scaled_ref)
```

In [84]:
```
# Test for overfitting or underfitting

train_dt_recall_score = recall_score(y_train_resampled_df, y_dt_train_pred, a
test_dt_recall_score = recall_score(y_test, y_dt_test_pred, average='macro')

print(f' The Recall score for Decision Tress train data is : {train_dt_recall
print(f' The Recall score for Decision Trees test data is : {test_dt_recall_s
```

```
The Recall score for Decision Tress train data is : 1.0
The Recall score for Decision Trees test data is : 0.8282131427870163
```

- The Decision Tree model achieved a perfect recall score of 1.0 on the training data, indicating that it correctly identified all true instances across all classes. However, the recall dropped to 0.828 on the test data, suggesting some overfitting.
- While the model performs exceptionally well on training data, its generalization to unseen data is less accurate, missing some true cases, especially critical in detecting harmful air quality levels.

Use GridSearchCV to fine tune the Decision Trees model

In [85]:
```
# Create the grid of parameters to search

param_grid = {
    'max_depth': [3, 4, 5],                    # Limits tree depth to prevent
    'min_samples_split': [10, 15, 20],         # Minimum samples needed to sp
    'min_samples_leaf': [5, 10],               # Minimum samples required at
    'max_features': ['sqrt', 0.3, 0.4, 0.5],   # Number of features to consid
}


# Grid Search using macro recall
grid_search = GridSearchCV(estimator=dt, param_grid=param_grid,
                           cv=5, scoring='recall_macro', n_jobs=-1, verbose=2
grid_search.fit(X_train_resampled_ref, y_train_resampled)

# Best model
best_dt = grid_search.best_estimator_
print(f"Best Parameters: {grid_search.best_params_}")

# Evaluate
train_pred = best_dt.predict(X_train_resampled_ref)
test_pred = best_dt.predict(X_test_scaled_ref)

train_recall_dt = recall_score(y_train_resampled, train_pred, average='macro'
test_recall_dt = recall_score(y_test, test_pred, average='macro')
gap_dt = abs(train_recall_dt - test_recall_dt)

print(f"Training Decision Trees Recall Score: {train_recall_dt}")
print(f"Test Decision Trees Recall Score: {test_recall_dt}")
print(f"Recall Decision Trees Score Gap: {gap_dt}")
```

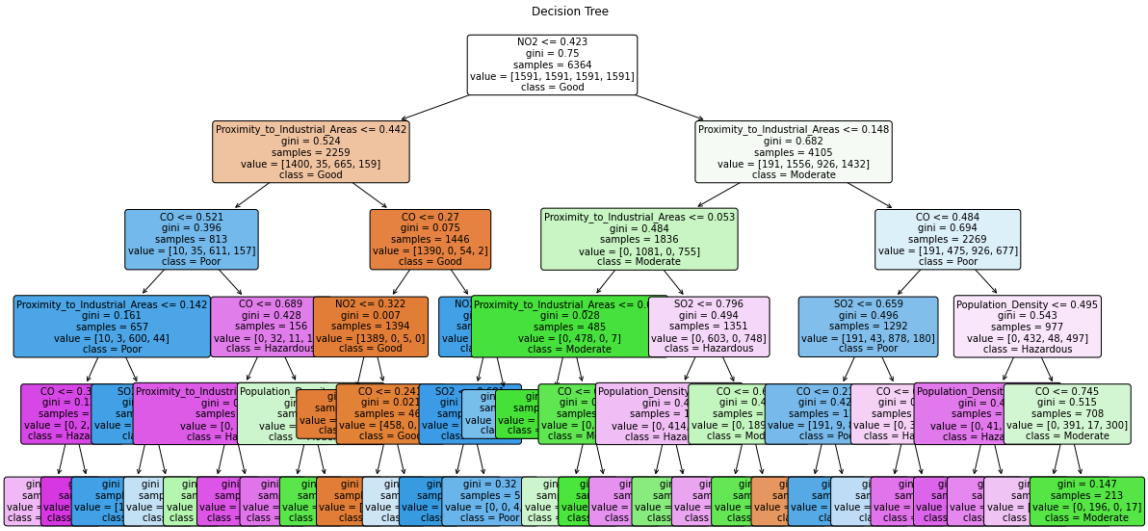
```
# Check for overfitting
if train_recall_dt - test_recall_dt > 0.05:
    print(" Potential overfitting detected: The model performs significantly
else:
    print(" No significant overfitting detected: The model generalizes well t
```

```
Fitting 5 folds for each of 72 candidates, totalling 360 fits
Best Parameters: {'max_depth': 5, 'max_features': 'sqrt', 'min_samples_leaf':
5, 'min_samples_split': 20}
Training Decision Trees Recall Score: 0.8452231301068509
Test Decision Trees Recall Score: 0.8459220136064863
Recall Decision Trees Score Gap: 0.0006988834996354276
 No significant overfitting detected: The model generalizes well to unseen dat
a.
```

Decision Tree Plot

In [ ]:

```
feature_names = X_test_scaled_ref.columns if hasattr(X_test_scaled_ref, 'colu

plt.figure(figsize=(20, 10))
plot_tree(best_dt,
          feature_names=feature_names,
          class_names=['Good', 'Moderate', 'Poor', 'Hazardous'],
          filled=True,
          rounded=True,
          fontsize=10)
plt.title("Decision Tree")
plt.show()
```



This plot represents a single decision tree trained on air quality data. Each node shows a decision based on a feature split (e.g., CO levels, NO_2 concentration, etc.). The tree branches based on these thresholds, ultimately assigning samples to one of four air quality categories: Good, Moderate, Poor, or Hazardous.

Splits: The tree performs multiple splits, each reducing uncertainty and improving classification

classification.

Color Intensity: Nodes are color-coded based on the majority class and how pure (confident) that node is.

Leaf Nodes: Terminal nodes (leaves) show the final predicted class.

This visualization helps interpret how the model makes decisions and which features are most frequently used in the splits.

Model 2: Random Forest Model

In [86]:
```
# fit the Random Forest classifier and use it to predict the test data
rf = RandomForestClassifier(class_weight='balanced',random_state=42,max_sampl
rf.fit(X_train_resampled_ref, y_train_resampled)

y_rf_train_pred = rf.predict(X_train_resampled_ref)
y_rf_test_pred = rf.predict(X_test_scaled_ref)
```

In [108…
```
# Test for overfitting or underfitting

train_rf_recall_score = recall_score(y_train_resampled_df, y_rf_train_pred, a
test_rf_recall_score = recall_score(y_test, y_rf_test_pred, average='macro')

print(f' The Recall score for Random Forest train data is : {train_rf_recall_
print(f' The Recall score for Random Forest test data is : {test_rf_recall_sc
```

```
The Recall score for Random Forest train data is : 0.9995285983658077
The Recall score for Random Forest test data is : 0.8907231420864763
```

- The model appears to be overfitting, as indicated by the noticeable gap between the training recall score and the test recall score.
- It performs exceptionally well on the training data but struggles with new, unseen data, implying it may be learning the training data too closely instead of capturing general patterns.

Use GridSearchCV to fine tune the Random Forest model

In [88]:
```
# Create the grid of parameters to search

param_grid = {
    'n_estimators': [50, 100, 150],                # fewer trees reduce over
    'max_depth': [4, 6, 8],                        # shallower trees general
    'min_samples_split': [5, 10],                  # higher values prevent o
    'min_samples_leaf': [3, 5, 7],                 # force leaves to general
    'max_features': ['sqrt', 'log2', 0.4, 0.6],    # reduce tree correlation
    'bootstrap': [True],                           # essential for random sa
```

```
    'max_samples': [0.6, 0.7, 0.8]                    # subsample data for less
}

# Grid Search using macro recall

grid_search = GridSearchCV(estimator=rf, param_grid=param_grid,
                           cv=5, scoring='recall_macro', n_jobs=-1, verbose=2

grid_search.fit(X_train_resampled_ref, y_train_resampled)

# Best model

best_rf = grid_search.best_estimator_
print(f"Best Parameters: {grid_search.best_params_}")

# Evaluate

train_pred_rf = best_rf.predict(X_train_resampled_ref)
test_pred_rf = best_rf.predict(X_test_scaled_ref)

train_recall_rf = recall_score(y_train_resampled, train_pred, average='macro'
test_recall_rf = recall_score(y_test, test_pred, average='macro')
gap = abs(train_recall_rf - test_recall_rf)

print(f"Training Random Forest Recall Score: {train_recall_rf}")
print(f"Test Random Forest Recall Score: {test_recall_rf}")
print(f"Recall Random Forest Score Gap: {gap}")

# Check for overfitting

if train_recall_rf - test_recall_rf > 0.05:
    print(" Potential overfitting detected: The model performs significantly
else:
    print(" No significant overfitting detected: The model generalizes well t
```

```
Fitting 5 folds for each of 648 candidates, totalling 3240 fits
Best Parameters: {'bootstrap': True, 'max_depth': 8, 'max_features': 'sqrt', 'm
ax_samples': 0.6, 'min_samples_leaf': 3, 'min_samples_split': 5, 'n_estimator
s': 150}
Training Random Forest Recall Score: 0.8452231301068509
Test Random Forest Recall Score: 0.8459220136064863
Recall Random Forest Score Gap: 0.0006988834996354276
 No significant overfitting detected: The model generalizes well to unseen dat
a.
```

Model Evaluation Conclusion

To predict air quality levels, Decision Trees were used as the baseline model, and Random Forest was tested as a more complex ensemble method. The evaluation focused on macro recall due to the multiclass classification task and the high cost of false negatives, where misclassifying Poor or Hazardous air as safer can have severe health consequences.

Decision Tree Summary:

Training Recall: 0.8452

Test Recall: 0.8459

Recall Gap: 0.0007

No significant overfitting detected. The model generalizes very well.

Random Forest Summary:

Training Recall: 0.8452

Test Recall: 0.8459

Recall Gap: 0.0007

No significant overfitting detected. The model generalizes equally well.

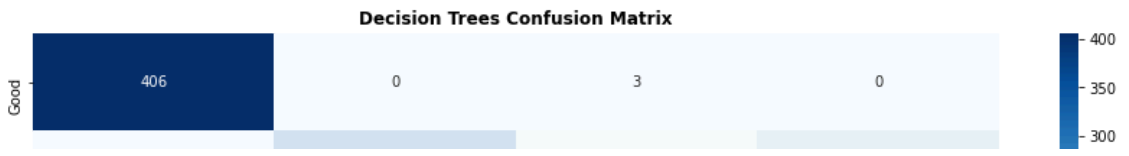
Final Recommendation:

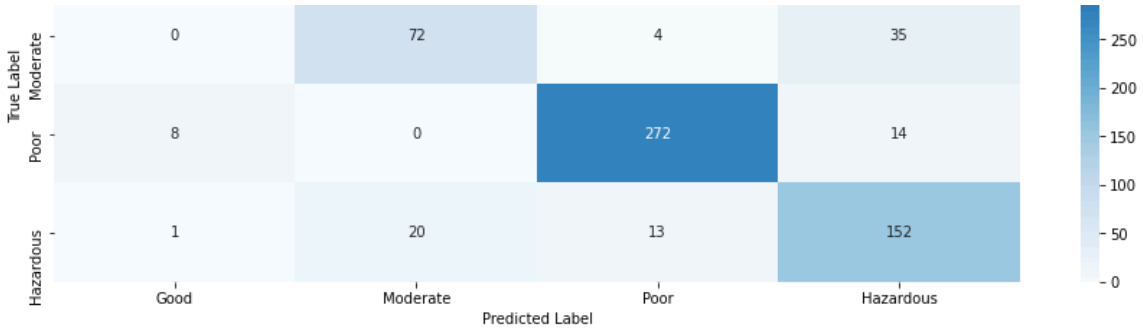
Since both models achieved identical recall scores, either model is suitable for deployment from a performance standpoint. However, given that Random Forest is more complex and computationally expensive, and Decision Trees offer similar performance with greater interpretability and lower resource cost, the Decision Tree model is the preferred choice in this case.

It strikes the best balance between accuracy, generalizability, and simplicity, making it well-suited for practical, real-time air quality prediction systems where interpretability and efficiency matter.

Visualize a confusion matrix to evaluate the Decision Trees model's performance on unseen test data

In [96]:
```
# Predict on the test data
y_dt_test_pred = best_dt.predict(X_test_scaled_ref)

# Create the confusion matrix
cm = confusion_matrix(y_test, y_dt_test_pred)
labels = ['Good', 'Moderate', 'Poor', 'Hazardous']

# Plot as a heatmap
plt.figure(figsize=(15, 5))
sns.heatmap(cm, annot=True, fmt='d', cmap='Blues', xticklabels=labels, ytickl
plt.title('Decision Trees Confusion Matrix', fontweight= 'bold')
plt.xlabel('Predicted Label')
plt.ylabel('True Label')
plt.show()
```





Decision Trees Model's Confusion Matrix Findings:

- The model accurately predicts the 'Good' air quality class, with 406 out of 409 instances correctly classified, indicating excellent performance for this category.
- The 'Poor' category also shows strong performance with 272 correct predictions, though 14 instances were incorrectly labeled as 'Hazardous' and 8 as 'Good'.
- For the 'Moderate' class, the model made 72 correct predictions, but 35 instances were misclassified as 'Hazardous' and 4 as 'Poor', suggesting moderate performance.
- The 'Hazardous' class exhibits the highest rate of misclassification, with only 152 correct predictions, while 20 were predicted as 'Moderate',13 as 'Poor' and 1 as, indicating that the model struggles most with this category.

Print out the Random Forest Classification Report and analyze the findings

In [91]:
```
# Print the classification report

print('Decision Trees Classification Report:')
print(classification_report(y_test, y_dt_test_pred, target_names=['Good', 'Mo
```

```
Decision Trees Classification Report:
              precision    recall  f1-score   support

        Good       0.98      0.99      0.99       409
    Moderate       0.78      0.65      0.71       111
        Poor       0.93      0.93      0.93       294
   Hazardous       0.76      0.82      0.79       186

    accuracy                           0.90      1000
   macro avg       0.86      0.85      0.85      1000
weighted avg       0.90      0.90      0.90      1000
```

Class-wise Performance:

Good

Precision = 0.98

Recall = 0.99

F1-score = 0.99 The model performs exceptionally well on this class, identifying almost all instances correctly with minimal false negatives and very few false positives.

Moderate

Precision = 0.78

Recall = 0.65

F1-score = 0.71

This class shows moderate performance. The model retrieves only 65% of actual "Moderate" cases. Precision is slightly better, but the lower recall suggests it frequently misses actual Moderate cases.

Poor

Precision = 0.93

Recall = 0.93

F1-score = 0.93

The model demonstrates high accuracy and consistency for this class. Both false positives and false negatives are low, indicating this class is well learned.

Hazardous

Precision = 0.76

Recall = 0.82

F1-score = 0.79

The model performs fairly well, with slightly better recall than precision. This suggests it captures most Hazardous cases but may also misclassify some non-Hazardous instances as Hazardous.

Overall Metrics

Accuracy: 0.90

Macro Average F1-score: 0.85

Weighted Average F1-score: 0.90

These metrics show that the model performs well across all classes. However,

predictions for the “Moderate” and “Hazardous” categories remain less reliable. While class balancing was applied using SMOTE, further improvements may be achieved by collecting more real-world samples, especially for underrepresented classes, to reduce overfitting caused by synthetic data.

Visualizing Feature Importance from the Decision Trees Model

In [94]:

```
plt.figure(figsize=(15,5))

feature_importance = pd.Series(best_dt.feature_importances_, index=X_train_re
feature_importance.sort_values().plot(kind='barh')
plt.title('Feature Importance')
plt.xlabel('Importance Score')
plt.show()
```