Machine_Learning_IoT_Application_Design_and_Implementation_Air_Qu

February 23, 2025

0.1 Introduction

The purpose of this notebook is to demonstrate a comprehensive data pipeline for an IoT sensorered Air Quality dataset, starting with data cleaning and EDA to address missing values, outliers, and proper datetime formatting. Two deep learning models were developed: an LSTM for time-series temperature prediction and a deep feed-forward neural network for NO2 forecasting.

```
[1]: import csv
     import numpy as np
     import pandas as pd
     import tensorflow as tf
     from google.colab import drive
     from tensorflow import keras
     from tensorflow.keras import layers
     from tensorflow.keras.callbacks import EarlyStopping, ReduceLROnPlateau
     from tensorflow.keras.layers import BatchNormalization, Dense, Dropout
     from tensorflow.keras.models import Sequential
     from tensorflow.keras.optimizers import Adam
     from tensorflow.keras.regularizers import 12
     from sklearn.metrics import mean_squared_error
     from sklearn.model_selection import train_test_split
     from sklearn.preprocessing import MinMaxScaler, StandardScaler
     drive.mount('/content/drive')
```

Mounted at /content/drive

```
[2]: !pip install openpyxl
```

```
Requirement already satisfied: openpyxl in /usr/local/lib/python3.11/dist-packages (3.1.5)
Requirement already satisfied: et-xmlfile in /usr/local/lib/python3.11/dist-packages (from openpyxl) (2.0.0)
```

##EDA Summary## The EDA carried out created a Datetime column, converted other columns into numerical data, dropped NaN/NaT rows (\sim 100). Two copies of that dataframe were created.

• df_no_outliers has removed rows with outliers in any column via IQR Method. The count for all rows decreased from 9357 to 5436 from this process. Outlier removal for any numerical

column can ommitted or re-added in the df_no_outliers module, which allows for increase the count value when priotizing certain sensor data over others.

• df_median replaced outliers with the median conserving the count, the number of data points becomes a priority during model training, testing and validation evaluation.

<ipython-input-4-871fd710467c>:10: UserWarning: Could not infer format, so each
element will be parsed individually, falling back to `dateutil`. To ensure
parsing is consistent and as-expected, please specify a format.

df_raw['Datetime'] = pd.to_datetime(df_raw['Date'].astype(str) + ' ' +
df_raw['Time'].astype(str), errors='coerce')

| | Date | Time | CO(GT) | PT08.S1(| CO) NMHC(GT) | C6H6(GT) \ | |
|---|-------------------|----------------|---------|----------|--------------|-------------|---|
| 0 | 2004-03-10 1900-0 | 01-01 18:00:00 | 2,6 | 136 | 0.0 150.0 | 11,9 | |
| 1 | 2004-03-10 1900-0 | 01-01 19:00:00 | 2 | 129 | 2.0 112.0 | 9,4 | |
| 2 | 2004-03-10 1900-0 |)1-01 20:00:00 | 2,2 | 140 | 2.0 88.0 | 9,0 | |
| 3 | 2004-03-10 1900-0 |)1-01 21:00:00 | 2,2 | 137 | 6.0 80.0 | 9,2 | |
| 4 | 2004-03-10 1900-0 |)1-01 22:00:00 | 1,6 | 127 | 2.0 51.0 | 6,5 | |
| | | | | | | | |
| | PT08.S2(NMHC) N | NOx(GT) PT08. | S3(NOx) | NO2(GT) | PT08.S4(NO2) | PT08.S5(03) | \ |
| 0 | 1046.0 | 166.0 | 1056.0 | 113.0 | 1692.0 | 1268.0 | |
| 1 | 955.0 | 103.0 | 1174.0 | 92.0 | 1559.0 | 972.0 | |
| 2 | 939.0 | 131.0 | 1140.0 | 114.0 | 1555.0 | 1074.0 | |
| 3 | 948.0 | 172.0 | 1092.0 | 122.0 | 1584.0 | 1203.0 | |

```
4
               836.0
                       131.0
                               1205.0
                                               116.0
                                                            1490.0
                                                                         1110.0
               RH
                       AΗ
                                           Datetime
    0 13,6 48,9 0,7578 2004-03-10 18:00:00-01:00
    1 13,3 47,7 0,7255 2004-03-10 19:00:00-01:00
    2 11,9 54,0 0,7502 2004-03-10 20:00:00-01:00
    3 11,0 60,0 0,7867 2004-03-10 21:00:00-01:00
    4 11,2 59,6 0,7888 2004-03-10 22:00:00-01:00
    Date
                                datetime64[ns]
    Time
                                datetime64[ns]
    CO(GT)
                                        object
    PT08.S1(CO)
                                       float64
    NMHC (GT)
                                       float64
    C6H6(GT)
                                        object
    PTO8.S2(NMHC)
                                       float64
    NOx (GT)
                                       float64
    PTO8.S3(NOx)
                                       float64
    NO2(GT)
                                       float64
    PT08.S4(NO2)
                                       float64
    PT08.S5(03)
                                       float64
    Т
                                        object
    RH
                                        object
    ΑH
                                        object
    Datetime
                     datetime64[ns, UTC-01:00]
    dtype: object
[5]: #Replacing commas with dots and convert to numeric for all applicable columns
    cols_before_conversion = ['CO(GT)', 'C6H6(GT)', 'T', 'RH', 'AH']
    for col in cols before conversion:
         # Converting the column to string type before applying str.replace
        df_raw[col] = df_raw[col].astype(str).str.replace(',', '.').astype(float)
     #Counts before converting commas to dots (then converting to numerical values_
      → in the next module), CO(GT)=2137, C6H6(GT)=NaN, T=366, RH=366, AH=366
[6]: #Converting all data columns (except 'Datetime', 'Date', and 'Time') to numeric
     #Again, the errors='coerce' argument handles potential conversion errors by
      ⇔setting invalid values to NaN (Not a Number)
    for col in df_raw.columns:
         if col not in ['Datetime', 'Date', 'Time']: #Exclude these columns, ___
      →converting them would provide large numbers that do not provide usefulu
      ⇔information, at least in this context
             df_raw[col] = pd.to_numeric(df_raw[col], errors='coerce') #Key step,__
      →converting all data in columns not excluded to numeric, helps guarantee data
      ⇔consistency through an explicit conversion
```

```
[7]: #Displaying the head of the DataFrame to confirm the changes
     print(df_raw.head())
     #Displaying the datatypes to verify the conversion
     print(df_raw.dtypes)
            Date
                                 Time CO(GT)
                                               PT08.S1(CO)
                                                            NMHC(GT)
                                                                       C6H6(GT)
    0 2004-03-10 1900-01-01 18:00:00
                                          2.6
                                                     1360.0
                                                                150.0
                                                                           11.9
    1 2004-03-10 1900-01-01 19:00:00
                                          2.0
                                                                112.0
                                                     1292.0
                                                                            9.4
    2 2004-03-10 1900-01-01 20:00:00
                                          2.2
                                                     1402.0
                                                                 88.0
                                                                            9.0
    3 2004-03-10 1900-01-01 21:00:00
                                          2.2
                                                     1376.0
                                                                 80.0
                                                                            9.2
    4 2004-03-10 1900-01-01 22:00:00
                                          1.6
                                                     1272.0
                                                                 51.0
                                                                            6.5
       PTO8.S2(NMHC)
                     NOx(GT)
                                PT08.S3(NOx) NO2(GT)
                                                                      PT08.S5(03)
                                                       PT08.S4(NO2)
    0
              1046.0
                         166.0
                                      1056.0
                                                113.0
                                                              1692.0
                                                                           1268.0
               955.0
                         103.0
                                      1174.0
                                                 92.0
                                                              1559.0
    1
                                                                            972.0
               939.0
    2
                         131.0
                                      1140.0
                                                114.0
                                                              1555.0
                                                                           1074.0
    3
               948.0
                         172.0
                                      1092.0
                                                122.0
                                                              1584.0
                                                                           1203.0
    4
               836.0
                         131.0
                                                116.0
                                      1205.0
                                                              1490.0
                                                                           1110.0
          Т
               RH
                        AΗ
                                            Datetime
      13.6 48.9 0.7578 2004-03-10 18:00:00-01:00
      13.3 47.7 0.7255 2004-03-10 19:00:00-01:00
    2 11.9 54.0 0.7502 2004-03-10 20:00:00-01:00
    3 11.0 60.0 0.7867 2004-03-10 21:00:00-01:00
    4 11.2 59.6 0.7888 2004-03-10 22:00:00-01:00
                                 datetime64[ns]
    Date
    Time
                                 datetime64[ns]
    CO(GT)
                                        float64
    PT08.S1(CO)
                                        float64
    NMHC(GT)
                                        float64
    C6H6(GT)
                                        float64
    PT08.S2(NMHC)
                                        float64
    NOx(GT)
                                        float64
    PT08.S3(NOx)
                                        float64
                                        float64
    NO2(GT)
    PT08.S4(NO2)
                                        float64
    PT08.S5(03)
                                        float64
    Т
                                        float64
    RH
                                        float64
    AH
                                        float64
                      datetime64[ns, UTC-01:00]
    Datetime
    dtype: object
```

[8]: df_raw.Date[0] #Prints out first date in the dataset

[8]: Timestamp('2004-03-10 00:00:00')

```
[9]: df_raw.Time[0] #Prints out first time in the dataset
 [9]: Timestamp('1900-01-01 18:00:00')
[10]: df_raw.Datetime[0] #Prints out datetime date in the dataset
[10]: Timestamp('2004-03-10 18:00:00-0100', tz='UTC-01:00')
[11]: df_raw.describe(include='all') #Includes all columns, including Datetime
      #describes dataset following conversions to numerical values, counts for all _{f L}
       ⇔categories have changed to 9357
      #Date, Time, Datetime were not converted to numerical values because of their
       →object-like datetime64[ns] datatype, so describe() carries out data analysis
       →on the other columns
                                                                             \
[11]:
                                       Date
                                                                        Time
      count
                                       9357
                                                                        9357
                                              1900-01-01 11:29:54.806028032
             2004-09-21 04:30:05.193972480
      mean
      min
                        2004-03-10 00:00:00
                                                        1900-01-01 00:00:00
      25%
                        2004-06-16 00:00:00
                                                        1900-01-01 05:00:00
      50%
                        2004-09-21 00:00:00
                                                        1900-01-01 11:00:00
      75%
                        2004-12-28 00:00:00
                                                        1900-01-01 18:00:00
                        2005-04-04 00:00:00
                                                        1900-01-01 23:00:00
      max
      std
                                        NaN
                                                                         NaN
                  CO(GT)
                           PT08.S1(CO)
                                                                   PTO8.S2(NMHC)
                                            NMHC(GT)
                                                         C6H6(GT)
             9357.000000
                           9357.000000
                                        9357.000000
                                                      9357.000000
                                                                      9357.000000
      count
              -34.207524
                           1048.990061
                                        -159.090093
                                                                       894.595276
      mean
                                                         1.865683
      min
             -200.000000
                           -200.000000
                                        -200.000000
                                                      -200.000000
                                                                      -200.000000
      25%
                0.600000
                           921.000000
                                        -200.000000
                                                         4.000000
                                                                       711.000000
      50%
                1.500000
                           1053.000000
                                        -200.000000
                                                         7.900000
                                                                       895.000000
      75%
                2.600000
                           1221.000000
                                        -200.000000
                                                        13.600000
                                                                      1105.000000
      max
               11.900000
                           2040.000000
                                        1189.000000
                                                        63.700000
                                                                      2214.000000
               77.657170
                                         139.789093
      std
                            329.832710
                                                        41.380206
                                                                       342.333252
                           PT08.S3(NOx)
                                                       PT08.S4(NO2)
                                                                      PT08.S5(03)
                 NOx(GT)
                                             NO2(GT)
             9357.000000
                            9357.000000
                                         9357.000000
                                                        9357.000000
                                                                      9357.000000
      count
              168.616971
                             794.990168
                                            58.148873
                                                        1391.479641
      mean
                                                                       975.072032
             -200.000000
      min
                            -200.000000
                                         -200.000000
                                                        -200.000000
                                                                      -200.000000
      25%
               50.000000
                             637.000000
                                            53.000000
                                                        1185.000000
                                                                       700.000000
      50%
                             794.000000
                                                        1446.000000
                                                                       942.000000
              141.000000
                                            96.000000
      75%
              284.000000
                             960.000000
                                          133.000000
                                                        1662.000000
                                                                      1255.000000
      max
             1479.000000
                            2683.000000
                                          340.000000
                                                        2775.000000
                                                                      2523.000000
      std
              257.433866
                             321.993552
                                          126.940455
                                                         467.210125
                                                                       456.938184
                        Τ
                                    RH
                                                  AΗ
                                                      \
             9357.000000
                           9357.000000
                                        9357.000000
      count
```

```
39.485380
                9.778305
                                         -6.837604
     mean
                         -200.000000 -200.000000
     min
             -200.000000
      25%
               10.900000
                            34.100000
                                           0.692300
      50%
               17.200000
                            48.600000
                                           0.976800
      75%
               24.100000
                            61.900000
                                           1.296200
               44.600000
     max
                            88.700000
                                          2.231000
      std
               43.203623
                            51.216145
                                         38.976670
                                        Datetime
     count
                                            9357
             2004-09-21 15:59:59.999999872-01:00
     mean
     min
                       2004-03-10 18:00:00-01:00
     25%
                       2004-06-16 05:00:00-01:00
     50%
                       2004-09-21 16:00:00-01:00
     75%
                       2004-12-28 03:00:00-01:00
                       2005-04-04 14:00:00-01:00
     max
      std
                                             NaN
[12]: df_raw.isna().sum().plot.bar()
      #df.isna creates True values for NaN/NaT values, false otherwise (not counted_
      →in the graph below)
      #In other words, this below graph illustrates the number of missing values
```

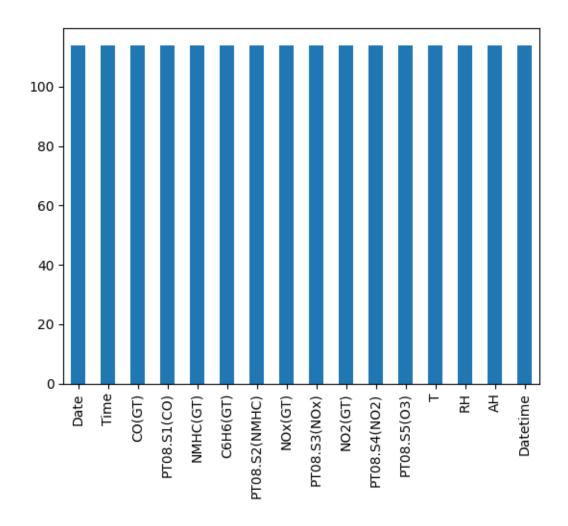
#It appears that there are approximately 110 rows in each category with NaN/Na T_{\sqcup}

#Removing about 100 rows out more than 9,000 will not likely distort, dropna()

[12]: <Axes: >

 $\rightarrow values$

⇒is an appropriate approach



```
[13]: # Drop rows with missing values, but exclude the 'Datetime' column
      df_dropna = df_raw.dropna(subset=df_raw.columns.difference(['Datetime']))
      #No NaT/NaN values detected after using dropna()
[14]:
     df_dropna.describe(include='all') #Includes all columns, including Datetime
[14]:
                                       Date
                                                                       Time
                                                                             \
                                       9357
                                                                       9357
      count
             2004-09-21 04:30:05.193972480
                                             1900-01-01 11:29:54.806028032
     mean
                       2004-03-10 00:00:00
                                                       1900-01-01 00:00:00
     min
      25%
                       2004-06-16 00:00:00
                                                       1900-01-01 05:00:00
                                                       1900-01-01 11:00:00
      50%
                       2004-09-21 00:00:00
      75%
                       2004-12-28 00:00:00
                                                       1900-01-01 18:00:00
     max
                       2005-04-04 00:00:00
                                                       1900-01-01 23:00:00
                                        NaN
                                                                       NaN
      std
                  CO(GT) PT08.S1(CO)
                                           NMHC(GT)
                                                        C6H6(GT) PT08.S2(NMHC)
```

```
9357.000000
                     9357.000000
                                  9357.000000
                                                9357.000000
                                                                9357.000000
count
mean
        -34.207524
                     1048.990061
                                   -159.090093
                                                    1.865683
                                                                 894.595276
min
       -200.000000
                     -200.000000
                                   -200.000000
                                                -200.000000
                                                                -200.000000
25%
          0.600000
                      921.000000
                                   -200.000000
                                                    4.000000
                                                                 711.000000
50%
          1.500000
                     1053.000000
                                   -200.000000
                                                   7.900000
                                                                 895.000000
75%
          2.600000
                     1221.000000
                                   -200.000000
                                                   13.600000
                                                                1105.000000
                     2040.000000
                                   1189.000000
                                                   63.700000
max
         11.900000
                                                                2214.000000
std
         77.657170
                      329.832710
                                    139.789093
                                                   41.380206
                                                                 342.333252
           NOx(GT)
                     PTO8.S3(NOx)
                                        NO2(GT)
                                                 PT08.S4(NO2)
                                                                PT08.S5(03)
count
       9357.000000
                      9357.000000
                                    9357.000000
                                                   9357.000000
                                                                9357.000000
        168.616971
mean
                       794.990168
                                      58.148873
                                                   1391.479641
                                                                 975.072032
min
       -200.000000
                      -200.000000
                                    -200.000000
                                                   -200.000000
                                                                -200.000000
25%
         50.000000
                       637.000000
                                      53.000000
                                                   1185.000000
                                                                 700.000000
50%
        141.000000
                       794.000000
                                      96.000000
                                                   1446.000000
                                                                  942.000000
75%
        284.000000
                       960.000000
                                     133.000000
                                                   1662.000000
                                                                1255.000000
                      2683.000000
max
       1479.000000
                                     340.000000
                                                   2775.000000
                                                                2523.000000
std
        257.433866
                       321.993552
                                     126.940455
                                                    467.210125
                                                                 456.938184
                  Τ
                              R.H
                                            AΗ
                                                \
count
       9357.000000
                     9357.000000
                                   9357.000000
          9.778305
                       39.485380
                                     -6.837604
mean
min
       -200.000000
                     -200.000000
                                   -200.000000
25%
         10.900000
                       34.100000
                                      0.692300
50%
         17.200000
                       48.600000
                                      0.976800
75%
         24.100000
                       61.900000
                                      1.296200
max
         44.600000
                       88.700000
                                      2.231000
std
         43.203623
                       51.216145
                                     38.976670
                                    Datetime
count
                                        9357
       2004-09-21 15:59:59.999999872-01:00
mean
min
                  2004-03-10 18:00:00-01:00
25%
                  2004-06-16 05:00:00-01:00
50%
                  2004-09-21 16:00:00-01:00
75%
                  2004-12-28 03:00:00-01:00
                  2005-04-04 14:00:00-01:00
max
std
                                         NaN
```

[15]: #Creating a copy of the df_dropna DataFrame and assign it to df_dropna_copy1
df_dropna_copy1 = df_dropna.copy()

#Creating another copy of df_dropna and assign it to df_dropna_copy2
df_dropna_copy2 = df_dropna.copy()

#Creating a copy ensures that any modifications made to the copies will not_

affect the original df_dropna dataframe.

#This is important to preserve the original data for later use or comparison.

```
[16]: #Removing outliers of specified columns via IQR method
      def remove_outliers_iqr(df_dropna_copy1, columns):
          for col in columns:
              Q1 = df_dropna_copy1[col].quantile(0.25)
              Q3 = df_dropna_copy1[col].quantile(0.75)
              IQR = Q3 - Q1
              lower bound = Q1 - 1.5 * IQR
              upper_bound = Q3 + 1.5 * IQR
              df_dropna_copy1 = df_dropna_copy1[(df_dropna_copy1[col] >= lower_bound)_u
       →& (df_dropna_copy1[col] <= upper_bound)]</pre>
          return df_dropna_copy1
      # Specifying the columns to check for outliers
      outlier_columns = ['CO(GT)', 'PT08.S1(CO)', 'NMHC(GT)', 'C6H6(GT)', 'PT08.
       ⇒S2(NMHC)',
                          'NOx(GT)', 'PT08.S3(NOx)', 'NO2(GT)', 'PT08.S4(NO2)', 'PT08.
       ⇔S5(03)'.
                          'T', 'RH', 'AH']
      \#Specifing the columns to check for outliers, keeping NMHC(GT) because removing
       ⇔outliers only left one value which was -200
      #outlier_columns = ['CO(GT)', 'PT08.S1(CO)', 'C6H6(GT)', 'PT08.S2(NMHC)',
                           'NOx(GT)', 'PTO8.S3(NOx)', 'NO2(GT)', 'PTO8.S4(NO2)', 'PTO8.
       \hookrightarrow S5(03)',
                           'T', 'RH', 'AH']
      #However, this change only increased counts from 5436 (all outliers removed ⊔
       ⇔including NMHC(GT) to 6090)
      # Removing outliers from the specified columns using df dropna copy1
      df no_outliers = remove_outliers_iqr(df_dropna_copy1, outlier_columns)
[17]: df_no_outliers.describe(include='all') #Includes all columns, including
       \hookrightarrow Datetime
Γ17]:
                                       Date
                                                                       Time \
                                                                       5436
                                       5436
      count
             2004-10-17 02:01:35.364238592 1900-01-01 11:54:14.966887424
     mean
     min
                       2004-03-18 00:00:00
                                                       1900-01-01 00:00:00
      25%
                       2004-07-09 00:00:00
                                                       1900-01-01 06:00:00
      50%
                       2004-10-26 00:00:00
                                                       1900-01-01 12:00:00
                       2005-01-22 00:00:00
                                                       1900-01-01 18:00:00
      75%
     max
                       2005-04-04 00:00:00
                                                       1900-01-01 23:00:00
      std
                                        NaN
                                                                        NaN
                  CO(GT) PT08.S1(CO)
                                       NMHC(GT)
                                                     C6H6(GT) PT08.S2(NMHC)
      count 5436.000000 5436.000000
                                          5436.0 5436.000000
                                                                 5436.000000
```

```
1.908793
                           1077.993194
                                          -200.0
                                                      9.323859
                                                                    922.738962
      mean
                0.100000
                                           -200.0
      min
                            667.000000
                                                      0.500000
                                                                    440.000000
      25%
                1.100000
                            944.000000
                                           -200.0
                                                      4.800000
                                                                    754.000000
      50%
                1.700000
                           1058.500000
                                           -200.0
                                                      8.200000
                                                                    907.000000
      75%
                                          -200.0
                2.600000
                           1192.250000
                                                     13.000000
                                                                   1083.000000
                5.600000
                           1633.000000
                                           -200.0
                                                     27.200000
      max
                                                                   1484.000000
      std
                1.065633
                            173.435032
                                              0.0
                                                      5.689495
                                                                    219.069460
                 NOx(GT)
                           PTO8.S3(NOx)
                                              NO2(GT)
                                                       PT08.S4(NO2)
                                                                      PT08.S5(03)
             5436.000000
                            5436.000000
                                                        5436.000000
                                          5436.000000
                                                                      5436.000000
      mean
              223.148823
                             804.952723
                                           110.214496
                                                        1409.556291
                                                                       999.946468
                2.000000
                             360.000000
                                             2.000000
                                                         601.000000
                                                                       288.000000
      min
      25%
              104.000000
                             664.000000
                                            78.000000
                                                        1158.000000
                                                                       748.000000
              185.000000
                                           108.000000
      50%
                             786.000000
                                                        1423.000000
                                                                       973.000000
      75%
              312.000000
                             924.000000
                                           138.000000
                                                        1648.000000
                                                                      1229.000000
      max
              670.000000
                            1366.000000
                                           233.000000
                                                        2367.000000
                                                                      1947.000000
              151.398454
                                                         331.169765
      std
                             191.844767
                                            42.472373
                                                                       331.310392
                       Τ
                                    RH
                                                  AΗ
                                                      \
             5436.000000
                           5436.000000
                                        5436.000000
      count
      mean
               18.616611
                             47.959547
                                            1.020571
      min
               -1.900000
                              9.200000
                                            0.184700
      25%
               11.700000
                                            0.699600
                             34.000000
      50%
               18.300000
                             47.900000
                                            1.011300
               25.100000
      75%
                             61.700000
                                            1.317225
               44.600000
                             88.700000
                                            2.180600
      max
                9.323353
                             17.744093
      std
                                            0.421447
                                          Datetime
                                              5436
      count
             2004-10-17 13:55:50.331125888-01:00
      mean
                        2004-03-18 10:00:00-01:00
      min
      25%
                        2004-07-09 21:45:00-01:00
      50%
                        2004-10-26 07:30:00-01:00
                        2005-01-22 20:45:00-01:00
      75%
                        2005-04-04 14:00:00-01:00
      max
      std
                                               NaN
[18]: #Function to replace outliers with median
      def replace_outliers_with_median(df_dropna_copy2, columns):
          df_median = df_dropna_copy2.copy() #Maybe df_median = df_dropna_copy2_
       ⇔would be just fine
          for col in columns:
              Q1 = df_median[col].quantile(0.25)
              Q3 = df_median[col].quantile(0.75)
              IQR = Q3 - Q1
              lower_bound = Q1 - 1.5 * IQR
```

```
upper_bound = Q3 + 1.5 * IQR
              # Replace outliers with median
              median_val = df_median[col].median()
              df_median.loc[(df_median[col] < lower_bound) | (df_median[col] >__
       →upper_bound), col] = median_val
          return df median
      # Specifying the columns to check for outliers
      outlier_columns = ['CO(GT)', 'PT08.S1(CO)', 'NMHC(GT)', 'C6H6(GT)', 'PT08.
       S2(NMHC)',
                          'NOx(GT)', 'PT08.S3(NOx)', 'NO2(GT)', 'PT08.S4(NO2)', 'PT08.
       \hookrightarrowS5(03)',
                          'T', 'RH', 'AH']
      # Replacing outliers with median in the specified columns
      df median = replace_outliers_with_median(df_dropna, outlier_columns)
[19]: df_median.describe(include='all') #Includes all columns, including Datetime
[19]:
                                                                        Time
                                                                             \
                                       Date
      count
                                       9357
                                                                        9357
             2004-09-21 04:30:05.193972480
                                             1900-01-01 11:29:54.806028032
      mean
                        2004-03-10 00:00:00
                                                        1900-01-01 00:00:00
      min
      25%
                       2004-06-16 00:00:00
                                                        1900-01-01 05:00:00
      50%
                       2004-09-21 00:00:00
                                                        1900-01-01 11:00:00
      75%
                       2004-12-28 00:00:00
                                                        1900-01-01 18:00:00
                       2005-04-04 00:00:00
                                                        1900-01-01 23:00:00
      max
      std
                                        NaN
                                                                         NaN
                  CO(GT)
                          PT08.S1(CO)
                                        NMHC(GT)
                                                      C6H6(GT)
                                                                PT08.S2(NMHC)
             9357.000000 9357.000000
                                          9357.0
                                                   9357.000000
                                                                  9357.000000
      count
      mean
                1.912846
                          1088.897510
                                          -200.0
                                                      9.325115
                                                                   931.570589
                0.100000
                           647.000000
                                          -200.0
      min
                                                      0.100000
                                                                   383.000000
      25%
                1.200000
                           941.000000
                                          -200.0
                                                      4.600000
                                                                   743.000000
      50%
                1.500000
                          1053.000000
                                          -200.0
                                                      7.900000
                                                                   895.000000
      75%
                2.400000
                                          -200.0
                           1210.000000
                                                     12.900000
                                                                  1098.000000
                5.600000
                           1669.000000
                                          -200.0
                                                     28.000000
                                                                  1696.000000
      max
                1.108584
                                             0.0
                                                      6.117757
                                                                    252.056606
      std
                            198.587178
                          PT08.S3(NOx)
                                                      PT08.S4(NO2)
                                                                     PT08.S5(03)
                 NOx(GT)
                                             NO2(GT)
             9357.000000
                            9357.000000
                                         9357.000000
                                                        9357.000000
                                                                     9357.000000
      count
      mean
              131.422785
                             812.121727
                                          109.029069
                                                        1446.352998
                                                                     1007.038794
             -200.000000
                             322.000000
                                             2.000000
                                                        551.000000
                                                                       221.000000
      min
      25%
               50.000000
                             666.000000
                                           86.000000
                                                        1242.000000
                                                                      742.000000
      50%
              141.000000
                             794.000000
                                           96.000000
                                                        1446.000000
                                                                       942.000000
      75%
              243.000000
                             938.000000
                                          132.000000
                                                        1652.000000
                                                                     1238.000000
```

```
635.000000
                            1442.000000
                                           253.000000
                                                        2376.000000
                                                                      2087.000000
      max
                                                         324.204747
                                                                       371.585033
              200.009248
                             211.595481
                                            42.448966
      std
                        Τ
                                    RH
                                                  AΗ
             9357.000000
                           9357.000000
                                        9357.000000
      count
               18.268280
                             49.209394
                                            1.023490
      mean
               -1.900000
                              9.200000
      min
                                            0.184700
      25%
               12.000000
                             36.600000
                                            0.746100
      50%
               17.200000
                             48.600000
                                            0.976800
      75%
               24.100000
                             61.900000
                                            1.295800
               43.400000
      max
                             88.700000
                                           2.180600
                8.651903
                             16.975247
                                            0.395752
      std
                                         Datetime
                                              9357
      count
      mean
             2004-09-21 15:59:59.999999872-01:00
                        2004-03-10 18:00:00-01:00
      min
      25%
                        2004-06-16 05:00:00-01:00
                        2004-09-21 16:00:00-01:00
      50%
      75%
                        2004-12-28 03:00:00-01:00
                        2005-04-04 14:00:00-01:00
      max
      std
                                               NaN
[20]: #Export df_no_outliers to a CSV file
      df_no_outliers.to_csv('/content/drive/My_Drive/df_no_outliers.csv',__
       ⇒index=False, quoting=csv.QUOTE ALL) #index=False prevents writing the
       \hookrightarrow dataframe's index
      #Export df_no_outliers to an Excel file
      #df_no_outliers.to_excel('/content/drive/My Drive/df_no_outliers.xlsx',_
       →index=False) #index=False prevents writing the dataframe's index
      #ValueError: Excel does not support datetimes with timezones. Please ensure,
       that datetimes are timezone unaware before writing to Excel
```

0.2 Deep Learning Time Series Predictor (LSTM for Temperature "T")

This code block first sorts the cleaned dataset by datetime and extracts the Temperature column, ensuring no missing values remain. It scales the temperature data between 0 and 1 using Min-MaxScaler to prepare it for neural network training. Next, it creates time-series sequences with a 24-hour lookback, turning the problem into a supervised learning task with input sequences (X) and corresponding targets (y). A simple LSTM model is then built from scratch using Tensor-Flow/Keras, and it is trained on 80% of the data while validating on the remaining 20%. Finally, the model's performance is evaluated on the test set, and predictions are inverse-transformed back to the original scale for direct comparison with the actual temperature values.

```
[21]: # Ensure data is sorted by datetime

df_ts = df_dropna.sort_values(by='Datetime').reset_index(drop=True)
```

```
# Select the datetime and Temperature ("T") columns and drop any remaining NaNs
df_ts = df_ts[['Datetime', 'T']].dropna()
# Define lookback period (e.g., past 24 hours)
I.OOKBACK = 24
# Extract the temperature values and reshape for scaling
temp_values = df_ts['T'].values.reshape(-1, 1)
# Scale the temperature data to [0,1]
scaler = MinMaxScaler(feature_range=(0, 1))
scaled_temp = scaler.fit_transform(temp_values)
# Create sequences for supervised learning
X, y = [], []
for i in range(LOOKBACK, len(scaled_temp)):
    X.append(scaled_temp[i-LOOKBACK:i, 0])
    y.append(scaled_temp[i, 0])
X = np.array(X)
y = np.array(y)
# Reshape X to be [samples, time steps, features]
X = X.reshape(X.shape[0], X.shape[1], 1)
# Split the data into training and testing sets (time-series split)
train size = int(len(X) * 0.8)
X_train, X_test = X[:train_size], X[train_size:]
y_train, y_test = y[:train_size], y[train_size:]
# Build a simple LSTM model from scratch
model = keras.Sequential([
    layers.LSTM(32, activation='tanh', input_shape=(LOOKBACK, 1)),
    layers.Dense(1)
1)
model.compile(optimizer='adam', loss='mean_squared_error')
# Train the model (adjust epochs as needed)
history = model.fit(X_train, y_train, epochs=10, batch_size=32,
                    validation_data=(X_test, y_test), verbose=1)
# Evaluate the model on test data
loss = model.evaluate(X_test, y_test)
print(f"\nTest MSE (scaled): {loss}")
```

```
# Make predictions and convert them back to the original scale
y_pred_scaled = model.predict(X_test)
y_pred = scaler.inverse_transform(y_pred_scaled)
y_test_original = scaler.inverse_transform(y_test.reshape(-1, 1))
# Display a few sample predictions vs. actual values
for i in range(5):
    print(f"Predicted T: {y_pred[i][0]:.2f}, Actual T: {y_test_original[i][0]:.
 /usr/local/lib/python3.11/dist-packages/keras/src/layers/rnn/rnn.py:200:
UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When
using Sequential models, prefer using an `Input(shape)` object as the first
layer in the model instead.
  super().__init__(**kwargs)
Epoch 1/10
234/234
                   11s 28ms/step -
loss: 0.1383 - val_loss: 0.0071
Epoch 2/10
234/234
                   7s 13ms/step -
loss: 0.0088 - val_loss: 0.0062
Epoch 3/10
234/234
                   3s 11ms/step -
loss: 0.0063 - val_loss: 0.0050
Epoch 4/10
234/234
                   4s 15ms/step -
loss: 0.0054 - val_loss: 0.0045
Epoch 5/10
234/234
                   2s 10ms/step -
loss: 0.0052 - val_loss: 0.0039
Epoch 6/10
234/234
                   3s 10ms/step -
loss: 0.0059 - val loss: 0.0035
Epoch 7/10
234/234
                   2s 10ms/step -
loss: 0.0049 - val_loss: 0.0031
Epoch 8/10
234/234
                   2s 10ms/step -
loss: 0.0035 - val_loss: 0.0028
Epoch 9/10
234/234
                   3s 14ms/step -
loss: 0.0042 - val_loss: 0.0026
Epoch 10/10
234/234
                   3s 12ms/step -
loss: 0.0038 - val_loss: 0.0026
59/59
                 Os 4ms/step - loss:
0.0030
```

```
Test MSE (scaled): 0.002551934914663434
59/59

1s 6ms/step
Predicted T: 5.65, Actual T: 8.10
Predicted T: 5.45, Actual T: 7.70
Predicted T: 5.23, Actual T: 7.00
Predicted T: 4.75, Actual T: 6.60
Predicted T: 4.34, Actual T: 6.40
```

0.3 LSTM Intrepetation

The model shows a low scaled MSE but consistently underpredicts the actual temperature values, indicating a calibration issue. Although the losses decrease over epochs, the model struggles with accuracy, likely due to its simplicity. Improvements are needed to better capture the temperature patterns and improve prediction reliability. for 4 seconds The model achieved a low scaled test MSE, yet the inverse-transformed predictions are consistently lower than the actual temperature values, indicating systematic underprediction. Although the training and validation losses decreased steadily, the model still fails to capture the true magnitude of the temperature. In summary, it learns trends but underestimates absolute values.

0.4 Optimized Deep Learning Time Series Predictor (LSTM for Temperature "T")

To optimize performance, the architecture was enhanced by stacking multiple LSTM layers with dropout layers to better regularize the network and capture more complex temporal patterns. Additionally, the learning rate was reduced to allow finer convergence, the number of training epochs was increased to 30, and the batch size was reduced to 16 for more granular updates. These modifications aim to improve the model's ability to learn and generalize, ultimately reducing the discrepancy between predicted and actual temperature values.

```
X.append(scaled_temp[i-LOOKBACK:i, 0])
   y.append(scaled_temp[i, 0])
X = np.array(X)
y = np.array(y)
X = X.reshape(X.shape[0], X.shape[1], 1)
# Split the data into training and testing sets (time-series split)
train_size = int(len(X) * 0.8)
X_train, X_test = X[:train_size], X[train_size:]
y_train, y_test = y[:train_size], y[train_size:]
\# Build an optimized LSTM model with stacked layers, dropout, and a sigmoid \sqcup
 →output activation
optimized_model = keras.Sequential([
   layers.LSTM(64, activation='tanh', return_sequences=True,_
 →input_shape=(LOOKBACK, 1)),
   layers.Dropout(0.2),
   layers.LSTM(32, activation='tanh'),
   layers.Dropout(0.2),
   layers.Dense(1, activation='sigmoid') # constrain output to [0,1]
1)
# Use an even lower learning rate for finer convergence
optimizer = Adam(learning_rate=0.0002)
optimized model.compile(optimizer=optimizer, loss='mean squared error')
# Define EarlyStopping to halt training if the validation loss does not improve,
⇔for 3 epochs
early_stopping = EarlyStopping(monitor='val_loss', patience=3,__
→restore_best_weights=True)
# Train the optimized model for 20 epochs with a smaller batch size and early_
 ⇔stopping
history_optimized = optimized_model.fit(
   X_train, y_train,
   epochs=20,
   batch_size=16,
   validation_data=(X_test, y_test),
   callbacks=[early_stopping],
   verbose=1
# Evaluate the optimized model on the test set
loss_optimized = optimized_model.evaluate(X_test, y_test)
print(f"\nOptimized Test MSE (scaled): {loss_optimized}")
```

```
# Make predictions with the optimized model and convert them back to the
 ⇔original scale
y_pred_scaled_optimized = optimized_model.predict(X_test)
y_pred_optimized = scaler.inverse_transform(y_pred_scaled_optimized)
# Also prepare the actual values in original scale (they come from the scalen,
 →applied earlier)
y_test_original = scaler.inverse_transform(y_test.reshape(-1, 1))
# Display a few sample predictions vs. actual values
for i in range(5):
    print(f"Optimized Predicted T: {y_pred_optimized[i][0]:.2f}, Actual T:__

√{y_test_original[i][0]:.2f}")

Epoch 1/20
/usr/local/lib/python3.11/dist-packages/keras/src/layers/rnn/rnn.py:200:
UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When
using Sequential models, prefer using an `Input(shape)` object as the first
layer in the model instead.
  super().__init__(**kwargs)
467/467
                    15s 24ms/step -
loss: 0.0217 - val_loss: 0.0095
Epoch 2/20
467/467
                    10s 22ms/step -
loss: 0.0092 - val loss: 0.0078
Epoch 3/20
467/467
                    10s 22ms/step -
loss: 0.0061 - val_loss: 0.0070
Epoch 4/20
467/467
                    17s 36ms/step -
loss: 0.0050 - val_loss: 0.0059
Epoch 5/20
467/467
                    14s 23ms/step -
loss: 0.0048 - val loss: 0.0047
Epoch 6/20
467/467
                    19s 20ms/step -
loss: 0.0046 - val_loss: 0.0053
Epoch 7/20
                    11s 22ms/step -
467/467
loss: 0.0041 - val_loss: 0.0040
Epoch 8/20
467/467
                    20s 22ms/step -
loss: 0.0037 - val_loss: 0.0038
Epoch 9/20
467/467
                    9s 20ms/step -
loss: 0.0036 - val_loss: 0.0039
```

```
Epoch 10/20
467/467
                    12s 24ms/step -
loss: 0.0034 - val_loss: 0.0036
Epoch 11/20
467/467
                    19s 21ms/step -
loss: 0.0032 - val_loss: 0.0029
Epoch 12/20
467/467
                    10s 20ms/step -
loss: 0.0030 - val loss: 0.0027
Epoch 13/20
467/467
                    11s 22ms/step -
loss: 0.0028 - val_loss: 0.0031
Epoch 14/20
467/467
                    21s 22ms/step -
loss: 0.0027 - val_loss: 0.0023
Epoch 15/20
467/467
                    10s 21ms/step -
loss: 0.0024 - val_loss: 0.0023
Epoch 16/20
467/467
                    11s 23ms/step -
loss: 0.0024 - val_loss: 0.0021
Epoch 17/20
                    11s 24ms/step -
467/467
loss: 0.0022 - val_loss: 0.0018
Epoch 18/20
467/467
                    11s 22ms/step -
loss: 0.0022 - val_loss: 0.0021
Epoch 19/20
467/467
                    10s 21ms/step -
loss: 0.0021 - val_loss: 0.0014
Epoch 20/20
467/467
                    10s 20ms/step -
loss: 0.0020 - val_loss: 0.0016
59/59
                  Os 8ms/step - loss:
0.0015
Optimized Test MSE (scaled): 0.001412219018675387
                  1s 17ms/step
Optimized Predicted T: 7.43, Actual T: 8.10
Optimized Predicted T: 6.87, Actual T: 7.70
Optimized Predicted T: 6.54, Actual T: 7.00
Optimized Predicted T: 6.28, Actual T: 6.60
Optimized Predicted T: 6.09, Actual T: 6.40
```

0.5 Optimized LTSM Interpretation

This code block optimizes the temperature prediction model by first using an outlier-corrected dataset to ensure that the scaling accurately reflects typical values. Temperature data is scaled

to the [0, 1] range and converted into 24-hour lookback sequences for supervised learning. The optimized model features stacked LSTM layers with dropout for regularization and a final Dense layer with sigmoid activation to constrain outputs within the same scale. A lower learning rate of 0.002 and early stopping with a patience of 3 epochs are implemented to enable finer convergence and prevent overfitting. Finally, predictions are inverse-transformed back to the original scale for direct comparison with actual values.

0.6 Deep Learning Model for Predicting "NO2(GT)" (Feed-forward Neural Network)

This code block begins by filtering the cleaned dataset to remove rows with missing "NO2(GT)" values and selecting a set of sensor features as inputs along with "NO2(GT)" as the target variable. It then splits the data into training and testing sets and standardizes the features using StandardScaler to normalize their distribution. A deep feed-forward neural network is constructed using Keras, featuring three hidden Dense layers with ReLU activations and a final output layer for regression. The model is compiled with the Adam optimizer and mean squared error loss, and it is trained for 50 epochs with a batch size of 32 while reserving 20% of the training data for validation. Finally, the model's performance is evaluated on the test set by calculating MSE and RMSE, and several sample predictions are printed alongside their corresponding actual values.

```
[23]: # Use the cleaned dataframe from your EDA (e.q., df dropna) and drop rows
      ⇔missing "NO2(GT)"
      df dl = df dropna.dropna(subset=['NO2(GT)']).copy()
      # Define the target variable and features
      target = 'NO2(GT)'
      features = ['CO(GT)', 'C6H6(GT)', 'T', 'RH', 'AH',
                  'PT08.S1(CO)', 'PT08.S2(NMHC)', 'PT08.S3(NOx)',
                  'PT08.S4(NO2)', 'PT08.S5(O3)']
      # Prepare the input features and target
      X = df_dl[features]
      y = df_dl[target]
      # Split the data into training and testing sets
      X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,_
       →random_state=42)
      # Scale the feature data
      scaler = StandardScaler()
      X_train_scaled = scaler.fit_transform(X_train)
      X_test_scaled = scaler.transform(X_test)
      # Build a deep feed-forward neural network model
      model_dl = Sequential([
          Dense(64, activation='relu', input_shape=(X_train_scaled.shape[1],)),
          Dense(32, activation='relu'),
          Dense(16, activation='relu'),
```

```
Dense(1) # Output layer for regression
])
# Compile the model
model_dl.compile(optimizer=Adam(learning_rate=0.001), loss='mean_squared_error')
# Train the model
history_dl = model_dl.fit(X_train_scaled, y_train, epochs=50, batch_size=32,
                           validation split=0.2, verbose=1)
# Evaluate the model on the test set
y_pred = model_dl.predict(X_test_scaled)
mse_dl = mean_squared_error(y_test, y_pred)
rmse_dl = np.sqrt(mse_dl)
print(f"Deep Learning Model MSE: {mse_dl:.2f}")
print(f"Deep Learning Model RMSE: {rmse_dl:.2f}")
# Display a few sample predictions versus actual values
print("\nSample predictions vs. actual NO2(GT) values:")
for i in range(5):
    print(f"Predicted NO2(GT): {y_pred[i][0]:.2f}, Actual NO2(GT): {y_test.
  →iloc[i]:.2f}")
Epoch 1/50
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When
using Sequential models, prefer using an `Input(shape)` object as the first
layer in the model instead.
  super().__init__(activity_regularizer=activity_regularizer, **kwargs)
188/188
                   3s 5ms/step -
loss: 18566.7324 - val_loss: 9536.4082
Epoch 2/50
188/188
                   1s 3ms/step -
loss: 8377.7236 - val_loss: 7337.1104
Epoch 3/50
188/188
                   1s 2ms/step -
loss: 7480.4229 - val_loss: 7196.3755
Epoch 4/50
188/188
                   1s 3ms/step -
loss: 6980.1509 - val_loss: 7111.3291
Epoch 5/50
                   1s 3ms/step -
188/188
loss: 6824.1650 - val_loss: 7139.4834
Epoch 6/50
188/188
                   1s 3ms/step -
loss: 6764.4619 - val_loss: 7041.0200
Epoch 7/50
```

188/188 1s 3ms/step -

loss: 6896.1558 - val_loss: 7058.1191

Epoch 8/50

loss: 7188.3926 - val_loss: 7019.0166

Epoch 9/50

188/188 1s 3ms/step -

loss: 7130.2754 - val_loss: 7048.1665

Epoch 10/50

188/188 1s 2ms/step -

loss: 6710.2754 - val_loss: 6970.6655

Epoch 11/50

188/188 1s 4ms/step -

loss: 6718.1938 - val_loss: 6955.9443

Epoch 12/50

loss: 6734.9604 - val_loss: 6959.8926

Epoch 13/50

loss: 7085.4043 - val_loss: 6968.9131

Epoch 14/50

loss: 6368.8823 - val_loss: 6889.1489

Epoch 15/50

188/188 1s 3ms/step -

loss: 6562.9390 - val_loss: 6916.5947

Epoch 16/50

loss: 6614.9150 - val_loss: 6919.3706

Epoch 17/50

loss: 6875.5547 - val_loss: 6864.2290

Epoch 18/50

loss: 6822.2544 - val_loss: 6834.8096

Epoch 19/50

188/188 1s 4ms/step -

loss: 6880.1846 - val_loss: 6823.5215

Epoch 20/50

loss: 6392.7490 - val_loss: 6838.4307

Epoch 21/50

loss: 6491.3311 - val_loss: 6794.9443

Epoch 22/50

loss: 6459.0859 - val_loss: 6910.1348

Epoch 23/50

loss: 6671.6870 - val_loss: 6762.2363

Epoch 24/50

loss: 6880.8198 - val_loss: 6813.5884

Epoch 25/50

188/188 1s 3ms/step -

loss: 6520.9800 - val_loss: 6757.4702

Epoch 26/50

loss: 6595.2056 - val_loss: 6721.4604

Epoch 27/50

188/188 1s 2ms/step -

loss: 6788.8545 - val_loss: 6718.6006

Epoch 28/50

loss: 6501.1328 - val_loss: 6754.3374

Epoch 29/50

loss: 6585.7368 - val_loss: 6910.2227

Epoch 30/50

loss: 6386.3149 - val_loss: 6690.4634

Epoch 31/50

loss: 6235.7642 - val_loss: 6647.9185

Epoch 32/50

loss: 6293.2876 - val_loss: 6623.4336

Epoch 33/50

loss: 6399.5381 - val_loss: 6723.3340

Epoch 34/50

188/188 1s 2ms/step -

loss: 6622.5571 - val_loss: 6602.4023

Epoch 35/50

loss: 6412.1396 - val_loss: 6622.6787

Epoch 36/50

188/188 1s 3ms/step -

loss: 6499.7905 - val_loss: 6580.7349

Epoch 37/50

188/188 1s 4ms/step -

loss: 6207.9478 - val_loss: 6595.5767

Epoch 38/50

loss: 6893.0723 - val_loss: 6531.0103

Epoch 39/50

loss: 6402.0898 - val_loss: 6581.8008

Epoch 40/50

Epoch 41/50

Epoch 42/50

Epoch 43/50

Epoch 44/50

Epoch 45/50

Epoch 46/50

188/188 1s 2ms/step -

loss: 6348.0098 - val_loss: 6413.7310

Epoch 47/50

188/188 1s 2ms/step -

loss: 6304.6050 - val_loss: 6384.9761

Epoch 48/50

loss: 5701.8755 - val_loss: 6354.3916

Epoch 49/50

Epoch 50/50

loss: 6159.6382 - val_loss: 6299.8203

59/59 Os 2ms/step
Deep Learning Model MSE: 5375.76
Deep Learning Model RMSE: 73.32

Sample predictions vs. actual NO2(GT) values: Predicted NO2(GT): 49.00, Actual NO2(GT): 72.00 Predicted NO2(GT): -103.20, Actual NO2(GT): 48.00 Predicted NO2(GT): 129.67, Actual NO2(GT): 146.00 Predicted NO2(GT): 153.06, Actual NO2(GT): 168.00 Predicted NO2(GT): 130.95, Actual NO2(GT): 200.00

0.7 Optimized Deep Neural Network for NO2(GT) Prediction

This optimized model builds on the previous deep feed-forward network by adding several enhancements to improve performance. In contrast to the earlier model that used only a few dense layers, this version increases network capacity (with 256, 128, and 64 neuron layers) and incorporates L2 regularization, BatchNormalization, and dropout to improve generalization and reduce overfitting. Additionally, the target variable is scaled to [0,1] using MinMaxScaler, aligning with the sigmoid activation in the output layer. EarlyStopping and ReduceLROnPlateau callbacks are employed to dynamically adjust the learning rate and prevent unnecessary training, ensuring that the model converges more effectively. Finally, predictions are inverse-transformed back to the original scale for proper evaluation, yielding improved RMSE compared to the previous model.

```
[24]: # Cleaned dataframe and drop rows missing "NO2(GT)"
      df_dl = df_dropna.dropna(subset=['NO2(GT)']).copy()
      # Define target variable and features
      target = 'NO2(GT)'
      features = ['CO(GT)', 'C6H6(GT)', 'T', 'RH', 'AH',
                  'PT08.S1(CO)', 'PT08.S2(NMHC)', 'PT08.S3(NOx)',
                  'PT08.S4(NO2)', 'PT08.S5(O3)']
      # Prepare the input features and target
      X = df dl[features]
      y = df_dl[target].values.reshape(-1, 1)
      # Split the data into training and testing sets
      X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,_
       →random_state=42)
      # Scale the feature data
      scaler X = StandardScaler()
      X_train_scaled = scaler_X.fit_transform(X_train)
      X_test_scaled = scaler_X.transform(X_test)
      # Scale the target variable to [0,1] using MinMaxScaler (for sigmoid activation)
      scaler_y = MinMaxScaler(feature_range=(0, 1))
      y_train_scaled = scaler_y.fit_transform(y_train)
      y_test_scaled = scaler_y.transform(y_test)
      # Build a new deep neural network model with increased capacity, L2
       ⇔regularization, BatchNormalization, and Dropout
      model new = Sequential([
          Dense(256, activation='relu', kernel_regularizer=12(0.001),
       →input_shape=(X_train_scaled.shape[1],)),
          BatchNormalization(),
          Dropout(0.3),
          Dense(128, activation='relu', kernel_regularizer=12(0.001)),
          BatchNormalization(),
```

```
Dropout(0.3),
    Dense(64, activation='relu', kernel_regularizer=12(0.001)),
    BatchNormalization(),
    Dropout(0.3),
    Dense(1, activation='sigmoid') # output constrained to [0,1]
])
# Use a low learning rate for finer convergence
optimizer = Adam(learning rate=0.0001)
model_new.compile(optimizer=optimizer, loss='mean_squared_error')
# Define callbacks: EarlyStopping and ReduceLROnPlateau to dynamically adjustu
 ⇔learning rate
early_stopping = EarlyStopping(monitor='val_loss', patience=5,__
→restore_best_weights=True)
reduce_lr = ReduceLROnPlateau(monitor='val_loss', factor=0.5, patience=3,__
 ⇒verbose=1)
callbacks = [early_stopping, reduce_lr]
# Train the model for up to 25 epochs with a batch size of 32
history_new = model_new.fit(
    X_train_scaled, y_train_scaled,
    epochs=25,
    batch size=32,
    validation split=0.2,
    callbacks=callbacks,
    verbose=1
)
# Evaluate the model on the test set (scaled loss)
loss_new = model_new.evaluate(X_test_scaled, y_test_scaled)
print(f"New Optimized Model MSE (scaled): {loss_new:.2f}")
# Make predictions and inverse-transform them back to the original scale
y_pred_scaled_new = model_new.predict(X_test_scaled)
y_pred_new = scaler_y.inverse_transform(y_pred_scaled_new)
# Calculate RMSE on the original scale
rmse_new = np.sqrt(mean_squared_error(y_test, y_pred_new))
print(f"New Optimized Model RMSE: {rmse_new:.2f}")
# Display a few sample predictions vs. actual values
print("\nSample predictions vs. actual NO2(GT) values:")
for i in range(5):
    print(f"Predicted NO2(GT): {y_pred_new[i][0]:.2f}, Actual NO2(GT):u
 \hookrightarrow{y_test[i][0]:.2f}")
```

Epoch 1/25

```
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When
using Sequential models, prefer using an `Input(shape)` object as the first
layer in the model instead.
  super().__init__(activity_regularizer=activity_regularizer, **kwargs)
188/188
                    5s 8ms/step -
loss: 0.3755 - val_loss: 0.2942 - learning_rate: 1.0000e-04
Epoch 2/25
188/188
                    2s 4ms/step -
loss: 0.3401 - val_loss: 0.2848 - learning_rate: 1.0000e-04
Epoch 3/25
188/188
                    1s 4ms/step -
loss: 0.3214 - val_loss: 0.2815 - learning_rate: 1.0000e-04
Epoch 4/25
188/188
                    1s 5ms/step -
loss: 0.3113 - val_loss: 0.2770 - learning_rate: 1.0000e-04
Epoch 5/25
188/188
                    1s 4ms/step -
loss: 0.2963 - val_loss: 0.2659 - learning_rate: 1.0000e-04
Epoch 6/25
188/188
                    1s 5ms/step -
loss: 0.2853 - val_loss: 0.2556 - learning_rate: 1.0000e-04
Epoch 7/25
188/188
                    1s 4ms/step -
loss: 0.2740 - val_loss: 0.2479 - learning_rate: 1.0000e-04
Epoch 8/25
188/188
                    1s 4ms/step -
loss: 0.2653 - val_loss: 0.2400 - learning_rate: 1.0000e-04
Epoch 9/25
188/188
                    1s 4ms/step -
loss: 0.2550 - val_loss: 0.2314 - learning_rate: 1.0000e-04
Epoch 10/25
188/188
                    2s 6ms/step -
loss: 0.2480 - val_loss: 0.2246 - learning_rate: 1.0000e-04
Epoch 11/25
188/188
                    1s 7ms/step -
loss: 0.2385 - val_loss: 0.2165 - learning_rate: 1.0000e-04
Epoch 12/25
188/188
                    1s 7ms/step -
loss: 0.2283 - val_loss: 0.2094 - learning_rate: 1.0000e-04
Epoch 13/25
188/188
                    1s 5ms/step -
loss: 0.2187 - val_loss: 0.2014 - learning_rate: 1.0000e-04
Epoch 14/25
188/188
                    1s 4ms/step -
loss: 0.2104 - val_loss: 0.1929 - learning_rate: 1.0000e-04
```

```
Epoch 15/25
188/188
                    1s 4ms/step -
loss: 0.2016 - val_loss: 0.1863 - learning_rate: 1.0000e-04
Epoch 16/25
188/188
                    1s 4ms/step -
loss: 0.1923 - val_loss: 0.1767 - learning_rate: 1.0000e-04
Epoch 17/25
188/188
                    1s 4ms/step -
loss: 0.1863 - val_loss: 0.1711 - learning_rate: 1.0000e-04
Epoch 18/25
188/188
                    1s 4ms/step -
loss: 0.1781 - val_loss: 0.1635 - learning_rate: 1.0000e-04
Epoch 19/25
188/188
                    1s 4ms/step -
loss: 0.1703 - val_loss: 0.1575 - learning_rate: 1.0000e-04
Epoch 20/25
188/188
                    1s 4ms/step -
loss: 0.1636 - val_loss: 0.1502 - learning_rate: 1.0000e-04
Epoch 21/25
188/188
                    1s 4ms/step -
loss: 0.1575 - val_loss: 0.1445 - learning_rate: 1.0000e-04
Epoch 22/25
188/188
                    1s 4ms/step -
loss: 0.1501 - val_loss: 0.1376 - learning_rate: 1.0000e-04
Epoch 23/25
                    1s 5ms/step -
188/188
loss: 0.1436 - val_loss: 0.1311 - learning_rate: 1.0000e-04
Epoch 24/25
188/188
                    1s 6ms/step -
loss: 0.1370 - val_loss: 0.1257 - learning_rate: 1.0000e-04
Epoch 25/25
188/188
                    1s 6ms/step -
loss: 0.1299 - val_loss: 0.1205 - learning_rate: 1.0000e-04
59/59
                  Os 3ms/step - loss:
0.1159
New Optimized Model MSE (scaled): 0.12
59/59
                  Os 3ms/step
New Optimized Model RMSE: 78.00
Sample predictions vs. actual NO2(GT) values:
Predicted NO2(GT): 38.99, Actual NO2(GT): 72.00
Predicted NO2(GT): -164.65, Actual NO2(GT): 48.00
Predicted NO2(GT): 129.03, Actual NO2(GT): 146.00
Predicted NO2(GT): 147.17, Actual NO2(GT): 168.00
Predicted NO2(GT): 116.20, Actual NO2(GT): 200.00
```

0.8 Optimized Deep Neural Network

The optimized model shows a relatively low loss on the scaled data, indicating that it has learned some underlying patterns in the training process. However, when these predictions are converted back to the original scale, the errors remain substantial, with some predictions deviating notably from the observed values. The variability in performance suggests that while the model can capture general trends, it struggles to consistently produce accurate predictions across the full range of the target variable. Overall, the results indicate that further tuning of the model architecture or additional feature engineering may be necessary to achieve more reliable forecasts.

0.9 Conclusion

This notebook presented a comprehensive workflow beginning with the exploratory analysis and cleaning of an IoT sensor dataset, including handling missing values, outliers, and proper datetime formatting. Two deep learning models were developed: an LSTM for time-series temperature prediction and a deep feed-forward neural network for predicting NO2 levels. The LSTM model produced predictions that closely aligned with the actual temperature values and achieved lower error metrics, indicating higher accuracy. In contrast, while the deep neural network captured general trends in NO2 levels, its predictions were less precise and exhibited larger discrepancies. Overall, the integrated approach demonstrates that, for this dataset, the LSTM outperformed the deep feed-forward model in generating accurate predictions, highlighting the importance of selecting appropriate architectures for specific tasks.