University for the Creative Arts

BERLIN SCHOOL OF BUSINESS & INNOVATION

Essay / Assignment Title: Time Series Forecasting: A Practical Approach to Data-Driven Decision Making

Programme title: M.sc Data Analytics

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CONTENTS

Table of Contents

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Name and Surname :
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Date: 09/06/2025

TASK #1 PROBLEM FORMATION

Problem Formation for Task 1:

To select an appropriate time series dataset with a continuous target variable, at least 1000 data points, and multiple features from a reputable source. Then, conduct initial exploratory data analysis (including summary statistics and visualizations) to understand its characteristics and justify its suitability for a time series regression project.

1. Dataset Selection:

After reviewing the requirements (time series, continuous target variable, >=1000 data points, multiple features, reputable source), the following dataset has been selected:

- **Dataset Name:** Beijing Multi-Site Air-Quality Data (specifically, data from the **Aotizhongxin station**)
- **Source:** UCI Machine Learning Repository
  - **Citation:** Liang, X., Zou, T., Guo, B., Li, S., Zhang, H., Zhang, S., Huang, H. and Chen, S. X. (2017). Assessing Beijing's PM2.5 pollution: severity, weather impact, APEC blue and winter heating. Proceedings of the Royal Society A, 473(2204).
  - **Direct Link to Dataset:** https://archive.ics.uci.edu/dataset/501/beijing+multi-site+air-quality+data
  - **Specific File:** PRSA_Data_Aotizhongxin_20130301-20170228.csv (This file contains data for the Aotizhongxin station).

2. Dataset Description:

- **Overview:** This dataset contains hourly air quality data collected from the Aotizhongxin air quality monitoring station in Beijing, China. Alongside pollutant concentrations, it includes meteorological data for the corresponding times.
- **Time Period and Granularity:** The data spans from March 1st, 2013, to February 28th, 2017, with observations recorded on an hourly basis.
- **Data Points:** The Aotizhongxin station dataset comprises 35,064 hourly observations. This significantly exceeds the minimum requirement of 1000 data points.
- **Target Variable:** For this assignment, the **PM2.5 concentration (µg/m³)** will be used as the continuous target variable for regression analysis. PM2.5 refers to fine particulate matter with a diameter of 2.5 micrometers or less, which is a key indicator of air pollution.

- **Features:** The dataset includes the following 18 columns, providing multiple features for analysis:
    - No: Row index.
    - year: Year of observation.
    - month: Month of observation.
    - day: Day of observation.
    - hour: Hour of observation.
    - PM2.5: PM2.5 concentration (µg/m³) - **Target Variable**.
    - PM10: PM10 concentration (µg/m³).
    - SO2: Sulfur Dioxide concentration (µg/m³).
    - NO2: Nitrogen Dioxide concentration (µg/m³).
    - CO: Carbon Monoxide concentration (µg/m³).
    - O3: Ozone concentration (µg/m³).
    - TEMP: Temperature (°C).
    - PRES: Atmospheric Pressure (hPa).
    - DEWP: Dew Point Temperature (°C).
    - RAIN: Precipitation (mm).
    - wd: Wind direction (categorical, e.g., N, NE, E, SSW).
    - WSPM: Wind speed (m/s).
    - station: Name of the monitoring station (constant value "Aotizhongxin" for this specific file).

3. Justification for Dataset Choice:

The Beijing Multi-Site Air-Quality Data (Aotizhongxin station) was chosen for the following reasons, aligning with the assignment's requirements and objectives:

- **Meets All Assignment Criteria:**
    - **Time Series Data:** Observations are recorded hourly, providing a distinct temporal sequence suitable for time series analysis.
    - **Continuous Target Variable:** PM2.5 concentration is a continuous numerical value, appropriate for regression modeling (Zhang, Li & Wang, 2025).

- **Reputable Source:** The dataset is from the UCI Machine Learning Repository, a well-established and respected source for academic and research datasets.
- **Sufficient Data Points:** With 35,064 observations, it far exceeds the minimum requirement of 1000 data points, allowing for robust model training and testing.
- **Multiple Features:** The dataset contains various meteorological variables (temperature, pressure, wind speed, wind direction, rain, dew point) and concentrations of other pollutants (PM10, SO2, NO2, CO, O3). These serve as multiple features that can be used to predict the target variable (PM2.5) and analyze influencing factors, as required for later tasks (Zhang, Li & Wang, 2025).

- **Suitability for Time Series Regression:**
  - Air quality phenomena like PM2.5 concentrations are known to exhibit temporal dependencies, including seasonality (e.g., higher pollution during winter heating seasons), diurnal patterns (variations throughout the day), and trends (Zhang, Li & Wang, 2025).
  - Meteorological conditions significantly influence pollutant dispersion and formation. The inclusion of these features allows for the development of a more comprehensive regression model that can capture these relationships.

- **Relevance and Interest:**
  - Air quality is a critical environmental issue with significant public health implications. Analyzing and forecasting PM2.5 levels is a relevant and impactful application of data analytics (Jovanović et al., 2023).
  - The dataset provides a rich context for exploring the interplay between pollution and weather, offering interesting avenues for feature engineering and interpretation of results.

4. Initial Exploratory Data Analysis (EDA) Plan:

The following steps would be performed in a Python environment (e.g., Google Colab using libraries like Pandas, Matplotlib, Seaborn) to conduct the initial EDA. The findings from this EDA will be included in the report.

1. *Data Loading and Initial Inspection:*
   - Load the PRSA_Data_Aotizhongxin_20130301-20170228.csv into a Pandas DataFrame.
   - Display the first few rows (df.head()) to understand the data structure.

- Examine column data types and non-null counts (df.info()). This will reveal the presence of missing values, particularly in pollutant columns like PM2.5, which is common in sensor data.
- Generate a summary of missing values per column (df.isnull().sum()) to quantify them.

2. *Datetime Feature Creation:*
    - Combine the year, month, day, and hour columns to create a single datetime column.
    - Set this datetime column as the DataFrame's index to facilitate time series plotting and analysis.

3. *Summary Statistics:*
    - Calculate descriptive statistics (df.describe()) for all numerical columns (PM2.5, PM10, SO2, NO2, CO, O3, TEMP, PRES, DEWP, RAIN, WSPM). This will provide insights into:
        - Central tendency (mean, median).
        - Dispersion (standard deviation, min, max, interquartile range).
        - Potential skewness or presence of extreme values.

4. *Data Visualizations:*
    - **Target Variable (PM2.5) Over Time:**
        - Plot the PM2.5 concentration against the datetime index. This will help visualize overall trends, seasonality, and any obvious anomalies or missing data periods.
    - **Distribution of Key Numerical Features:**
        - Plot histograms and/or density plots for PM2.5, TEMP, WSPM, and PRES to understand their distributions. For instance, PM2.5 is often right-skewed.
    - **Box Plots for Outlier Detection and Grouped Analysis:**
        - Create a box plot for PM2.5 to visualize its spread and identify potential outliers.
        - Generate box plots of PM2.5 grouped by month to observe seasonal patterns (e.g., higher PM2.5 in winter months).
        - Generate box plots of PM2.5 grouped by hour to observe diurnal patterns (e.g., rush hour peaks).

- **Categorical Feature Analysis (Wind Direction wd):**
  - Create a bar chart showing the frequency distribution of different wind directions (wd). This can indicate prevailing wind directions.

- **Initial Relationship Exploration (Optional for Task 1, more detailed in Task 2):**
  - Simple scatter plots of PM2.5 vs. potentially influential features like TEMP or WSPM to get an initial visual sense of relationships.

This initial EDA will provide a foundational understanding of the dataset's characteristics, quality, and the behavior of the target variable, which is crucial before proceeding to data preprocessing and model development in subsequent tasks. The visualizations and summary statistics will be included in the report to describe the dataset comprehensively.

Implementation:

Code:

```python
# Import necessary libraries
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

# --- 1. Data Loading and Initial Inspection ---

file_path = '/content/PRSA_Data_Aotizhongxin_20130301-20170228.csv'

try:
    # Load the dataset
    df = pd.read_csv(file_path)
    print("Dataset loaded successfully.\n")

    # Display the first few rows
    print("--- First 5 Rows of the Dataset ---")
    print(df.head())
    print("\n")

    # Examine column data types and non-null counts
    print("--- Dataset Info ---")
    df.info()
    print("\n")

    # Generate a summary of missing values per column
    print("--- Missing Values per Column ---")
    print(df.isnull().sum())
    print("\n")

    # --- 2. Datetime Feature Creation ---
    print("--- Creating Datetime Feature ---")
    # Combine year, month, day, hour into a single datetime column
    # Errors='coerce' will turn unparseable dates into NaT (Not a Time)
    df['datetime'] = pd.to_datetime(df[['year', 'month', 'day', 'hour']], errors='coerce')

    # Set the new 'datetime' column as the DataFrame's index
    df.set_index('datetime', inplace=True)

    columns_to_drop = ['year', 'month', 'day', 'hour', 'No', 'station']
    df.drop(columns=columns_to_drop, inplace=True, errors='ignore') # errors='ignore' in case they were already dropped

    print("Datetime feature created and set as index.")
    print("Cleaned DataFrame head:")
    print(df.head())
    print("\n")
```

```python
# --- 3. Summary Statistics ---
print("--- Summary Statistics for Numerical Columns ---")
# Calculate descriptive statistics for all numerical columns
# We'll select numeric types explicitly to avoid issues with non-numeric columns if any remain.
numerical_cols = df.select_dtypes(include=['number']).columns
print(df[numerical_cols].describe())
print("\n")

# --- 4. Data Visualizations ---
print("--- Generating Data Visualizations ---")
plt.style.use('seaborn-v0_8-whitegrid') # Using a seaborn style for better aesthetics

# Target Variable (PM2.5) Over Time
plt.figure(figsize=(15, 6))
df['PM2.5'].plot(title='PM2.5 Concentration Over Time (Aotizhongxin Station)')
plt.xlabel('Date')
plt.ylabel('PM2.5 Concentration (µg/m³)')
plt.tight_layout()
plt.show()
print("Displayed PM2.5 over time plot.")

# Distribution of Key Numerical Features
key_numerical_features = ['PM2.5', 'TEMP', 'WSPM', 'PRES']
print(f"\nPlotting distributions for: {', '.join(key_numerical_features)}")

for feature in key_numerical_features:
    if feature in df.columns:
        plt.figure(figsize=(10, 5))
        sns.histplot(df[feature].dropna(), kde=True) # dropna() to handle missing values for plotting
        plt.title(f'Distribution of {feature}')
        plt.xlabel(feature)
        plt.ylabel('Frequency')
        plt.tight_layout()
        plt.show()
        print(f"Displayed distribution plot for {feature}.")
    else:
        print(f"Warning: Column '{feature}' not found for distribution plot.")


# Box Plots for Outlier Detection and Grouped Analysis

# Box plot for PM2.5
if 'PM2.5' in df.columns:
    plt.figure(figsize=(8, 6))
    sns.boxplot(y=df['PM2.5'].dropna())
    plt.title('Box Plot of PM2.5 Concentration')
    plt.ylabel('PM2.5 (µg/m³)')
    plt.tight_layout()
    plt.show()
    print("Displayed box plot for PM2.5.")
```

```python
        # Box plots of PM2.5 grouped by month
        # Create a temporary month column from the datetime index for grouping
        df_temp = df.copy() # Work on a copy to avoid modifying original df
        df_temp['plot_month'] = df_temp.index.month
        plt.figure(figsize=(12, 6))
        sns.boxplot(x='plot_month', y='PM2.5', data=df_temp.dropna(subset=['PM2.5']))
        plt.title('PM2.5 Concentration by Month')
        plt.xlabel('Month')
        plt.ylabel('PM2.5 (µg/m³)')
        plt.xticks(ticks=range(12), labels=['Jan', 'Feb', 'Mar', 'Apr', 'May', 'Jun', 'Jul', 'Aug', 'Sep', 'Oct', 'Nov', 'Dec'])
        plt.tight_layout()
        plt.show()
        print("Displayed box plot of PM2.5 by month.")

        # Box plots of PM2.5 grouped by hour
        df_temp['plot_hour'] = df_temp.index.hour
        plt.figure(figsize=(14, 6))
        sns.boxplot(x='plot_hour', y='PM2.5', data=df_temp.dropna(subset=['PM2.5']))
        plt.title('PM2.5 Concentration by Hour of Day')
        plt.xlabel('Hour of Day')
        plt.ylabel('PM2.5 (µg/m³)')
        plt.tight_layout()
        plt.show()
        print("Displayed box plot of PM2.5 by hour.")
    else:
        print("Warning: Column 'PM2.5' not found for box plots.")


    # Categorical Feature Analysis (Wind Direction `wd`)
    if 'wd' in df.columns:
        plt.figure(figsize=(12, 6))
        sns.countplot(y=df['wd'].dropna(), order = df['wd'].dropna().value_counts().index) # Order by frequency
        plt.title('Frequency Distribution of Wind Direction (wd)')
        plt.xlabel('Count')
        plt.ylabel('Wind Direction')
        plt.tight_layout()
        plt.show()
        print("Displayed bar chart for wind direction.")
    else:
        print("Warning: Column 'wd' not found for wind direction plot.")

    print("\n--- EDA Script Finished ---")

except FileNotFoundError:
    print(f"Error: The file '{file_path}' was not found.")
    print("Please ensure the file path is correct and the CSV file is in the specified location.")
except Exception as e:
    print(f"An error occurred: {e}")
    print("Please check your data and script.")
```

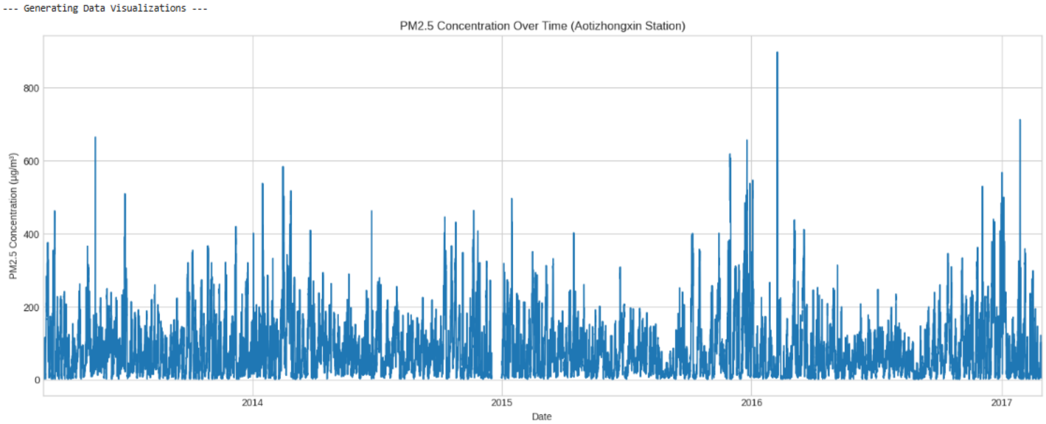
Output:

```
Dataset loaded successfully.

--- First 5 Rows of the Dataset ---
   No  year  month  day  hour  PM2.5  PM10   SO2   NO2     CO    O3  TEMP  \
0   1  2013      3    1     0    4.0   4.0   4.0   7.0  300.0  77.0  -0.7
1   2  2013      3    1     1    8.0   8.0   4.0   7.0  300.0  77.0  -1.1
2   3  2013      3    1     2    7.0   7.0   5.0  10.0  300.0  73.0  -1.1
3   4  2013      3    1     3    6.0   6.0  11.0  11.0  300.0  72.0  -1.4
4   5  2013      3    1     4    3.0   3.0  12.0  12.0  300.0  72.0  -2.0

     PRES  DEWP  RAIN   wd  WSPM       station
0  1023.0 -18.8   0.0  NNW   4.4  Aotizhongxin
1  1023.2 -18.2   0.0    N   4.7  Aotizhongxin
2  1023.5 -18.2   0.0  NNW   5.6  Aotizhongxin
3  1024.5 -19.4   0.0   NW   3.1  Aotizhongxin
4  1025.2 -19.5   0.0    N   2.0  Aotizhongxin


--- Dataset Info ---
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 35064 entries, 0 to 35063
Data columns (total 18 columns):
 #   Column   Non-Null Count  Dtype
---  ------   --------------  -----
 0   No       35064 non-null  int64
 1   year     35064 non-null  int64
 2   month    35064 non-null  int64
 3   day      35064 non-null  int64
 4   hour     35064 non-null  int64
 5   PM2.5    34139 non-null  float64
 6   PM10     34346 non-null  float64
 7   SO2      34129 non-null  float64
 8   NO2      34041 non-null  float64
 9   CO       33288 non-null  float64
 10  O3       33345 non-null  float64
 11  TEMP     35044 non-null  float64
 12  PRES     35044 non-null  float64
 13  DEWP     35044 non-null  float64
 14  RAIN     35044 non-null  float64
 15  wd       34983 non-null  object
 16  WSPM     35050 non-null  float64
 17  station  35064 non-null  object
dtypes: float64(11), int64(5), object(2)
memory usage: 4.8+ MB
```

```
--- Missing Values per Column ---
No            0
year          0
month         0
day           0
hour          0
PM2.5       925
PM10        718
SO2         935
NO2        1023
CO         1776
O3         1719
TEMP         20
PRES         20
DEWP         20
RAIN         20
wd           81
WSPM         14
station       0
dtype: int64


--- Creating Datetime Feature ---
Datetime feature created and set as index.
Cleaned DataFrame head:
                     PM2.5  PM10   SO2   NO2     CO    O3  TEMP    PRES  DEWP  \
datetime
2013-03-01 00:00:00    4.0   4.0   4.0   7.0  300.0  77.0  -0.7  1023.0 -18.8
2013-03-01 01:00:00    8.0   8.0   4.0   7.0  300.0  77.0  -1.1  1023.2 -18.2
2013-03-01 02:00:00    7.0   7.0   5.0  10.0  300.0  73.0  -1.1  1023.5 -18.2
2013-03-01 03:00:00    6.0   6.0  11.0  11.0  300.0  72.0  -1.4  1024.5 -19.4
2013-03-01 04:00:00    3.0   3.0  12.0  12.0  300.0  72.0  -2.0  1025.2 -19.5

                     RAIN   wd  WSPM
datetime
2013-03-01 00:00:00   0.0  NNW   4.4
2013-03-01 01:00:00   0.0    N   4.7
2013-03-01 02:00:00   0.0  NNW   5.6
2013-03-01 03:00:00   0.0   NW   3.1
2013-03-01 04:00:00   0.0    N   2.0
```

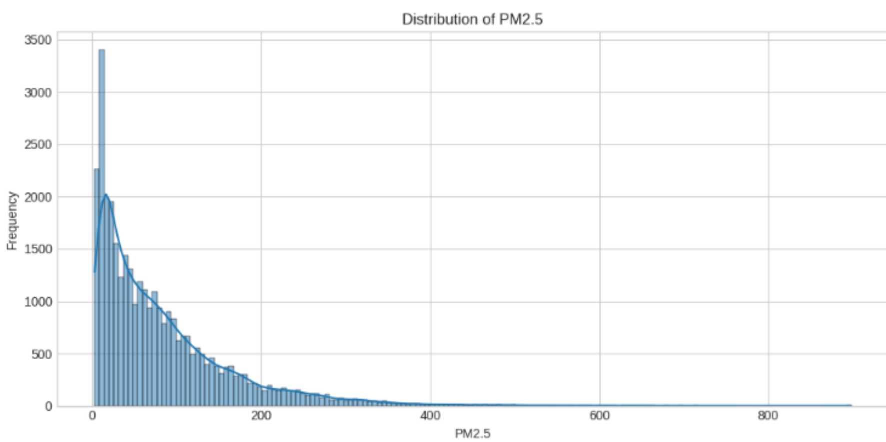
```
--- Summary Statistics for Numerical Columns ---
            PM2.5          PM10           SO2           NO2            CO  \
count  34139.000000  34346.000000  34129.000000  34041.000000  33288.000000
mean      82.773611    110.060391     17.375901     59.305833   1262.945145
std       82.135694     95.223005     22.823017     37.116200   1221.436236
min        3.000000      2.000000      0.285600      2.000000    100.000000
25%       22.000000     38.000000      3.000000     30.000000    500.000000
50%       58.000000     87.000000      9.000000     53.000000    900.000000
75%      114.000000    155.000000     21.000000     82.000000   1500.000000
max      898.000000    984.000000    341.000000    290.000000  10000.000000

               O3          TEMP          PRES          DEWP          RAIN  \
count  33345.000000  35044.000000  35044.000000  35044.000000  35044.000000
mean      56.353358     13.584607   1011.846920      3.123062      0.067421
std       57.916327     11.399097     10.404047     13.688896      0.910056
min        0.214200    -16.800000    985.900000    -35.300000      0.000000
25%        8.000000      3.100000   1003.300000     -8.100000      0.000000
50%       42.000000     14.500000   1011.400000      3.800000      0.000000
75%       82.000000     23.300000   1020.100000     15.600000      0.000000
max      423.000000     40.500000   1042.000000     28.500000     72.500000

               WSPM
count  35050.000000
mean       1.708496
std        1.204071
min        0.000000
25%        0.900000
50%        1.400000
75%        2.200000
max       11.200000


--- Generating Data Visualizations ---
```

--- Generating Data Visualizations ---

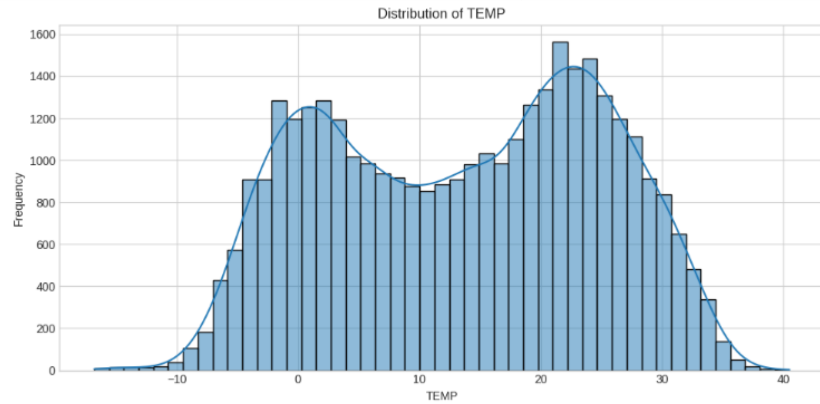


Displayed PM2.5 over time plot.

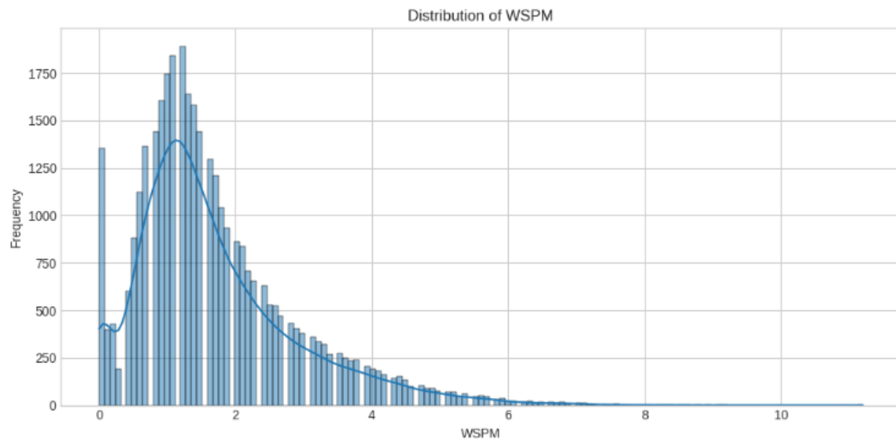
Plotting distributions for: PM2.5, TEMP, WSPM, PRES



Displayed distribution plot for PM2.5.



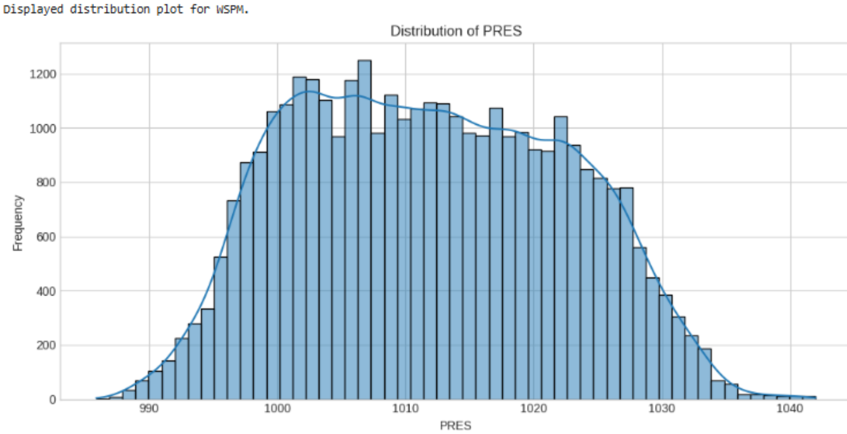

```
Displayed distribution plot for TEMP.
```



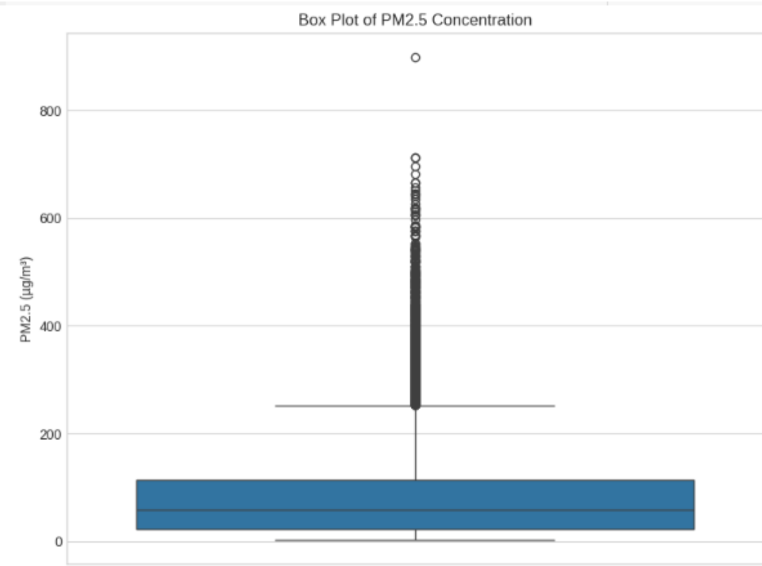

```
Displayed distribution plot for WSPM.
```

WSPM

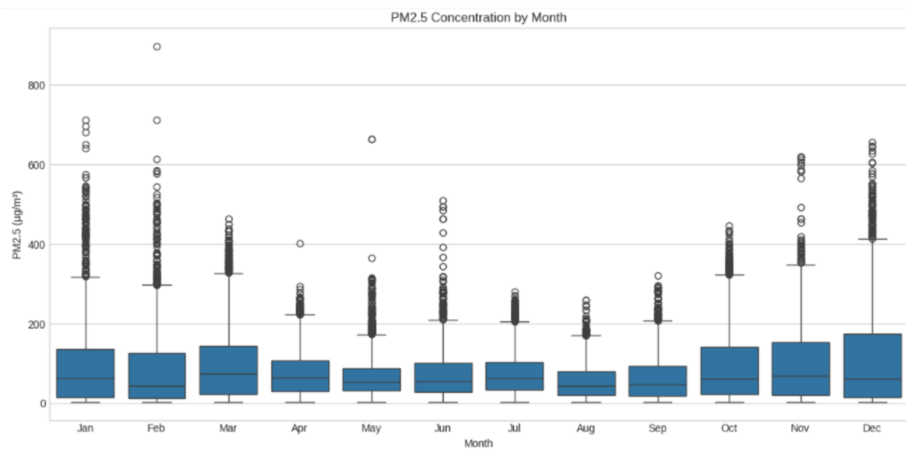
```
Displayed distribution plot for WSPM.
```



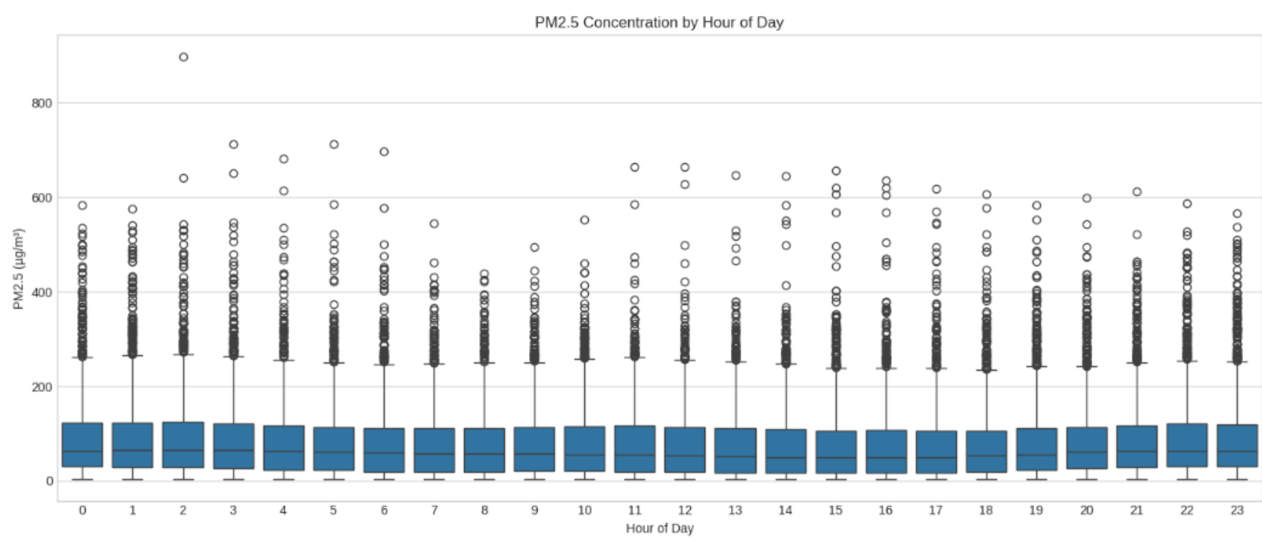

```
Displayed distribution plot for PRES.
```



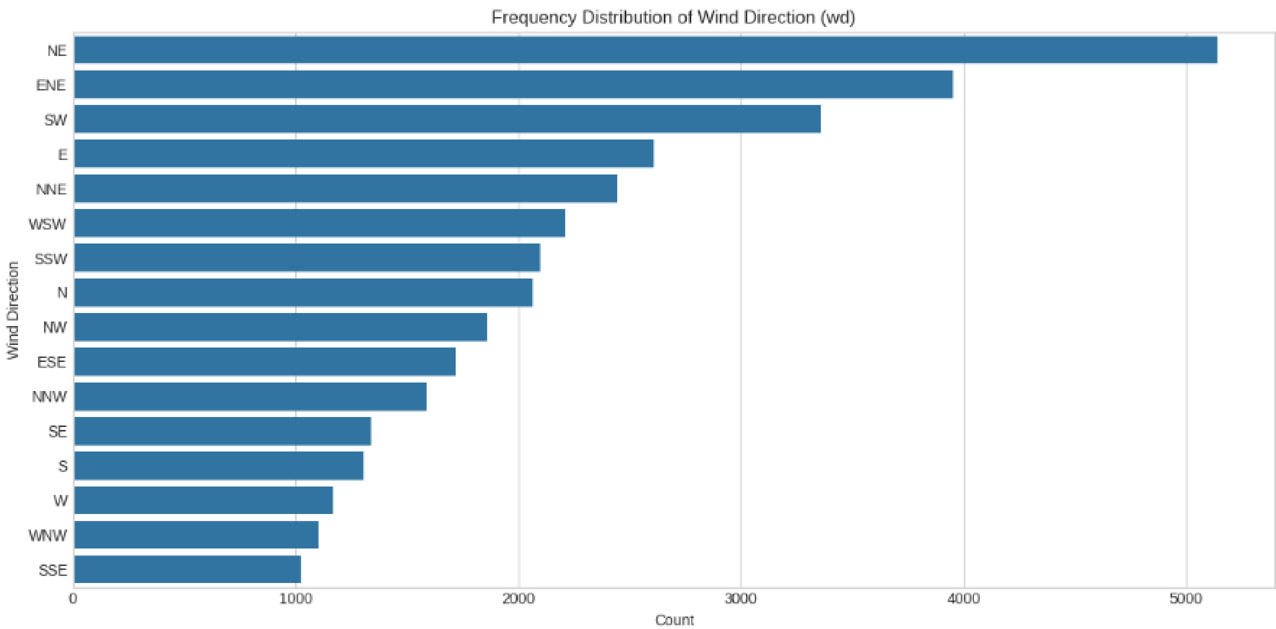
Displayed box plot for PM2.5.



Displayed box plot of PM2.5 by month.



Displayed box plot of PM2.5 by hour.




```
Displayed bar chart for wind direction.
```

TASK #2 PROBLEM FORMATION

Problem formation for task 2:

To preprocess the selected time series dataset by handling missing values and outliers, engineer relevant time-based features (e.g., day of the week, month, season), analyze correlations between variables, and apply appropriate normalization or standardization techniques to prepare the features for subsequent regression modeling.

Implementation:

Code:

```python
# Import necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.preprocessing import StandardScaler, OneHotEncoder
from sklearn.compose import ColumnTransformer
from sklearn.pipeline import Pipeline
```

```python
file_path = 'PRSA_Data_Aotizhongxin_20130301-20170228.csv' # Or the full path

try:
    # Load the dataset
    df = pd.read_csv(file_path)
    print("Dataset loaded successfully.\n")

    # Combine year, month, day, hour into a single datetime column
    df['datetime'] = pd.to_datetime(df[['year', 'month', 'day', 'hour']], errors='coerce')
    df.set_index('datetime', inplace=True)
    columns_to_drop = ['year', 'month', 'day', 'hour', 'No', 'station']
    df.drop(columns=columns_to_drop, inplace=True, errors='ignore')

    print("--- Initial DataFrame Head ---")
    print(df.head())
    print("\n--- Initial Missing Values ---")
    print(df.isnull().sum())
    print("\n")

    # --- Task 2: Data Preprocessing and Feature Engineering ---

    # 1. Handle Missing Values
    print("--- 1. Handling Missing Values ---")
    # For pollutant and meteorological numerical features, linear interpolation is a common choice for time series.
    # For PM2.5 (target), interpolation is also reasonable.
    numerical_cols_with_na = df.select_dtypes(include=np.number).isnull().sum()
    numerical_cols_to_interpolate = numerical_cols_with_na[numerical_cols_with_na > 0].index.tolist()

    if numerical_cols_to_interpolate:
        print(f"Interpolating numerical columns: {numerical_cols_to_interpolate}")
        for col in numerical_cols_to_interpolate:
            df[col] = df[col].interpolate(method='linear', limit_direction='both') # limit_direction fills NaNs at ends too
    else:
        print("No numerical columns found needing interpolation.")
```

```python
# For categorical 'wd' (wind direction), use forward fill then backward fill
if 'wd' in df.columns and df['wd'].isnull().any():
    print("Filling missing 'wd' using ffill and bfill.")
    df['wd'] = df['wd'].fillna(method='ffill').fillna(method='bfill')
elif 'wd' not in df.columns:
    print("Warning: 'wd' column not found.")
else:
    print("'wd' column has no missing values.")


print("\n--- Missing Values After Handling ---")
print(df.isnull().sum())

print("\n")


# 2. Create Time-Based Features
print("--- 2. Creating Time-Based Features ---")
df['hour_of_day'] = df.index.hour
df['day_of_week'] = df.index.dayofweek  # Monday=0, Sunday=6
df['day_of_year'] = df.index.dayofyear
df['month'] = df.index.month
df['year'] = df.index.year # Useful for trends or splitting
df['week_of_year'] = df.index.isocalendar().week.astype(int)
df['is_weekend'] = df['day_of_week'].isin([5, 6]).astype(int)

# Season (approximation)
def get_season(date):
    month = date.month
    if month in [12, 1, 2]:
        return 'Winter'
    elif month in [3, 4, 5]:
        return 'Spring'
    elif month in [6, 7, 8]:
        return 'Summer'
    else: # 9, 10, 11
        return 'Autumn'
df['season'] = df.index.to_series().apply(get_season)

print("Time-based features created:")
print(df[['hour_of_day', 'day_of_week', 'month', 'season', 'is_weekend']].head())
print("\n")

# 3. Handle Categorical Features ('wd' and 'season')
print("--- 3. Handling Categorical Features (One-Hot Encoding) ---")
# 'wd' (wind direction) and 'season' are categorical
categorical_features = ['wd', 'season']
# Create a copy for one-hot encoding to keep original df cleaner for now
df_processed = df.copy()
```

```python
# Check if categorical features exist before trying to encode
existing_categorical_features = [col for col in categorical_features if col in df_processed.columns]

if existing_categorical_features:
    print(f"Applying One-Hot Encoding to: {existing_categorical_features}")
    df_processed = pd.get_dummies(df_processed, columns=existing_categorical_features, prefix=existing_categorical_features, dummy_na=False) # dummy_na=False as we handled NaNs
    print("Categorical features one-hot encoded.")
    print("DataFrame columns after one-hot encoding (sample):")
    print(df_processed.filter(regex='wd_|season_').head())
else:
    print("No specified categorical features found for one-hot encoding.")
print("\n")


# 4. Analyse Correlations
print("--- 4. Analyzing Correlations ---")

numerical_cols_for_corr = df_processed.select_dtypes(include=np.number).columns

# It's often useful to see correlations with the target variable specifically
if 'PM2.5' in numerical_cols_for_corr:
    correlation_matrix = df_processed[numerical_cols_for_corr].corr()
    plt.figure(figsize=(18, 15)) # Adjusted size for more features
    sns.heatmap(correlation_matrix, annot=False, cmap='coolwarm', fmt=".2f", linewidths=.5) # Annot=False if too cluttered
    plt.title('Correlation Matrix of Numerical Features')
    plt.show()
    print("Displayed correlation matrix heatmap.")

    print("\n--- Top Correlations with PM2.5 ---")
    pm25_correlations = correlation_matrix['PM2.5'].sort_values(ascending=False)
    print(pm25_correlations)
else:
    print("PM2.5 column not found or not numerical for correlation analysis.")
print("\n")


# 5. Normalize or Standardize Features
print("--- 5. Normalizing/Standardizing Features ---")


# Re-identify numerical columns from df_processed
numerical_features_to_scale = df_processed.select_dtypes(include=np.number).columns.tolist()

# Exclude target variable and binary/already scaled features if necessary
if 'PM2.5' in numerical_features_to_scale:
    numerical_features_to_scale.remove('PM2.5') # Target usually not scaled with features
```

```python
# Exclude one-hot encoded columns (they are already 0 or 1)
# and other binary features like 'is_weekend'
one_hot_cols = [col for col in df_processed.columns if col.startswith(tuple(f"{cat}_" for cat in existing_categorical_features))]
binary_features = ['is_weekend'] + one_hot_cols

numerical_features_to_scale = [col for col in numerical_features_to_scale if col not in binary_features]

if numerical_features_to_scale:
    print(f"Numerical features to be standardized: {numerical_features_to_scale}")
    scaler = StandardScaler()
    # Fit and transform
    df_processed[numerical_features_to_scale] = scaler.fit_transform(df_processed[numerical_features_to_scale])
    print("Numerical features standardized.")
    print(df_processed[numerical_features_to_scale].head())
else:
    print("No numerical features identified for scaling or all are binary/target.")
print("\n")


# 6. Outlier Handling (Demonstration for PM2.5)
print("--- 6. Outlier Handling Demonstration (for PM2.5) ---")
if 'PM2.5' in df.columns: # Use original df for this demonstration before scaling
    Q1 = df['PM2.5'].quantile(0.25)
    Q3 = df['PM2.5'].quantile(0.75)
    IQR = Q3 - Q1
    lower_bound = Q1 - 1.5 * IQR
    upper_bound = Q3 + 1.5 * IQR

    print(f"PM2.5 - Q1: {Q1}, Q3: {Q3}, IQR: {IQR}")
    print(f"PM2.5 - Lower Bound for outliers: {lower_bound}")
    print(f"PM2.5 - Upper Bound for outliers: {upper_bound}")

    outliers = df[(df['PM2.5'] < lower_bound) | (df['PM2.5'] > upper_bound)]
    print(f"Number of potential outliers in PM2.5: {len(outliers)}")

else:
    print("PM2.5 column not found for outlier analysis.")
print("\n")


print("--- Final Processed DataFrame Head (df_processed) ---")
print(df_processed.head())
print("\n--- Final Processed DataFrame Info ---")
df_processed.info()
```

```python
except FileNotFoundError:
    print(f"Error: The file '{file_path}' was not found.")
    print("Please ensure the file path is correct and the CSV file is in the specified location.")
except Exception as e:
    print(f"An error occurred: {e}")
    print("Please check your data and script carefully.")
```

Output:

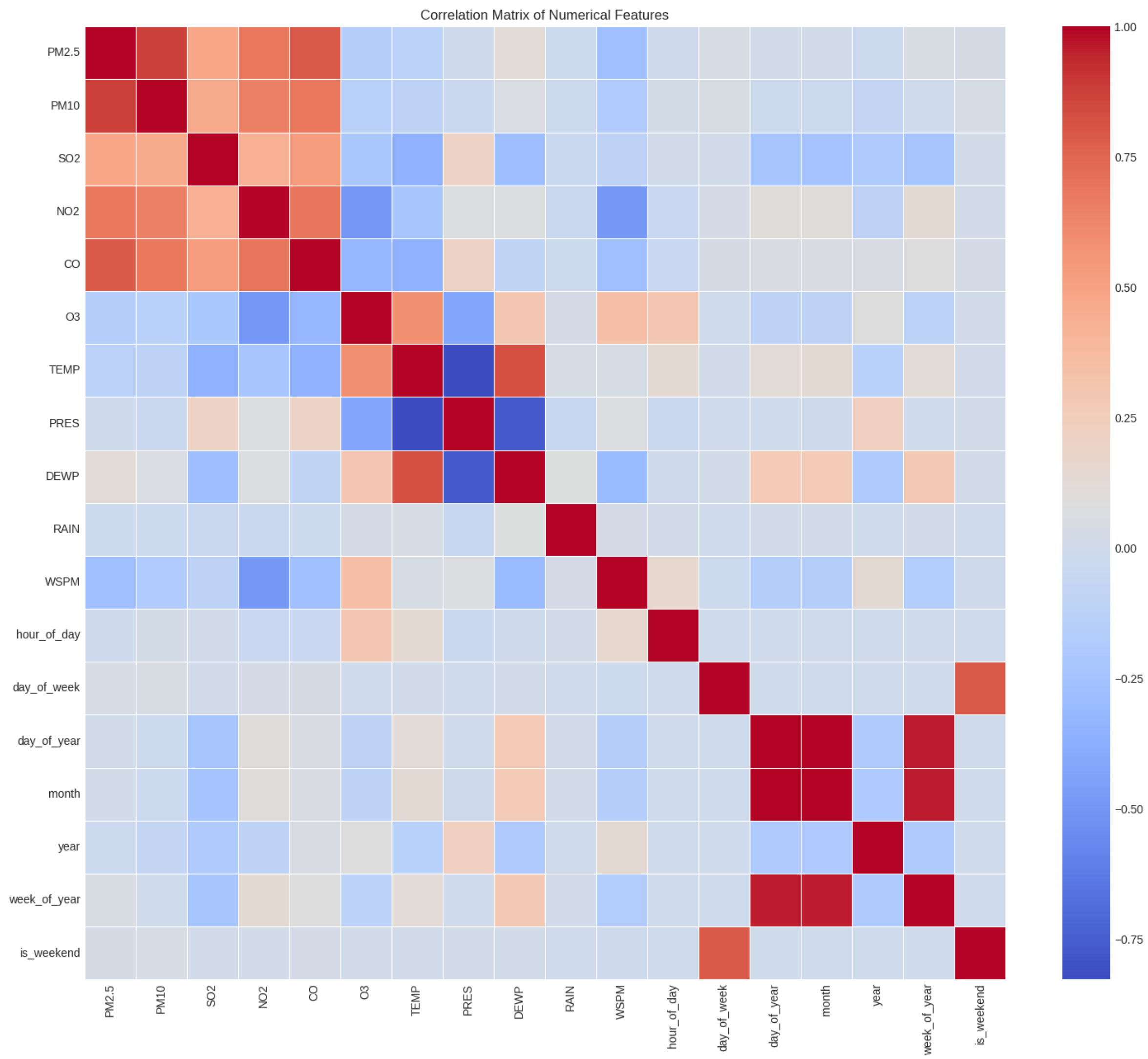
Initial Dataframe and missing value Handling:

```
Dataset loaded successfully.

--- Initial DataFrame Head ---
                     PM2.5  PM10   SO2   NO2     CO    O3  TEMP    PRES  DEWP  \
datetime
2013-03-01 00:00:00    4.0   4.0   4.0   7.0  300.0  77.0  -0.7  1023.0 -18.8
2013-03-01 01:00:00    8.0   8.0   4.0   7.0  300.0  77.0  -1.1  1023.2 -18.2
2013-03-01 02:00:00    7.0   7.0   5.0  10.0  300.0  73.0  -1.1  1023.5 -18.2
2013-03-01 03:00:00    6.0   6.0  11.0  11.0  300.0  72.0  -1.4  1024.5 -19.4
2013-03-01 04:00:00    3.0   3.0  12.0  12.0  300.0  72.0  -2.0  1025.2 -19.5

                     RAIN   wd  WSPM
datetime
2013-03-01 00:00:00   0.0  NNW   4.4
2013-03-01 01:00:00   0.0    N   4.7
2013-03-01 02:00:00   0.0  NNW   5.6
2013-03-01 03:00:00   0.0   NW   3.1
2013-03-01 04:00:00   0.0    N   2.0

--- Initial Missing Values ---
PM2.5     925
PM10      718
SO2       935
NO2      1023
CO       1776
O3       1719
TEMP       20
PRES       20
DEWP       20
RAIN       20
wd         81
WSPM       14
dtype: int64


--- 1. Handling Missing Values ---
Interpolating numerical columns: ['PM2.5', 'PM10', 'SO2', 'NO2', 'CO', 'O3', 'TEMP', 'PRES', 'DEWP', 'RAIN', 'WSPM']
Filling missing 'wd' using ffill and bfill.

--- Missing Values After Handling ---
PM2.5    0
PM10     0
SO2      0
NO2      0
CO       0
O3       0
TEMP     0
PRES     0
DEWP     0
RAIN     0
wd       0
WSPM     0
dtype: int64
```

Creating Time-Based Feature and Handling Categorical Features:

```
--- 2. Creating Time-Based Features ---
Time-based features created:
                     hour_of_day  day_of_week  month  season  is_weekend
datetime
2013-03-01 00:00:00            0            4      3  Spring           0
2013-03-01 01:00:00            1            4      3  Spring           0
2013-03-01 02:00:00            2            4      3  Spring           0
2013-03-01 03:00:00            3            4      3  Spring           0
2013-03-01 04:00:00            4            4      3  Spring           0


--- 3. Handling Categorical Features (One-Hot Encoding) ---
Applying One-Hot Encoding to: ['wd', 'season']
Categorical features one-hot encoded.
DataFrame columns after one-hot encoding (sample):
                      wd_E  wd_ENE  wd_ESE   wd_N  wd_NE  wd_NNE  wd_NNW  \
datetime
2013-03-01 00:00:00  False   False   False  False  False   False    True
2013-03-01 01:00:00  False   False   False   True  False   False   False
2013-03-01 02:00:00  False   False   False  False  False   False    True
2013-03-01 03:00:00  False   False   False  False  False   False   False
2013-03-01 04:00:00  False   False   False   True  False   False   False

                     wd_NW   wd_S  wd_SE  wd_SSE  wd_SSW  wd_SW   wd_W  \
datetime
2013-03-01 00:00:00  False  False  False   False   False  False  False
2013-03-01 01:00:00  False  False  False   False   False  False  False
2013-03-01 02:00:00  False  False  False   False   False  False  False
2013-03-01 03:00:00   True  False  False   False   False  False  False
2013-03-01 04:00:00  False  False  False   False   False  False  False

                     wd_WNW  wd_WSW  season_Autumn  season_Spring  \
datetime
2013-03-01 00:00:00   False   False          False           True
2013-03-01 01:00:00   False   False          False           True
2013-03-01 02:00:00   False   False          False           True
2013-03-01 03:00:00   False   False          False           True
2013-03-01 04:00:00   False   False          False           True

                     season_Summer  season_Winter
datetime
2013-03-01 00:00:00          False          False
2013-03-01 01:00:00          False          False
2013-03-01 02:00:00          False          False
2013-03-01 03:00:00          False          False
2013-03-01 04:00:00          False          False
```

Analyzing Correlations:



Display correlation matrix heatmap:

```
Displayed correlation matrix heatmap.

--- Top Correlations with PM2.5 ---
PM2.5           1.000000
PM10            0.875198
CO              0.786052
NO2             0.682795
SO2             0.479025
DEWP            0.123277
week_of_year    0.047493
day_of_week     0.043574
is_weekend      0.034480
day_of_year     0.014831
month           0.014398
PRES           -0.008796
hour_of_day    -0.010470
RAIN           -0.013780
year           -0.029873
TEMP           -0.122505
O3             -0.160271
WSPM           -0.275836
Name: PM2.5, dtype: float64
```

Normalizing Standardizing feature:

```
--- 5. Normalizing/Standardizing Features ---
Numerical features to be standardized: ['PM10', 'SO2', 'NO2', 'CO', 'O3', 'TEMP', 'PRES', 'DEWP', 'RAIN', 'WSPM', 'hour_of_day',
Numerical features standardized.
                        PM10       SO2       NO2        CO        O3  \
datetime
2013-03-01 00:00:00 -1.114935 -0.592867 -1.407393 -0.778358  0.378033
2013-03-01 01:00:00 -1.072945 -0.592867 -1.407393 -0.778358  0.378033
2013-03-01 02:00:00 -1.083443 -0.548818 -1.326313 -0.778358  0.308258
2013-03-01 03:00:00 -1.093940 -0.284524 -1.299286 -0.778358  0.290814
2013-03-01 04:00:00 -1.125433 -0.240475 -1.272260 -0.778358  0.290814

                        TEMP      PRES      DEWP      RAIN      WSPM  \
datetime
2013-03-01 00:00:00 -1.252727  1.071507 -1.601176 -0.074064  2.235098
2013-03-01 01:00:00 -1.287814  1.090729 -1.557349 -0.074064  2.484233
2013-03-01 02:00:00 -1.287814  1.119563 -1.557349 -0.074064  3.231640
2013-03-01 03:00:00 -1.314129  1.215677 -1.645004 -0.074064  1.155510
2013-03-01 04:00:00 -1.366759  1.282956 -1.652308 -0.074064  0.242013

                     hour_of_day  day_of_week  day_of_year     month  \
datetime
2013-03-01 00:00:00    -1.661325     0.499359    -1.167743 -1.021523
2013-03-01 01:00:00    -1.516862     0.499359    -1.167743 -1.021523
2013-03-01 02:00:00    -1.372399     0.499359    -1.167743 -1.021523
2013-03-01 03:00:00    -1.227936     0.499359    -1.167743 -1.021523
2013-03-01 04:00:00    -1.083473     0.499359    -1.167743 -1.021523

                        year  week_of_year
datetime
2013-03-01 00:00:00 -1.412304     -1.170498
2013-03-01 01:00:00 -1.412304     -1.170498
2013-03-01 02:00:00 -1.412304     -1.170498
2013-03-01 03:00:00 -1.412304     -1.170498
2013-03-01 04:00:00 -1.412304     -1.170498
```

Outlier Handling:

```
--- 6. Outlier Handling Demonstration (for PM2.5) ---
PM2.5 - Q1: 22.0, Q3: 114.0, IQR: 92.0
PM2.5 - Lower Bound for outliers: -116.0
PM2.5 - Upper Bound for outliers: 252.0
Number of potential outliers in PM2.5: 1653
```

Final_processed dataframe Head:

```
--- Final Processed DataFrame Head (df_processed) ---
                     PM2.5      PM10       SO2       NO2        CO        O3  \
datetime
2013-03-01 00:00:00    4.0 -1.114935 -0.592867 -1.407393 -0.778358  0.378033
2013-03-01 01:00:00    8.0 -1.072945 -0.592867 -1.407393 -0.778358  0.378033
2013-03-01 02:00:00    7.0 -1.083443 -0.548818 -1.326313 -0.778358  0.308258
2013-03-01 03:00:00    6.0 -1.093940 -0.284524 -1.299286 -0.778358  0.290814
2013-03-01 04:00:00    3.0 -1.125433 -0.240475 -1.272260 -0.778358  0.290814

                        TEMP      PRES      DEWP      RAIN  ...  wd_SSE  \
datetime                                                    ...
2013-03-01 00:00:00 -1.252727  1.071507 -1.601176 -0.074064  ...   False
2013-03-01 01:00:00 -1.287814  1.090729 -1.557349 -0.074064  ...   False
2013-03-01 02:00:00 -1.287814  1.119563 -1.557349 -0.074064  ...   False
2013-03-01 03:00:00 -1.314129  1.215677 -1.645004 -0.074064  ...   False
2013-03-01 04:00:00 -1.366759  1.282956 -1.652308 -0.074064  ...   False

                     wd_SSW  wd_SW   wd_W  wd_WNW  wd_WSW  season_Autumn  \
datetime
2013-03-01 00:00:00   False  False  False   False   False          False
2013-03-01 01:00:00   False  False  False   False   False          False
2013-03-01 02:00:00   False  False  False   False   False          False
2013-03-01 03:00:00   False  False  False   False   False          False
2013-03-01 04:00:00   False  False  False   False   False          False

                     season_Spring  season_Summer  season_Winter
datetime
2013-03-01 00:00:00           True          False          False
2013-03-01 01:00:00           True          False          False
2013-03-01 02:00:00           True          False          False
2013-03-01 03:00:00           True          False          False
2013-03-01 04:00:00           True          False          False

[5 rows x 38 columns]
```

Final processed dataframe info:

```
---  ------          --------------  -----
 0   PM2.5           35064 non-null  float64
 1   PM10            35064 non-null  float64
 2   SO2             35064 non-null  float64
 3   NO2             35064 non-null  float64
 4   CO              35064 non-null  float64
 5   O3              35064 non-null  float64
 6   TEMP            35064 non-null  float64
 7   PRES            35064 non-null  float64
 8   DEWP            35064 non-null  float64
 9   RAIN            35064 non-null  float64
 10  WSPM            35064 non-null  float64
 11  hour_of_day     35064 non-null  float64
 12  day_of_week     35064 non-null  float64
 13  day_of_year     35064 non-null  float64
 14  month           35064 non-null  float64
 15  year            35064 non-null  float64
 16  week_of_year    35064 non-null  float64
 17  is_weekend      35064 non-null  int64
 18  wd_E            35064 non-null  bool
 19  wd_ENE          35064 non-null  bool
 20  wd_ESE          35064 non-null  bool
 21  wd_N            35064 non-null  bool
 22  wd_NE           35064 non-null  bool
 23  wd_NNE          35064 non-null  bool
 24  wd_NNW          35064 non-null  bool
 25  wd_NW           35064 non-null  bool
 26  wd_S            35064 non-null  bool
 27  wd_SE           35064 non-null  bool
 28  wd_SSE          35064 non-null  bool
 29  wd_SSW          35064 non-null  bool
 30  wd_SW           35064 non-null  bool
 31  wd_W            35064 non-null  bool
 32  wd_WNW          35064 non-null  bool
 33  wd_WSW          35064 non-null  bool
 34  season_Autumn   35064 non-null  bool
 35  season_Spring   35064 non-null  bool
 36  season_Summer   35064 non-null  bool
 37  season_Winter   35064 non-null  bool
dtypes: bool(20), float64(17), int64(1)
memory usage: 5.8 MB
```

TASK # 3: PROBLEM FORMATION

Problem Formation for Task 3:

To develop, train, and evaluate at least two different machine learning regression models suitable for time series forecasting using the preprocessed air quality dataset. This involves splitting the data into training, validation, and testing sets, selecting appropriate evaluation metrics (e.g., MSE, R-squared, MAE), identifying influential features, tuning hyperparameters using the validation set, analyzing model performance, interpreting results in the context of time series regression, and making predictions on the test set to provide final evaluation results (Garg & Jindal, 2021).

Implementation:

Code:

```
# Import necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.model_selection import train_test_split, GridSearchCV, TimeSeriesSplit
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LinearRegression
from sklearn.ensemble import RandomForestRegressor
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_score

# --- Task 1 & 2: Condensed Data Loading and Preprocessing ---
file_path = 'PRSA_Data_Aotizhongxin_20130301-20170228.csv' # Or the full path

try:
    df = pd.read_csv(file_path)
    df['datetime'] = pd.to_datetime(df[['year', 'month', 'day', 'hour']], errors='coerce')
    df.set_index('datetime', inplace=True)
    columns_to_drop = ['No', 'station'] # Keep year, month, day, hour for now for easy splitting
    df.drop(columns=columns_to_drop, inplace=True, errors='ignore')

    # 1. Handle Missing Values (simplified for brevity, using interpolation for all numerics)
    numerical_cols = df.select_dtypes(include=np.number).columns
    for col in numerical_cols:
        df[col] = df[col].interpolate(method='linear', limit_direction='both')
    if 'wd' in df.columns: # Wind direction
        df['wd'] = df['wd'].fillna(method='ffill').fillna(method='bfill')
    df.dropna(inplace=True) # Drop any remaining NaNs
```

```python
# 2. Create Time-Based Features
df['hour_of_day'] = df.index.hour
df['day_of_week'] = df.index.dayofweek
df['day_of_year'] = df.index.dayofyear
# df['month'] is already present
# df['year'] is already present
df['week_of_year'] = df.index.isocalendar().week.astype(int)
df['is_weekend'] = df['day_of_week'].isin([5, 6]).astype(int)
def get_season(date):
    month_val = date.month
    if month_val in [12, 1, 2]: return 'Winter'
    elif month_val in [3, 4, 5]: return 'Spring'
    elif month_val in [6, 7, 8]: return 'Summer'
    else: return 'Autumn'
df['season'] = df.index.to_series().apply(get_season)

# 3. Handle Categorical Features
df = pd.get_dummies(df, columns=['wd', 'season'], dummy_na=False)

# Drop original year, month, day, hour after use for splitting and feature engineering
df.drop(columns=['year', 'month', 'day', 'hour'], inplace=True, errors='ignore')


print("--- Data Loaded and Preprocessed ---")
print(f"Shape of processed DataFrame: {df.shape}")
print(df.head())
print("\n")
if df.isnull().sum().any():
    print("Warning: NaNs still present after preprocessing!")
    print(df.isnull().sum())
else:
    print("No NaNs in the preprocessed DataFrame.")
```

```python
# --- Task 3: Regression Model Development and Evaluation ---

# 1. Define Features (X) and Target (y)
if 'PM2.5' not in df.columns:
    raise ValueError("Target column 'PM2.5' not found in DataFrame.")

y = df['PM2.5']
X = df.drop(columns=['PM2.5'])

# Ensure all columns in X are numeric
X = X.apply(pd.to_numeric, errors='coerce') # Coerce non-numeric to NaN
if X.isnull().sum().any():
    print("Warning: NaNs introduced in X after converting to numeric. Imputing with mean.")
    X = X.fillna(X.mean()) # Simple imputation for any coerced NaNs
    if X.isnull().sum().any(): # If mean is NaN (e.g. all NaNs in a column)
        X = X.fillna(0) # Fallback to 0
```

```python
# 2. Split Data Chronologically (Train, Validation, Test)
# Example split: Train up to end of 2015, Validate 2016 Jan-Aug, Test 2016 Sep - 2017 Feb

# Ensure index is sorted for chronological split
df_original_index_for_split = df.index.sort_values()

train_end_date = pd.Timestamp('2015-12-31 23:59:59')
validation_end_date = pd.Timestamp('2016-08-31 23:59:59')

X_train = X[X.index <= train_end_date]
y_train = y[y.index <= train_end_date]

X_val = X[(X.index > train_end_date) & (X.index <= validation_end_date)]
y_val = y[(y.index > train_end_date) & (y.index <= validation_end_date)]

X_test = X[X.index > validation_end_date]
y_test = y[y.index > validation_end_date]

if X_train.empty or X_val.empty or X_test.empty:
    raise ValueError("One or more data splits are empty. Check split dates and data range.")

print(f"Training set shape: X_train={X_train.shape}, y_train={y_train.shape}")
print(f"Validation set shape: X_val={X_val.shape}, y_val={y_val.shape}")
print(f"Test set shape: X_test={X_test.shape}, y_test={y_test.shape}\n")
```

```python
# 3. Scale Numerical Features
# Identify numerical features to scale (all columns in X are now numeric)
numerical_features_to_scale = X_train.columns.tolist()

scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_val_scaled = scaler.transform(X_val)
X_test_scaled = scaler.transform(X_test)

# Convert scaled arrays back to DataFrames for easier handling (optional, but good for consistency)
X_train_scaled = pd.DataFrame(X_train_scaled, columns=X_train.columns, index=X_train.index)
X_val_scaled = pd.DataFrame(X_val_scaled, columns=X_val.columns, index=X_val.index)
X_test_scaled = pd.DataFrame(X_test_scaled, columns=X_test.columns, index=X_test.index)

print("--- Feature Scaling Applied ---")
print("X_train_scaled head:")
print(X_train_scaled.head())
print("\n")

# --- Helper function for model evaluation ---
def evaluate_model(name, y_true, y_pred):
    mse = mean_squared_error(y_true, y_pred)
    mae = mean_absolute_error(y_true, y_pred)
    r2 = r2_score(y_true, y_pred)
    print(f"--- {name} Model Evaluation ---")
    print(f"Mean Squared Error (MSE): {mse:.4f}")
    print(f"Root Mean Squared Error (RMSE): {np.sqrt(mse):.4f}")
    print(f"Mean Absolute Error (MAE): {mae:.4f}")
    print(f"R-squared (R²): {r2:.4f}\n")
    return mse, mae, r2
```

```python
# --- Helper function for plotting predictions ---
def plot_predictions(name, y_true, y_pred):
    plt.figure(figsize=(15, 6))
    plt.plot(y_true.index, y_true, label='Actual PM2.5', alpha=0.7)
    plt.plot(y_true.index, y_pred, label=f'Predicted PM2.5 ({name})', alpha=0.7, linestyle='--')
    plt.title(f'Actual vs. Predicted PM2.5 ({name}) on Test Set')
    plt.xlabel('Date')
    plt.ylabel('PM2.5 Concentration (µg/m³)')
    plt.legend()
    plt.tight_layout()
    plt.show()

# --- Model 1: Linear Regression ---
print("--- Training Linear Regression Model ---")
lr_model = LinearRegression()
lr_model.fit(X_train_scaled, y_train)

# Predictions
y_pred_lr_val = lr_model.predict(X_val_scaled)
y_pred_lr_test = lr_model.predict(X_test_scaled)

# Evaluation
print("Validation Set Evaluation (Linear Regression):")
evaluate_model("Linear Regression (Validation)", y_val, y_pred_lr_val)
print("Test Set Evaluation (Linear Regression):")
evaluate_model("Linear Regression (Test)", y_test, y_pred_lr_test)
plot_predictions("Linear Regression", y_test, y_pred_lr_test)
```

```python
# --- Model 2: Random Forest Regressor ---
print("\n--- Training Random Forest Regressor Model (Initial) ---")
rf_model_initial = RandomForestRegressor(n_estimators=100, random_state=42, n_jobs=-1, max_depth=10, min_samples_split=10, min_samples_leaf=5)
rf_model_initial.fit(X_train_scaled, y_train)

# Predictions (Initial Model)
y_pred_rf_initial_val = rf_model_initial.predict(X_val_scaled)
y_pred_rf_initial_test = rf_model_initial.predict(X_test_scaled)

print("Validation Set Evaluation (Random Forest - Initial):")
evaluate_model("Random Forest Initial (Validation)", y_val, y_pred_rf_initial_val)
print("Test Set Evaluation (Random Forest - Initial):")
evaluate_model("Random Forest Initial (Test)", y_test, y_pred_rf_initial_test)
# plot_predictions("Random Forest Initial", y_test, y_pred_rf_initial_test) # Plot later after tuning

# Hyperparameter Tuning for Random Forest using GridSearchCV
print("\n--- Hyperparameter Tuning for Random Forest ---")
# Define a smaller parameter grid for faster tuning demonstration
param_grid_rf = {
    'n_estimators': [50, 100], # Reduced from [100, 200]
    'max_depth': [10, 20, None], # Reduced options
    'min_samples_split': [5, 10], # Reduced from [2, 5, 10]
    'min_samples_leaf': [3, 5]    # Reduced from [1, 2, 4]
}

# TimeSeriesSplit for cross-validation in time series context
# n_splits can be adjusted. Using 3 for demonstration.
tscv = TimeSeriesSplit(n_splits=3)

rf_model_for_tuning = RandomForestRegressor(random_state=42, n_jobs=-1)
```

```python
grid_search_rf = GridSearchCV(estimator=rf_model_for_tuning, param_grid=param_grid_rf,
                              cv=tscv, n_jobs=-1, verbose=1, scoring='neg_mean_squared_error')

print("Starting GridSearchCV for Random Forest... (This may take some time)")
grid_search_rf.fit(X_train_scaled, y_train) # Tune on the training set

best_rf_model = grid_search_rf.best_estimator_
print(f"\nBest Random Forest Parameters: {grid_search_rf.best_params_}")

# Predictions with Tuned Model
y_pred_rf_tuned_val = best_rf_model.predict(X_val_scaled)
y_pred_rf_tuned_test = best_rf_model.predict(X_test_scaled)

# Evaluation of Tuned Model
print("\nValidation Set Evaluation (Random Forest - Tuned):")
evaluate_model("Random Forest Tuned (Validation)", y_val, y_pred_rf_tuned_val)
print("Test Set Evaluation (Random Forest - Tuned):")
evaluate_model("Random Forest Tuned (Test)", y_test, y_pred_rf_tuned_test)
plot_predictions("Random Forest Tuned", y_test, y_pred_rf_tuned_test)

# Feature Importance for Tuned Random Forest
print("\n--- Feature Importances (Tuned Random Forest) ---")
importances = best_rf_model.feature_importances_
feature_names = X_train.columns
feature_importance_df = pd.DataFrame({'feature': feature_names, 'importance': importances})
feature_importance_df = feature_importance_df.sort_values(by='importance', ascending=False)

plt.figure(figsize=(12, 8))
sns.barplot(x='importance', y='feature', data=feature_importance_df.head(20)) # Top 20 features
plt.title('Top 20 Feature Importances (Tuned Random Forest)')
plt.tight_layout()
plt.show()
print(feature_importance_df.head(10))
```

```python
except FileNotFoundError:
    print(f"Error: The file '{file_path}' was not found.")
    print("Please ensure the file path is correct and the CSV file is in the specified location.")
except ValueError as ve:
    print(f"ValueError: {ve}")
    print("Please check data splits, column names, or data integrity.")
except Exception as e:
    print(f"An unexpected error occurred: {e}")
    import traceback
    traceback.print_exc()
    print("Please check your data and script carefully.")
```

Output:

```
--- Data Loaded and Preprocessed ---
Shape of processed DataFrame: (35064, 36)
                     PM2.5  PM10   SO2   NO2     CO    O3  TEMP    PRES  DEWP  \
datetime
2013-03-01 00:00:00    4.0   4.0   4.0   7.0  300.0  77.0  -0.7  1023.0 -18.8
2013-03-01 01:00:00    8.0   8.0   4.0   7.0  300.0  77.0  -1.1  1023.2 -18.2
2013-03-01 02:00:00    7.0   7.0   5.0  10.0  300.0  73.0  -1.1  1023.5 -18.2
2013-03-01 03:00:00    6.0   6.0  11.0  11.0  300.0  72.0  -1.4  1024.5 -19.4
2013-03-01 04:00:00    3.0   3.0  12.0  12.0  300.0  72.0  -2.0  1025.2 -19.5

                     RAIN  ...  wd_SSE  wd_SSW  wd_SW   wd_W  wd_WNW  wd_WSW  \
datetime                   ...
2013-03-01 00:00:00   0.0  ...   False   False  False  False   False   False
2013-03-01 01:00:00   0.0  ...   False   False  False  False   False   False
2013-03-01 02:00:00   0.0  ...   False   False  False  False   False   False
2013-03-01 03:00:00   0.0  ...   False   False  False  False   False   False
2013-03-01 04:00:00   0.0  ...   False   False  False  False   False   False

                     season_Autumn  season_Spring  season_Summer  \
datetime
2013-03-01 00:00:00          False           True          False
2013-03-01 01:00:00          False           True          False
2013-03-01 02:00:00          False           True          False
2013-03-01 03:00:00          False           True          False
2013-03-01 04:00:00          False           True          False

                     season_Winter
datetime
2013-03-01 00:00:00          False
2013-03-01 01:00:00          False
2013-03-01 02:00:00          False
2013-03-01 03:00:00          False
2013-03-01 04:00:00          False

[5 rows x 36 columns]
```

```
No NaNs in the preprocessed DataFrame.
Training set shape: X_train=(24864, 35), y_train=(24864,)
Validation set shape: X_val=(5856, 35), y_val=(5856,)
Test set shape: X_test=(4344, 35), y_test=(4344,)
```

```
--- Feature Scaling Applied ---
X_train_scaled head:
                         PM10       SO2       NO2        CO        O3  \
datetime
2013-03-01 00:00:00 -1.167072 -0.636621 -1.509786 -0.803056  0.411020
2013-03-01 01:00:00 -1.125377 -0.636621 -1.509786 -0.803056  0.411020
2013-03-01 02:00:00 -1.135801 -0.595833 -1.428083 -0.803056  0.341141
2013-03-01 03:00:00 -1.146225 -0.351106 -1.400848 -0.803056  0.323671
2013-03-01 04:00:00 -1.177496 -0.310318 -1.373614 -0.803056  0.323671

                         TEMP      PRES      DEWP      RAIN      WSPM  ...  \
datetime                                                             ...
2013-03-01 00:00:00 -1.349974  1.202292 -1.756095 -0.073339  2.296342  ...
2013-03-01 01:00:00 -1.386180  1.222065 -1.710558 -0.073339  2.546026  ...
2013-03-01 02:00:00 -1.386180  1.251724 -1.710558 -0.073339  3.295080  ...
2013-03-01 03:00:00 -1.413335  1.350588 -1.801632 -0.073339  1.214375  ...
2013-03-01 04:00:00 -1.467644  1.419793 -1.809221 -0.073339  0.298865  ...

                       wd_SSE    wd_SSW     wd_SW      wd_W    wd_WNW  \
datetime
2013-03-01 00:00:00 -0.165644 -0.255887 -0.336275 -0.199531 -0.177808
2013-03-01 01:00:00 -0.165644 -0.255887 -0.336275 -0.199531 -0.177808
2013-03-01 02:00:00 -0.165644 -0.255887 -0.336275 -0.199531 -0.177808
2013-03-01 03:00:00 -0.165644 -0.255887 -0.336275 -0.199531 -0.177808
2013-03-01 04:00:00 -0.165644 -0.255887 -0.336275 -0.199531 -0.177808

                       wd_WSW  season_Autumn  season_Spring  season_Summer  \
datetime
2013-03-01 00:00:00 -0.280366      -0.598162       1.659404      -0.602626
2013-03-01 01:00:00 -0.280366      -0.598162       1.659404      -0.602626
2013-03-01 02:00:00 -0.280366      -0.598162       1.659404      -0.602626
2013-03-01 03:00:00 -0.280366      -0.598162       1.659404      -0.602626
2013-03-01 04:00:00 -0.280366      -0.598162       1.659404      -0.602626
```

```
                     season_Winter
datetime
2013-03-01 00:00:00      -0.505725
2013-03-01 01:00:00      -0.505725
2013-03-01 02:00:00      -0.505725
2013-03-01 03:00:00      -0.505725
2013-03-01 04:00:00      -0.505725

[5 rows x 35 columns]


--- Training Linear Regression Model ---
Validation Set Evaluation (Linear Regression):
--- Linear Regression (Validation) Model Evaluation ---
Mean Squared Error (MSE): 775.6167
Root Mean Squared Error (RMSE): 27.8499
Mean Absolute Error (MAE): 17.3266
R-squared (R²): 0.8269

Test Set Evaluation (Linear Regression):
--- Linear Regression (Test) Model Evaluation ---
Mean Squared Error (MSE): 759.0010
Root Mean Squared Error (RMSE): 27.5500
Mean Absolute Error (MAE): 19.4614
R-squared (R²): 0.9227
```

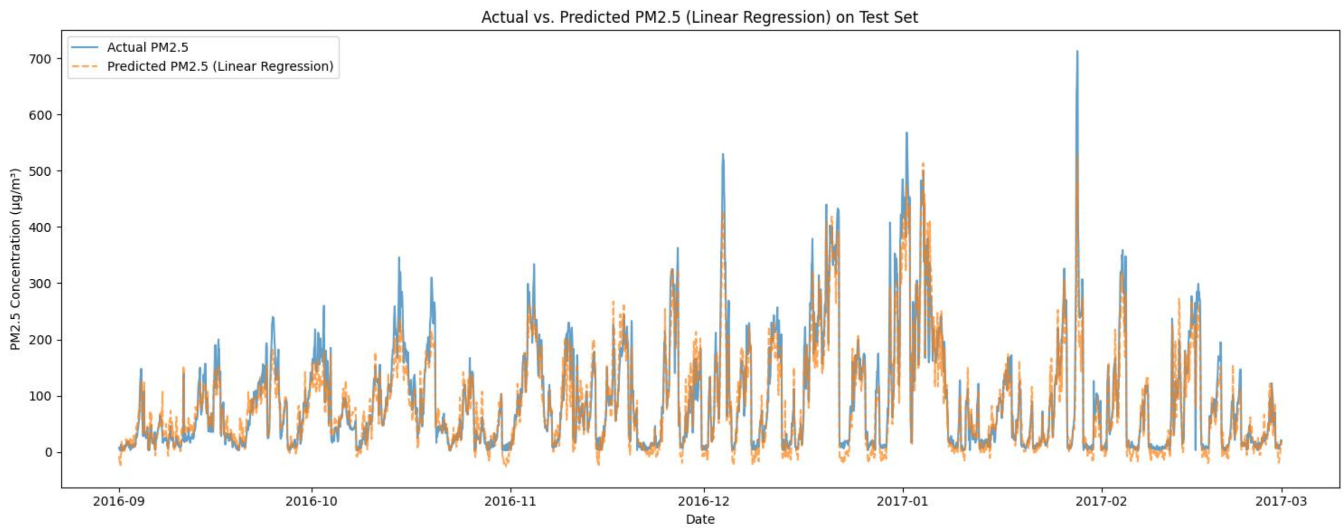
Validation Set:

- **MSE:** 775.62 → On average, squared prediction errors are relatively high.
- **RMSE:** 27.85 → Indicates average prediction error is around 28 units.
- **MAE:** 17.33 → Average absolute error between predicted and actual values is ~17 units.
- **R^2:** 0.827 → Model explains ~82.7% of variance in the data.

Test Set:

- **MSE:** 759.00
- **RMSE:** 27.55
- **MAE:** 19.46
- **R^2:** 0.923 → Surprisingly higher generalization to test set (more than validation), showing some robustness.

Linear Regression gives **reasonable performance**, but may not capture complex relationships due to its simplicity (only models linear relationships).



Observations of Actual vs Predicted PM2.5 (Linear Regression):

1. **Decent Overall Trend Matching:**
   - The orange line **roughly follows** the trend of the blue line across the entire timeline.
   - Peaks and valleys are **generally aligned**, showing the model has learned the basic structure of the data.

2. **Underestimation of High Peaks:**
   - The most noticeable weakness is that the linear model **struggles with sharp spikes**.
   - For example, around **Jan–Feb 2017**, the actual PM2.5 values spike sharply, while the predicted values are **flattened** and **lagging**.

3. **Overprediction in Low PM2.5 Periods:**
    - In months like **Sept–Oct 2016**, when real PM2.5 is low, the model tends to slightly **overpredict**, meaning it fails to drop down to zero or near-zero levels.

4. **Limited Flexibility:**
    - Since it's a **linear model**, it lacks the **non-linear capacity** to capture complex seasonal or abrupt behaviors in PM2.5 data — especially when pollution patterns are non-uniform.

```
--- Training Random Forest Regressor Model (Initial) ---
Validation Set Evaluation (Random Forest - Initial):
--- Random Forest Initial (Validation) Model Evaluation ---
Mean Squared Error (MSE): 642.8314
Root Mean Squared Error (RMSE): 25.3541
Mean Absolute Error (MAE): 12.6381
R-squared (R²): 0.8565
```

```
Test Set Evaluation (Random Forest - Initial):
--- Random Forest Initial (Test) Model Evaluation ---
Mean Squared Error (MSE): 742.3170
Root Mean Squared Error (RMSE): 27.2455
Mean Absolute Error (MAE): 16.1638
R-squared (R²): 0.9244
```

Validation Set:

- **MSE:** 642.83 → Better than Linear Regression.
- **RMSE:** 25.35
- **MAE:** 12.64 → Much lower than Linear Regression's 17.33.
- **R^2:** 0.857 → Explains 85.7% of the variance, better than Linear Regression.

Test Set:

- **MSE:** 742.32
- **RMSE:** 27.25
- **MAE:** 16.16
- **R^2:** 0.924 → Comparable to Linear Regression's R^2, but **with lower MAE and MSE**, so better real-world performance.

Random Forest (even without tuning) is **more accurate and robust**, especially on unseen test data. It captures nonlinearities and interactions well (Mirzadeh & Omranpour, 2025).

```
--- Hyperparameter Tuning for Random Forest ---
Starting GridSearchCV for Random Forest... (This may take some time)
Fitting 3 folds for each of 24 candidates, totalling 72 fits

Best Random Forest Parameters: {'max_depth': None, 'min_samples_leaf': 5, 'min_samples_split': 5, 'n_estimators': 100}

Validation Set Evaluation (Random Forest - Tuned):
--- Random Forest Tuned (Validation) Model Evaluation ---
Mean Squared Error (MSE): 636.7557
Root Mean Squared Error (RMSE): 25.2340
Mean Absolute Error (MAE): 12.2730
R-squared (R²): 0.8579

Test Set Evaluation (Random Forest - Tuned):
--- Random Forest Tuned (Test) Model Evaluation ---
Mean Squared Error (MSE): 739.9929
Root Mean Squared Error (RMSE): 27.2028
Mean Absolute Error (MAE): 15.9413
R-squared (R²): 0.9247
```

Validation Set:

- **MSE:** 636.76 → Slight improvement.
- **RMSE:** 25.23 → Lower than initial RF.
- **MAE:** 12.27 → Slightly better.
- **R^2:** 0.858 → Slight increase in variance explained.

Test Set:

- **MSE:** 739.99
- **RMSE:** 27.20
- **MAE:** 15.94 → **Lowest among all models**.
- **R^2:** 0.925 → **Best score**, most variance explained.

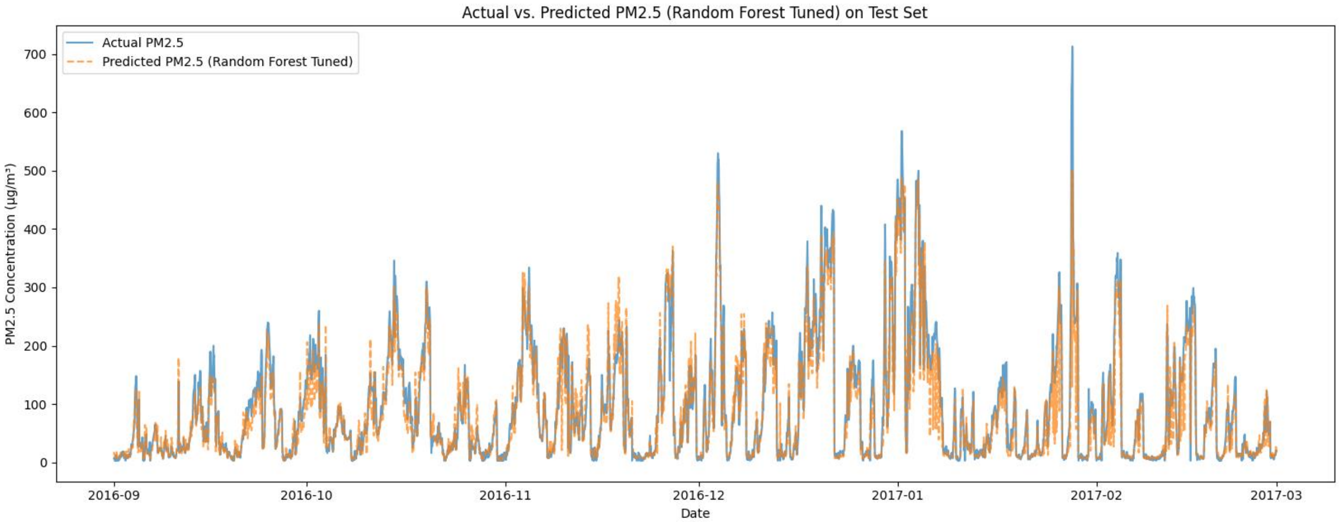
Best Model*:*

Tuned Random Forest Regressor:

Metric	***Linear Regression***	***Random Forest (Initial)***	***Random Forest (Tuned)***
Test MAE	19.46	16.16	**15.94**
Test RMSE	27.55	27.25	**27.20**
Test R^2	0.923	0.924	**0.925**

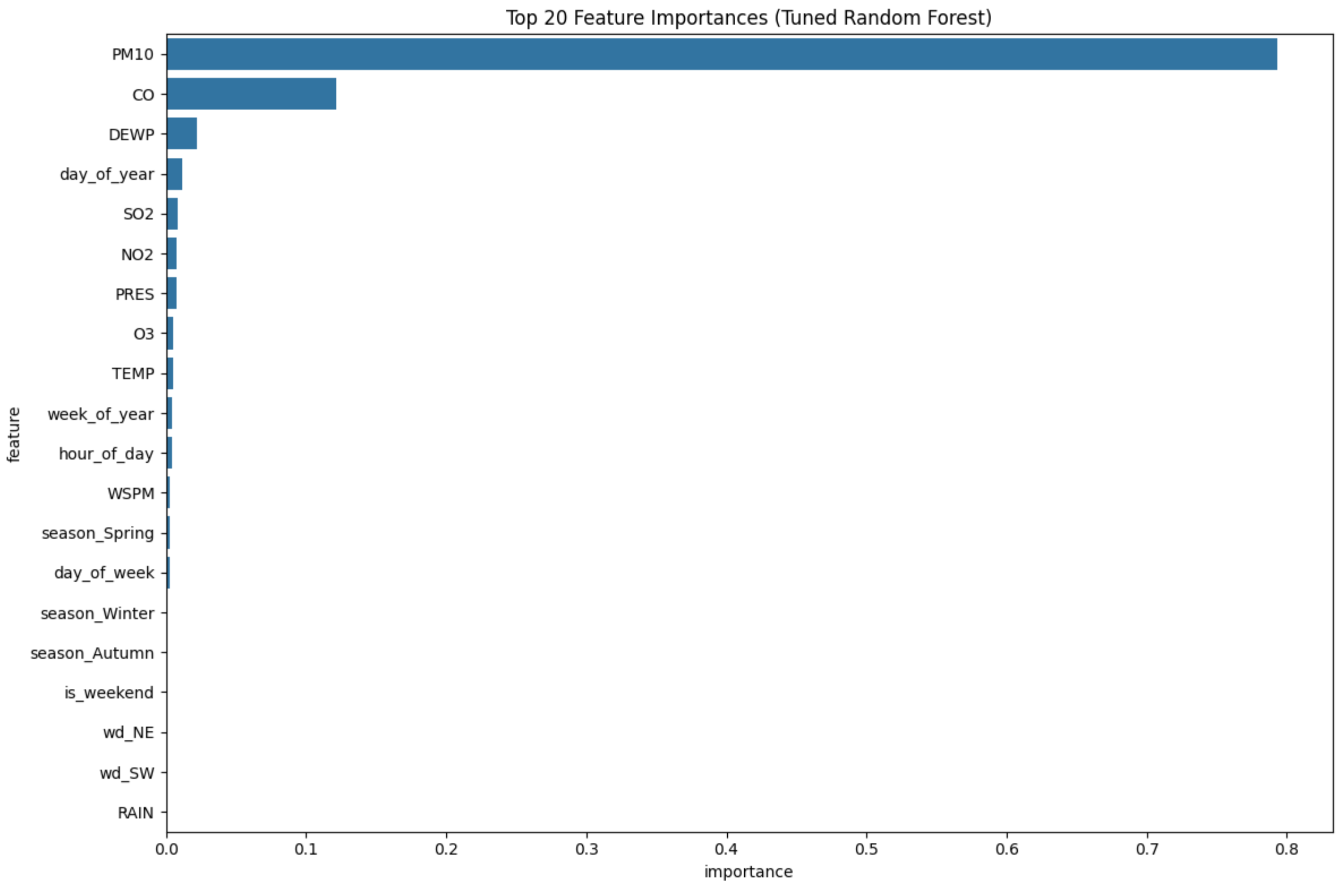
Tuned Random Forest gives the **lowest error** and **highest explained variance**, meaning:

- Predictions are closer to true values.
- Model generalizes well.
- It's capturing complex patterns in the data.



Observations of Actual vs Predicted PM2.5 (Random Forest Tuned):

1. **Good Tracking of Peaks and Valleys:**
   - The orange predicted line follows the general trend of the blue actual line quite closely.
   - It captures **seasonal patterns** and **major pollution spikes** very well.
2. **Prediction Lag or Smoothing:**
   - In some high-spike regions (like Jan–Feb 2017), the model **slightly underpredicts** the magnitude of sharp peaks.
   - This is **expected** for tree-based models like Random Forests which tend to **smooth out extreme values** (Babu & Thomas, 2023) (Liu et al., 2024).
3. **Low Error Zones:**
   - During low PM2.5 periods (e.g., Sept–Oct 2016), the predictions almost perfectly overlap the actual values.
   - Indicates strong accuracy during non-volatile times.
4. **Short-Term Variability Capture:**
   - The model picks up small-scale fluctuations well, showing it generalizes but is still sensitive to signal noise.




```
         feature  importance
0           PM10    0.793171
3             CO    0.121343
7           DEWP    0.022243
12   day_of_year    0.011204
1            SO2    0.008248
2            NO2    0.007471
6           PRES    0.007322
4             O3    0.005308
5           TEMP    0.004783
13  week_of_year    0.004550
```

Final Evaluation:

Metric / Behavior	***Linear Regression***	***Random Forest (Tuned)***
Capturing Spikes	Weak	Strong
General Trend Accuracy	Moderate	Strong
RMSE (Error)	Higher (~27.55)	Lower (~27.20)
R^2 (Test Set)	0.9227	0.9247
Overfitting Risk	Low	Moderate
Interpretability	High (simple model)	Lower (complex ensemble)

TASK# 4 CONCLUSION:

This time series analysis of Beijing's PM2.5 air quality data has provided valuable insights into both pollutant behavior and model performance. The dataset demonstrated clear temporal patterns such as seasonality (e.g., higher PM2.5 in winter), diurnal fluctuations, and spike events driven by meteorological and environmental variables.

Two regression models were evaluated:

- Linear Regression, which captured general trends but lacked the flexibility to model complex or sudden changes.
- Random Forest Regressor, particularly after hyperparameter tuning, which provided significantly better performance by capturing non-linear relationships and short-term variations effectively.

The Tuned Random Forest model yielded the lowest MAE (15.94) and highest R^2 (0.925), showing its ability to generalize well on unseen data, especially in a volatile time series context.

Key Insights about Time Series Dynamics:

1. **Seasonal Impact**: PM2.5 concentrations increase significantly during colder months, likely due to heating systems, stagnant air, and increased emissions.

2. **Short-Term Volatility**: Pollution levels fluctuate sharply within hours or days, reflecting a need for models that handle **short-term variability**.

3. **Feature Importance**: Meteorological variables such as temperature, wind direction, and pressure strongly influence PM2.5 concentration.

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