MaterialsZone - The Lean R&D Solution

Technical Exercise for Lead AI Engineer Position

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```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from scipy.spatial.distance import pdist
from sklearn.preprocessing import LabelEncoder,StandardScaler
import statsmodels.api as sm
from sklearn.model_selection import train_test_split
from statsmodels.stats.outliers_influence import OLSInfluence
from sklearn.linear_model import LinearRegression
from sklearn.ensemble import RandomForestRegressor
from sklearn.svm import SVR
import xgboost as xgb
from catboost import CatBoostRegressor
from sklearn.linear_model import LinearRegression, Lasso, Ridge,
ElasticNet,BayesianRidge
from sklearn.metrics import mean_absolute_error, mean_squared_error,
r2_score
from hyperopt import hp, fmin, tpe, STATUS_OK, Trials
from typing import Dict, Union, Any, Callable

sns.set()
```

Load both datasets

```
raw_materials_path = 'datasets/raw_materials.csv'
formulations_path = 'datasets/formulations.csv'

raw_materials_df = pd.read_csv(raw_materials_path)
formulations_df = pd.read_csv(formulations_path)
formulations_df_final = formulations_df.copy()
```

Data exploration

```
# Check for missing values and data types in both datasets
missing_values_raw = raw_materials_df.isnull().sum().sum()
data_types_raw = raw_materials_df.dtypes
print(f'\nMissing values in raw_materials : {missing_values_raw}\n')

print(data_types_raw)
missing_values_formulations = formulations_df.isnull().sum().sum()
```

```
data_types_formulations = formulations_df.dtypes

print(f'\nMissing values in formulations :
{missing_values_formulations}\n')
print(data_types_formulations)
```

```
Missing values in raw_materials : 0

Raw_Material_ID       object
Raw_Material_Name     object
Melting_Point        float64
Density              float64
Purity               float64
dtype: object

Missing values in formulations : 5

Formulation_ID             object
Formulation_Name           object
Processing_Temperature    float64
Processing_Time           float64
Processing_Pressure       float64
RM1                       float64
RM2                       float64
RM3                       float64
RM4                       float64
RM5                       float64
RM6                       float64
RM7                       float64
RM8                       float64
RM9                       float64
RM10                      float64
RM11                      float64
RM12                      float64
RM13                      float64
RM14                      float64
RM15                      float64
RM16                      float64
RM17                      float64
RM18                      float64
RM19                      float64
RM20                      float64
RM21                      float64
RM22                      float64
RM23                      float64
RM24                      float64
RM25                      float64
RM26                      float64
RM27                      float64
```

```
RM28                        float64
RM29                        float64
RM30                        float64
Number_of_Materials           int64
Percentage_Sum              float64
Tensile_Strength            float64
dtype: object
```

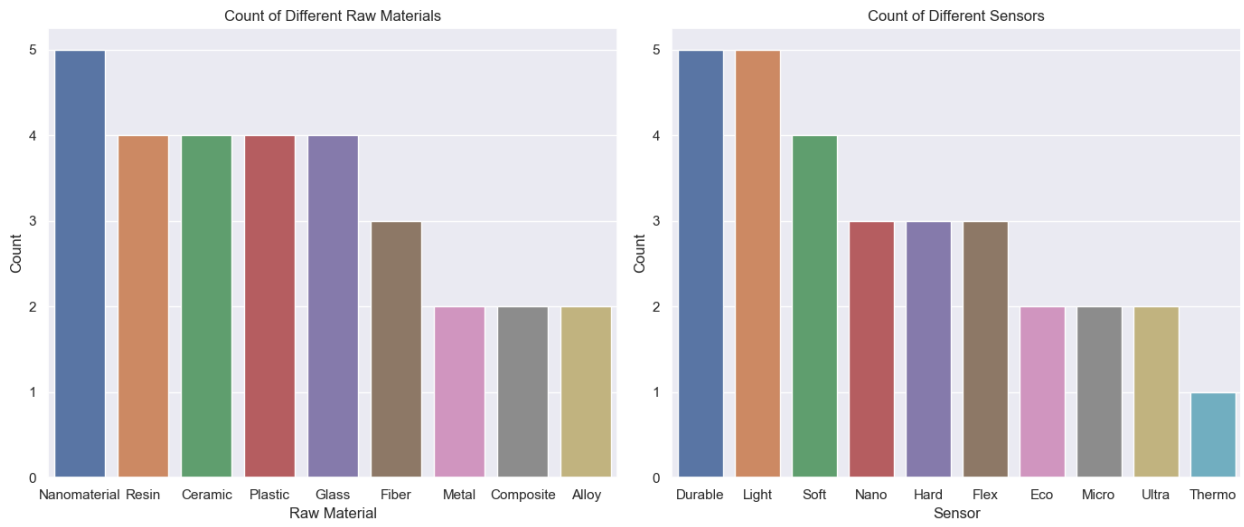
```
formulations_df =
formulations_df.set_index(formulations_df.Formulation_ID)
RM_df = formulations_df[['RM'+str(i)for i in range(1,31)]]
experiment_df = formulations_df[['Processing_Temperature',
       'Processing_Time', 'Processing_Pressure']]
Target = formulations_df[["Tensile_Strength"]]
raw_materials_df[["Raw_Material","Sensor"]] =
raw_materials_df.Raw_Material_Name.str.split('-', expand=True)
raw_materials_df = raw_materials_df.drop("Raw_Material_Name",axis = 1)
```

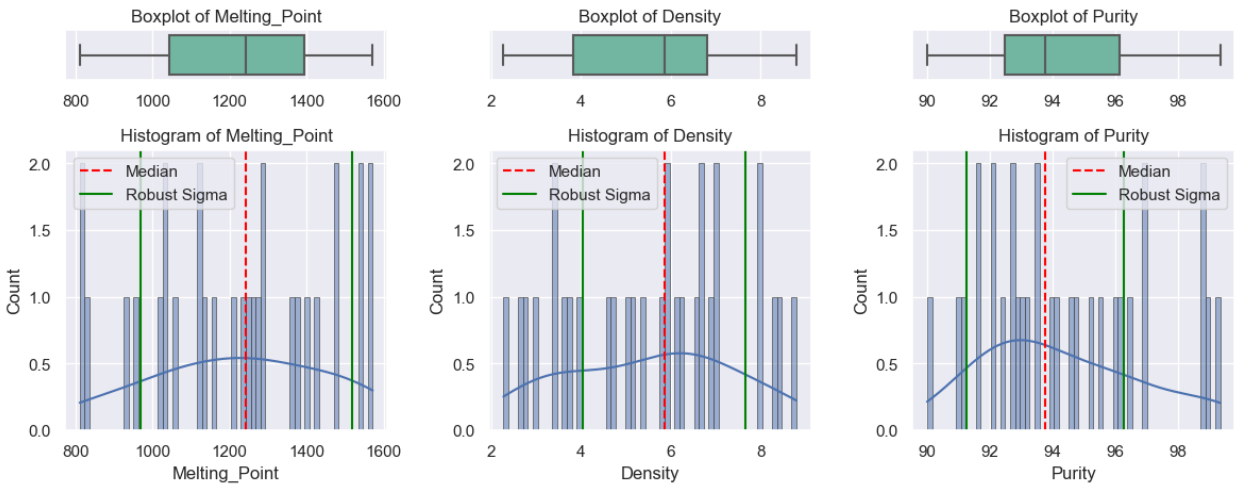
Visualization

```
class Visualization:

    def __init__(self,df: pd.DataFrame):
        self.df = df

    # Function to calculate robust sigma
    def calculate_robust_sigma(self,data):
        scaling_factor = 1.4826
        return scaling_factor * np.median(np.abs(data -
np.median(data)))

    def plot_histograms(self,rows,cols, bins: int = 30) -> None:
        np.random.seed(10)  # For reproducibility

        fig, axs = plt.subplots(rows, cols, figsize=(int(12*(cols/3)),
int(15*(rows/6))), gridspec_kw={"height_ratios": (.15,
.85)*int(rows/2) })

        # Iterate over the features to plot boxplot and histogram for
each
        for i, feature in enumerate(self.df.columns):
            row = (i // 3) * 2  # Determine row for boxplot
            col = i % 3         # Determine column

            # Boxplot
            sns.boxplot(data=self.df, x=feature, ax=axs[row, col],
orient="h", palette="Set2")
            axs[row, col].set(xlabel='', title=f'Boxplot of
{feature}')
```

```
            # Histogram
            sns.histplot(data=self.df[feature], ax=axs[row+1, col],
bins=bins, kde=True, edgecolor=".3", linewidth=.5)
            axs[row+1, col].set(title=f'Histogram of {feature}')
            robust_sigma =
self.calculate_robust_sigma(self.df[feature])
            median = np.median(self.df[feature])
            axs[row+1, col].axvline(median, color='red',
linestyle='--', label='Median')
            axs[row+1, col].axvline(median + robust_sigma,
color='green', linestyle='-', label='Robust Sigma')
            axs[row+1, col].axvline(median - robust_sigma,
color='green', linestyle='-', label=None)
            axs[row+1, col].legend()
        plt.tight_layout(rect=[0, 0, 1, 0.96])  # Adjust layout to
make room for the title
        plt.show()

    def pairplot_histograms(self, plot_features: list[str],hue_column:
str = None) -> None:

        sns.pairplot(self.df[plot_features], corner=True, hue =
hue_column)
        plt.show()

    def plot_correlation_matrix(self) -> None:
        cor = self.df.corr().round(2)
        mask = np.zeros_like(cor)
        mask[np.triu_indices_from(mask)] = True
        cmap = sns.diverging_palette(220, 10, as_cmap=True)
        plt.figure()
        sns.heatmap(cor, mask=mask, annot=True, annot_kws={"size":
10},
                    center=0, cmap=cmap, square=False, linewidths=.5,
                    cbar_kws={"shrink": .5}, yticklabels=1,
xticklabels=1, vmin=-1, vmax=1)
        plt.title("correlation matrix", fontsize='xx-large',
fontweight='bold')

        plt.show()

# Set up the matplotlib figure
plt.figure(figsize=(14, 6))

# Plotting countplot for Raw_Material sorted by frequency
plt.subplot(1, 2, 1)  # 1 row, 2 columns, 1st subplot
raw_material_order =
raw_materials_df['Raw_Material'].value_counts().index
sns.countplot(x='Raw_Material', data=raw_materials_df,
order=raw_material_order)
```

```
plt.title('Count of Different Raw Materials')
plt.xlabel('Raw Material')
plt.ylabel('Count')

# Plotting countplot for Sensor sorted by frequency
plt.subplot(1, 2, 2)  # 1 row, 2 columns, 2nd subplot
sensor_order = raw_materials_df['Sensor'].value_counts().index
sns.countplot(x='Sensor', data=raw_materials_df, order=sensor_order)
plt.title('Count of Different Sensors')
plt.xlabel('Sensor')
plt.ylabel('Count')

# Show the plot
plt.tight_layout()
plt.show()

vis_raw_materials_df = Visualization(df =
raw_materials_df.select_dtypes(include=[np.number]))
vis_raw_materials_df.plot_histograms(bins = 60,rows= 2,cols = 3)
```





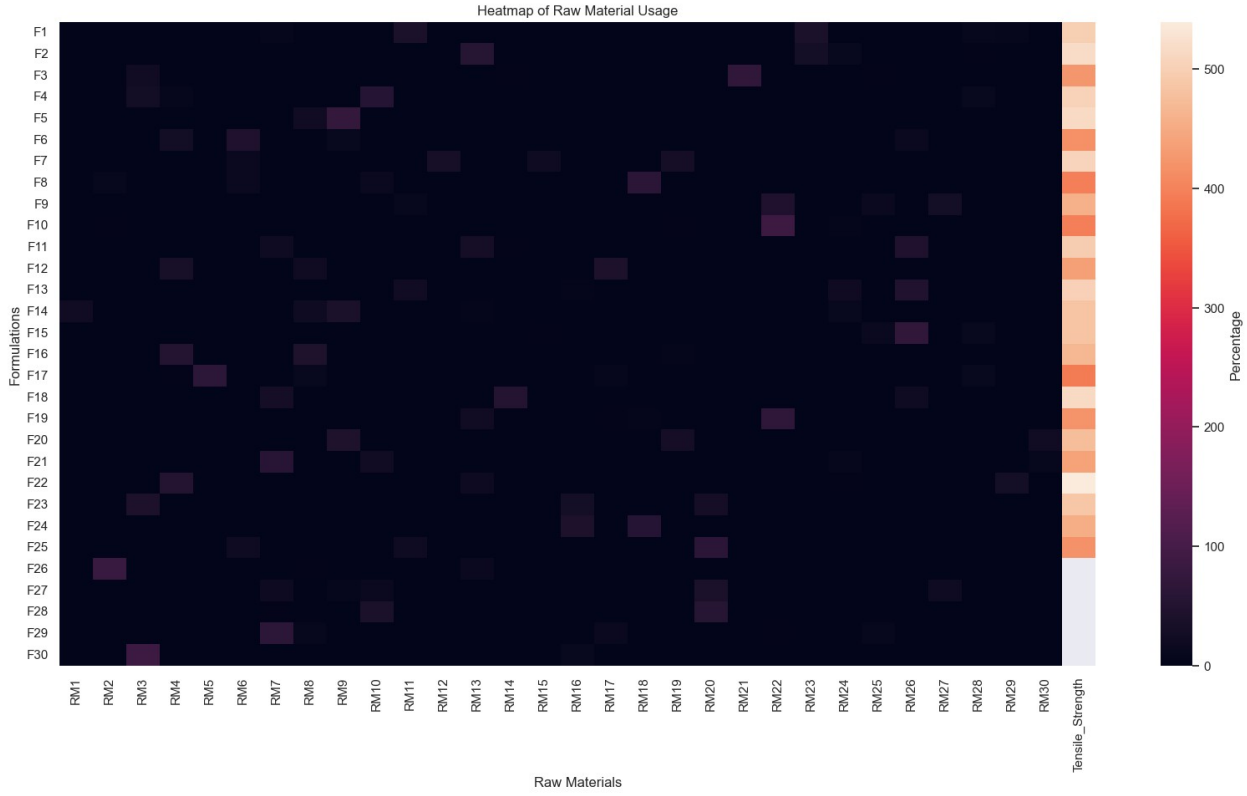
Heatmap showing RM's percentages in each formulation

```
Target.column
```

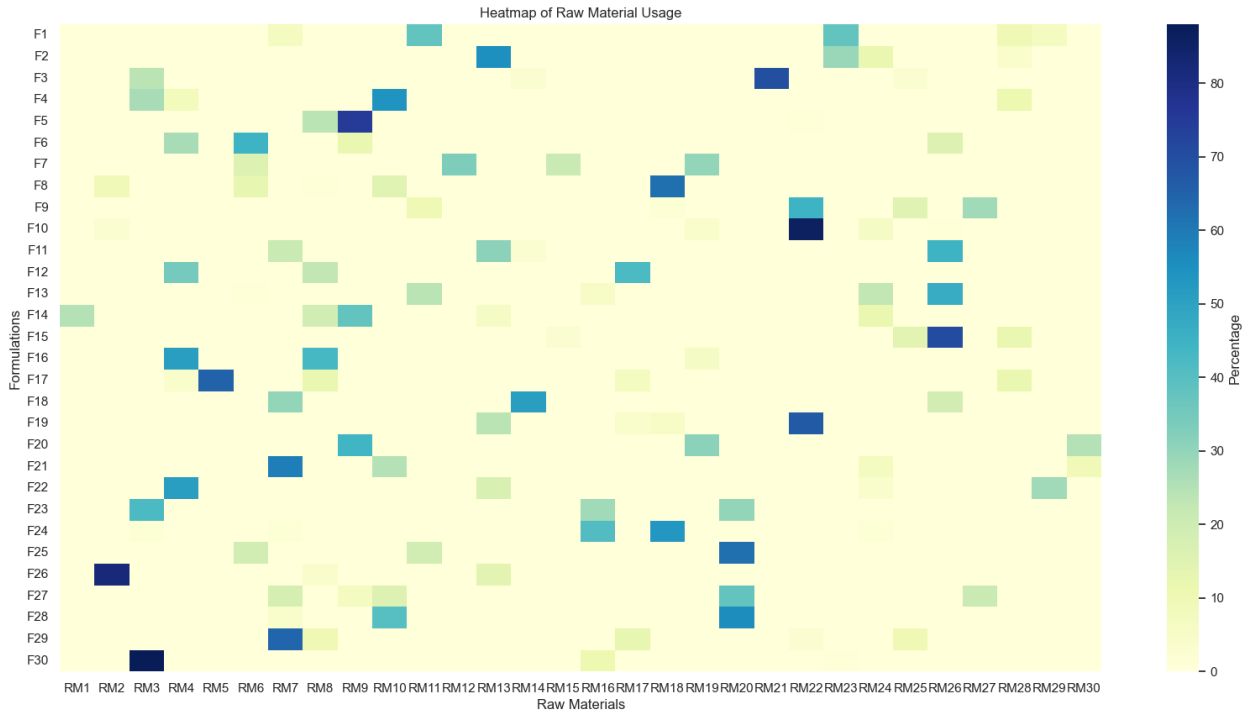
Formulation_ID	Tensile_Strength
F1	498.05
F2	517.93
F3	425.43
F4	505.06
F5	515.62
F6	416.85
F7	506.26
F8	395.90
F9	459.15
F10	394.19
F11	496.10
F12	435.29
F13	503.71
F14	483.13
F15	483.55
F16	466.47
F17	390.67
F18	515.58
F19	419.60
F20	476.08
F21	439.63
F22	539.57
F23	488.67
F24	453.53
F25	419.21
F26	NaN
F27	NaN
F28	NaN

```
F29                             NaN
F30                             NaN
```

```
RM_df_tar = RM_df.copy()
RM_df_tar["Tensile_Strength"] = Target

plt.figure(figsize=(20, 10))
sns.heatmap(RM_df_tar,  cbar_kws={'label': 'Percentage'})
plt.title('Heatmap of Raw Material Usage')
plt.xlabel('Raw Materials')
plt.ylabel('Formulations')
plt.show()
```




```
plt.figure(figsize=(20, 10))
sns.heatmap(RM_df, cmap="YlGnBu", cbar_kws={'label': 'Percentage'})
plt.title('Heatmap of Raw Material Usage')
plt.xlabel('Raw Materials')
plt.ylabel('Formulations')
plt.show()
```



Preprocessing

```
# Dictionary to hold the non-zero RM values for each row
non_zero_rm_dict = {}

# Iterate over each row in RM_df
for index, row in RM_df.iterrows():
    # Filter out columns where the value is not zero
    non_zero_values = row[row != 0]
    # Store in dictionary: key is the row index, and value is another
dictionary of RM names and their values
    non_zero_rm_dict[index] = dict(non_zero_values)

def formulations_dict_to_dataframe(formulations_dict):
    # Create a list to hold the data
    data = []

    # Iterate over each formulation in the dictionary
    for formulation_id, materials in formulations_dict.items():
        # Iterate over each material in the formulation
        for raw_material_id, percentage in materials.items():
            # Append each item as a row in the data list
            data.append({
                'Formulation_ID': formulation_id,
                'Raw_Material_ID': raw_material_id,
                'Percentage': percentage
            })
```

```
    # Convert the list of data into a DataFrame
    return pd.DataFrame(data)

agg_RM_df = formulations_dict_to_dataframe(non_zero_rm_dict)

agg_RM_df
```

	Formulation_ID	Raw_Material_ID	Percentage
0	F1	RM7	7.0
1	F1	RM11	38.0
2	F1	RM23	38.0
3	F1	RM28	10.0
4	F1	RM29	7.0
..	...	...	...
115	F29	RM22	3.0
116	F29	RM25	10.0
117	F30	RM3	88.0
118	F30	RM16	11.0
119	F30	RM23	1.0

[120 rows x 3 columns]

The melting point of a pure substance is always higher

and has a smaller range than the melting point of an impure substance or, more generally, of mixtures.

```
formulations_with_properties = agg_RM_df.merge(raw_materials_df,
on='Raw_Material_ID', how='left')
formulations_with_properties
```

	Formulation_ID	Raw_Material_ID	Percentage	Melting_Point	Density
\					
0	F1	RM7	7.0	1381.8	6.68
1	F1	RM11	38.0	1568.9	5.93
2	F1	RM23	38.0	1115.9	8.27
3	F1	RM28	10.0	1432.1	6.23
4	F1	RM29	7.0	1284.8	5.78
..	...	...	...	...	...
115	F29	RM22	3.0	1138.7	3.41
116	F29	RM25	10.0	811.3	5.94
117	F30	RM3	88.0	1473.8	7.95

```
118            F30            RM16         11.0          1572.2      3.65

119            F30            RM23          1.0          1115.9      8.27


     Purity  Raw_Material   Sensor
0     91.04         Resin     Soft
1     98.74         Alloy     Flex
2     94.80       Plastic    Light
3     92.17         Resin  Durable
4     95.53       Ceramic    Ultra
..      ...           ...      ...
115   95.29       Plastic   Thermo
116   92.67  Nanomaterial     Nano
117   96.88  Nanomaterial      Eco
118   92.69         Glass     Soft
119   94.80       Plastic    Light

[120 rows x 8 columns]
```

Feature Engineering

```
formulations_with_properties["Partial_Density"] =
0.01*formulations_with_properties["Percentage"]*formulations_with_prop
erties["Density"]
formulations_with_properties["Partial_Melting_Point"] =
0.01*formulations_with_properties["Percentage"]*formulations_with_prop
erties["Melting_Point"]
formulations_with_properties["Partial_Purity"] =
0.01*formulations_with_properties["Percentage"]*formulations_with_prop
erties["Purity"]

formulations_with_properties =
formulations_with_properties.drop(["Melting_Point","Purity","Density",
"Percentage"],axis = 1)

formulations_with_properties
```

```
    Formulation_ID Raw_Material_ID  Raw_Material   Sensor
Partial_Density  \
0               F1             RM7         Resin     Soft
0.4676
1               F1            RM11         Alloy     Flex
2.2534
2               F1            RM23       Plastic    Light
3.1426
3               F1            RM28         Resin  Durable
0.6230
4               F1            RM29       Ceramic    Ultra
0.4046
```

```
..              ...              ...           ...      ...
...
115             F29             RM22       Plastic   Thermo
0.1023
116             F29             RM25  Nanomaterial     Nano
0.5940
117             F30              RM3  Nanomaterial      Eco
6.9960
118             F30             RM16         Glass     Soft
0.4015
119             F30             RM23       Plastic    Light
0.0827

     Partial_Melting_Point  Partial_Purity
0                   96.726          6.3728
1                  596.182         37.5212
2                  424.042         36.0240
3                  143.210          9.2170
4                   89.936          6.6871
..                     ...             ...
115                 34.161          2.8587
116                 81.130          9.2670
117               1296.944         85.2544
118                172.942         10.1959
119                 11.159          0.9480

[120 rows x 7 columns]
```

Label encode each of the categorical columns

```
# Initialize LabelEncoder
le = LabelEncoder()

formulations_with_properties['Formulation_ID_encoded'] =
le.fit_transform(formulations_with_properties['Formulation_ID'])
formulations_with_properties['Raw_Material_ID_encoded'] =
le.fit_transform(formulations_with_properties['Raw_Material_ID'])
#formulations_with_properties['Raw_Material_encoded'] =
le.fit_transform(formulations_with_properties['Raw_Material']) #Apply
only when data is real
#formulations_with_properties['Sensor_encoded'] =
le.fit_transform(formulations_with_properties['Sensor']) #Apply only
when data is real

# Drop original categorical columns if no longer needed
formulations_with_properties.drop(["Formulation_ID",'Raw_Material_ID',
'Raw_Material', 'Sensor'], axis=1, inplace=True)
formulations_with_properties
```

```
     Partial_Density  Partial_Melting_Point  Partial_Purity  \
0             0.4676                 96.726          6.3728
1             2.2534                596.182         37.5212
2             3.1426                424.042         36.0240
3             0.6230                143.210          9.2170
4             0.4046                 89.936          6.6871
..               ...                    ...             ...
115           0.1023                 34.161          2.8587
116           0.5940                 81.130          9.2670
117           6.9960               1296.944         85.2544
118           0.4015                172.942         10.1959
119           0.0827                 11.159          0.9480

     Formulation_ID_encoded  Raw_Material_ID_encoded
0                         0                       27
1                         0                        2
2                         0                       15
3                         0                       20
4                         0                       21
..                      ...                      ...
115                      21                       14
116                      21                       17
117                      23                       22
118                      23                        7
119                      23                       15

[120 rows x 5 columns]
```

Calculate cosine distances

```
def calculate_average_distance(group):

    distances = pdist(group, metric='cosine')
    # Calculate the average of these distances
    average_distance = distances.sum()
    return average_distance
cols = 3
# Group by Formulation_ID and apply the average distance calculation
experiment_df = experiment_df.reset_index(drop = False)
experiment_df["sum_distances"] =
formulations_with_properties.groupby('Formulation_ID_encoded').apply(c
alculate_average_distance)
experiment_df["Number_of_Materials"] =
formulations_df["Number_of_Materials"].values
experiment_df[["wheighted_"+i[8:] for i in
formulations_with_properties.columns[:cols]]] =
formulations_with_properties.groupby('Formulation_ID_encoded').sum()
[formulations_with_properties.columns[:cols]].values
```

```
experiment_df = experiment_df.set_index("Formulation_ID")
experiment_df
```

Formulation_ID	Processing_Temperature	Processing_Time	Processing_Pressure
F1	213.0	4.43	4.64
F2	250.8	2.30	8.99
F3	249.4	1.88	8.66
F4	339.3	3.84	9.42
F5	342.5	4.24	8.07
F6	229.6	2.39	7.02
F7	399.5	1.38	6.23
F8	253.4	4.76	4.35
F9	395.3	2.59	9.46
F10	282.2	3.07	9.76
F11	206.6	4.35	3.56
F12	269.0	3.70	3.75
F13	326.9	3.94	5.37
F14	336.1	1.84	5.04
F15	306.2	3.17	9.95
F16	289.6	3.78	2.58
F17	310.6	1.91	1.16
F18	318.5	1.70	5.45
F19	216.2	4.93	2.61
F20	273.9	3.07	4.30
F21	248.4	2.04	7.70
F22	360.6	4.99	

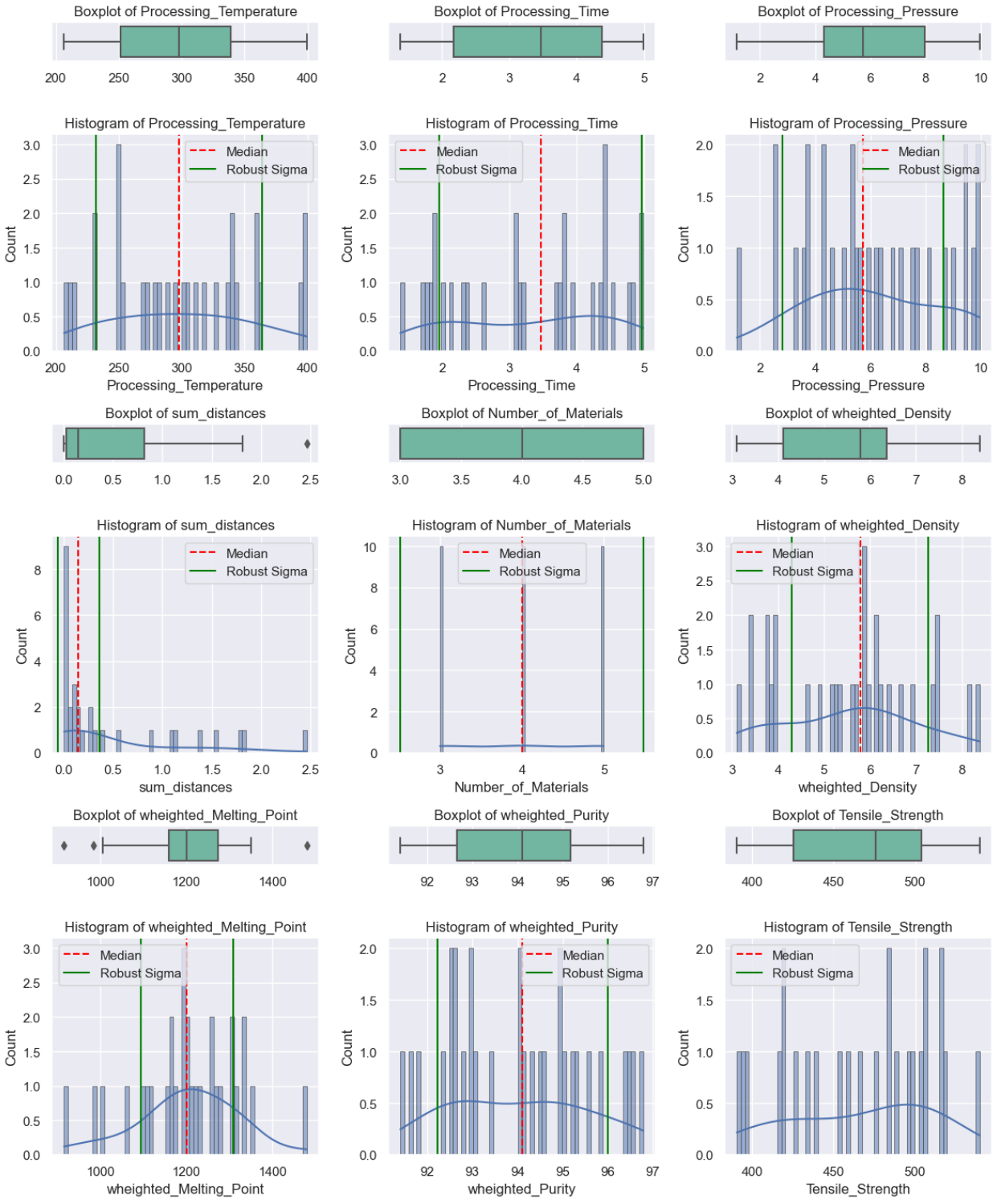
```
7.49
F23                                294.1              4.86
3.77
F24                                396.7              3.23
5.88
F25                                279.8              4.53
5.58
F26                                363.3              1.75
6.73
F27                                359.7              2.12
3.25
F28                                230.1              3.80
6.31
F29                                301.6              4.39
9.81
F30                                339.2              4.43
5.38

                 sum_distances  Number_of_Materials  wheighted_Density
\
Formulation_ID

F1                    0.137207                    5             6.8912

F2                    1.551091                    4             3.8519

F3                    0.022937                    4             7.4605

F4                    0.007573                    4             4.9261

F5                    1.810380                    3             6.1065

F6                    0.038286                    4             6.4062

F7                    0.047928                    4             6.6684

F8                    0.021271                    5             5.9085

F9                    0.327725                    5             3.7536

F10                   0.007927                    5             7.3587

F11                   0.101175                    4             4.6623

F12                   0.160343                    3             8.1271

F13                   0.001491                    5             5.7173

F14                   0.091639                    5             5.6021

F15                   0.261123                    4             5.9541
```

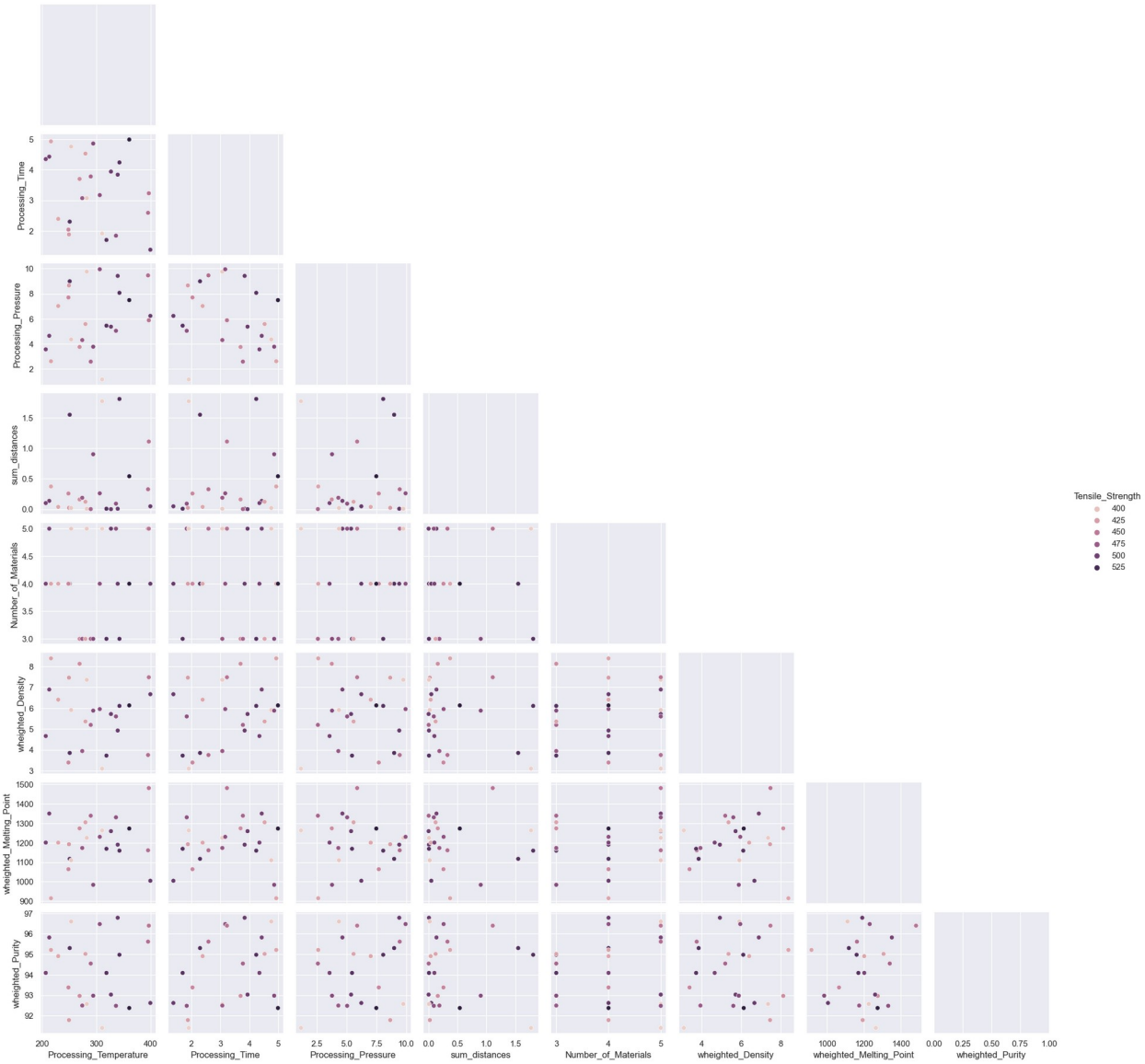
F16	0.002654	3	5.1950
F17	1.773062	5	3.1041
F18	0.007932	3	3.7243
F19	0.373488	4	8.3864
F20	0.187941	3	3.9416
F21	0.257808	4	3.3920
F22	0.541176	4	6.1302
F23	0.903222	3	5.8804
F24	1.110882	5	7.4802
F25	0.122599	3	5.3606
F26	1.106146	3	6.2375
F27	0.051103	5	5.2965
F28	0.015758	3	5.8519
F29	2.466774	5	3.4222
F30	1.375620	3	3.8985

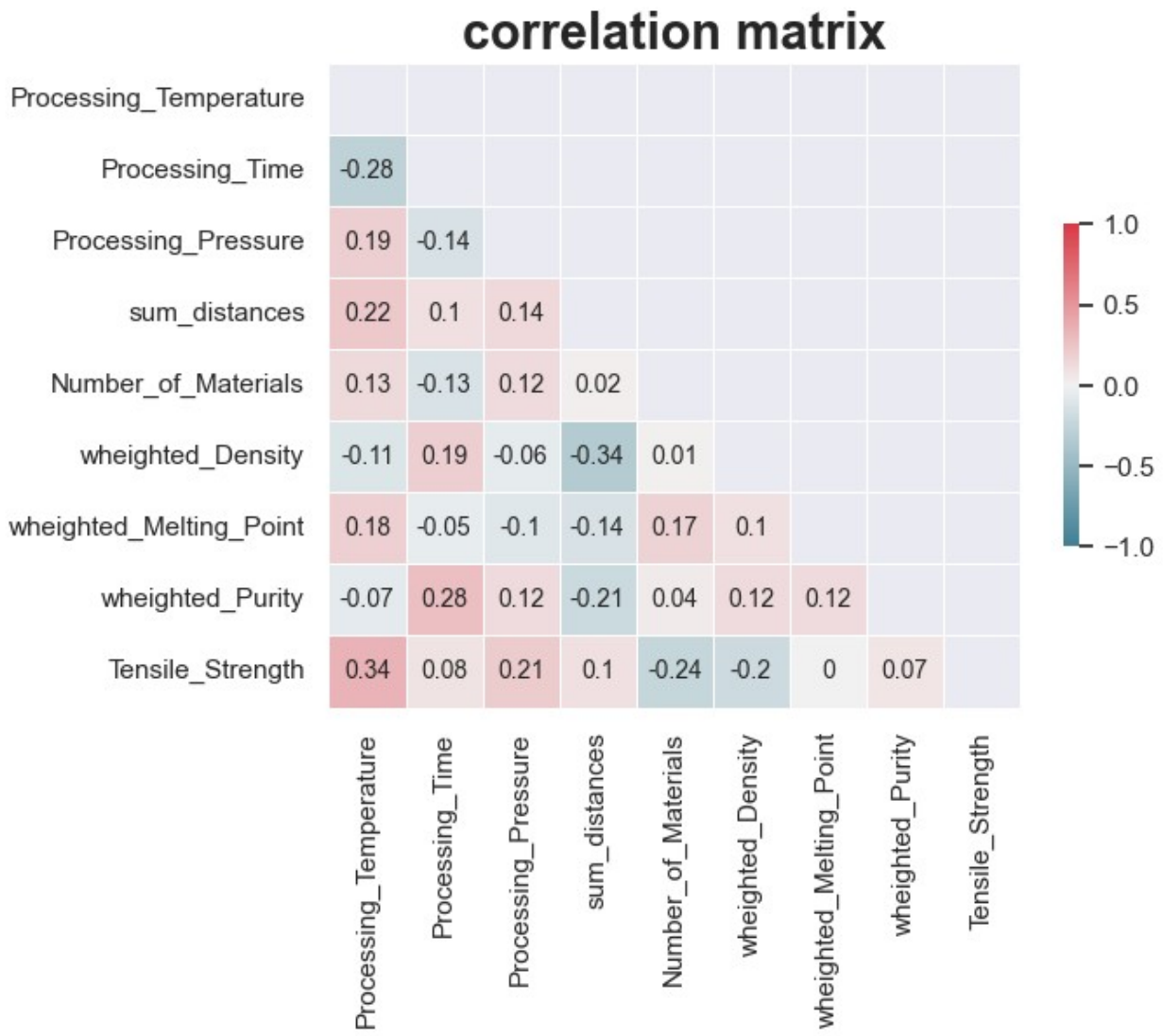
Formulation_ID	wheighted_Melting_Point	wheighted_Purity
F1	1350.096	95.8221
F2	1117.194	95.3027
F3	1192.076	91.7884
F4	1189.958	96.7838
F5	1159.340	94.9766
F6	1200.660	94.9079
F7	1004.477	92.6218
F8	1110.034	96.6002
F9	1161.045	95.6173
F10	1224.987	92.5721
F11	1200.889	94.0916
F12	1273.916	92.9675
F13	1259.536	93.0323
F14	1330.563	92.4838
F15	1230.277	96.4757
F16	1338.872	94.5488
F17	1263.434	91.4038

```
F18                                1168.902           94.0897
F19                                 914.736           95.2128
F20                                1173.091           92.4959
F21                                1063.984           93.3808
F22                                1272.891           92.3766
F23                                 983.755           92.9782
F24                                1481.045           96.3983
F25                                1305.259           95.0187
F26                                1208.375           92.7577
F27                                1310.955           94.3193
F28                                1311.230           94.4609
F29                                1100.641           91.5840
F30                                1194.764           94.1228
```

```
experiment_df_with_target = experiment_df.copy()
experiment_df_with_target["Tensile_Strength"] = Target
vis_raw_materials_df = Visualization(df = experiment_df_with_target)
vis_raw_materials_df.plot_histograms(bins = 60,rows= 6,cols = 3)

vis_raw_materials_df.pairplot_histograms(plot_features =
experiment_df_with_target.columns,hue_column="Tensile_Strength")

vis_raw_materials_df.plot_correlation_matrix()
```


Boxplot of Processing_Temperature
Boxplot of Processing_Time
Boxplot of Processing_Pressure
Histogram of Processing_Temperature
Histogram of Processing_Time
Histogram of Processing_Pressure
Median
Robust Sigma
Count
Processing_Temperature
Processing_Time
Processing_Pressure
Boxplot of sum_distances
Boxplot of Number_of_Materials
Boxplot of wheighted_Density
Histogram of sum_distances
Histogram of Number_of_Materials
Histogram of wheighted_Density
sum_distances
Number_of_Materials
wheighted_Density
Boxplot of wheighted_Melting_Point
Boxplot of wheighted_Purity
Boxplot of Tensile_Strength
Histogram of wheighted_Melting_Point
Histogram of wheighted_Purity
Histogram of Tensile_Strength
wheighted_Melting_Point
wheighted_Purity
Tensile_Strength


Tensile_Strength
400
425
450
475
500
525
Processing_Temperature
Processing_Time
Processing_Pressure
sum_distances
Number_of_Materials
wheighted_Density
wheighted_Melting_Point
wheighted_Purity




```
modeling_df = experiment_df.copy()
modeling_df["Melting_Point_pured"] =
100*modeling_df["wheighted_Melting_Point"]/modeling_df["wheighted_Puri
ty"]
modeling_df["Melting_Point_pressure_Time"] =
modeling_df["Melting_Point_pured"]/(modeling_df["Processing_Pressure"]
*(modeling_df["Processing_Time"]))
modeling_df["Melting_Point_Temp_Time"] =
modeling_df["Melting_Point_pured"]/(modeling_df["Processing_Temperatur
e"]*(modeling_df["Processing_Time"]))

modeling_df["Density_Temp_Time"] =
modeling_df["wheighted_Density"]/(modeling_df["Processing_Temperature"
])
modeling_df["avg_distances"] =
modeling_df["sum_distances"]/modeling_df["Number_of_Materials"]
```

```
modeling_df.drop(["wheighted_Melting_Point",'wheighted_Purity',"Proces
sing_Time","Processing_Temperature","wheighted_Density","avg_distances
",
                                      'Melting_Point_pured',
'Processing_Pressure',"sum_distances","Number_of_Materials"], axis=1,
inplace=True)
modeling_df.describe()
```

```
       Melting_Point_pressure_Time  Melting_Point_Temp_Time
Density_Temp_Time
count                    30.000000                30.000000
30.000000
mean                     96.461915                 1.502767
0.019382
std                     107.546174                 0.578386
0.007138
min                      27.905676                 0.740243
0.009496
25%                      53.531125                 0.977294
0.014570
50%                      70.540868                 1.398448
0.017659
75%                      98.087551                 2.015936
0.023129
max                     623.874094                 2.769886
0.038790
```

Creating a new DataFrame for the normalized features

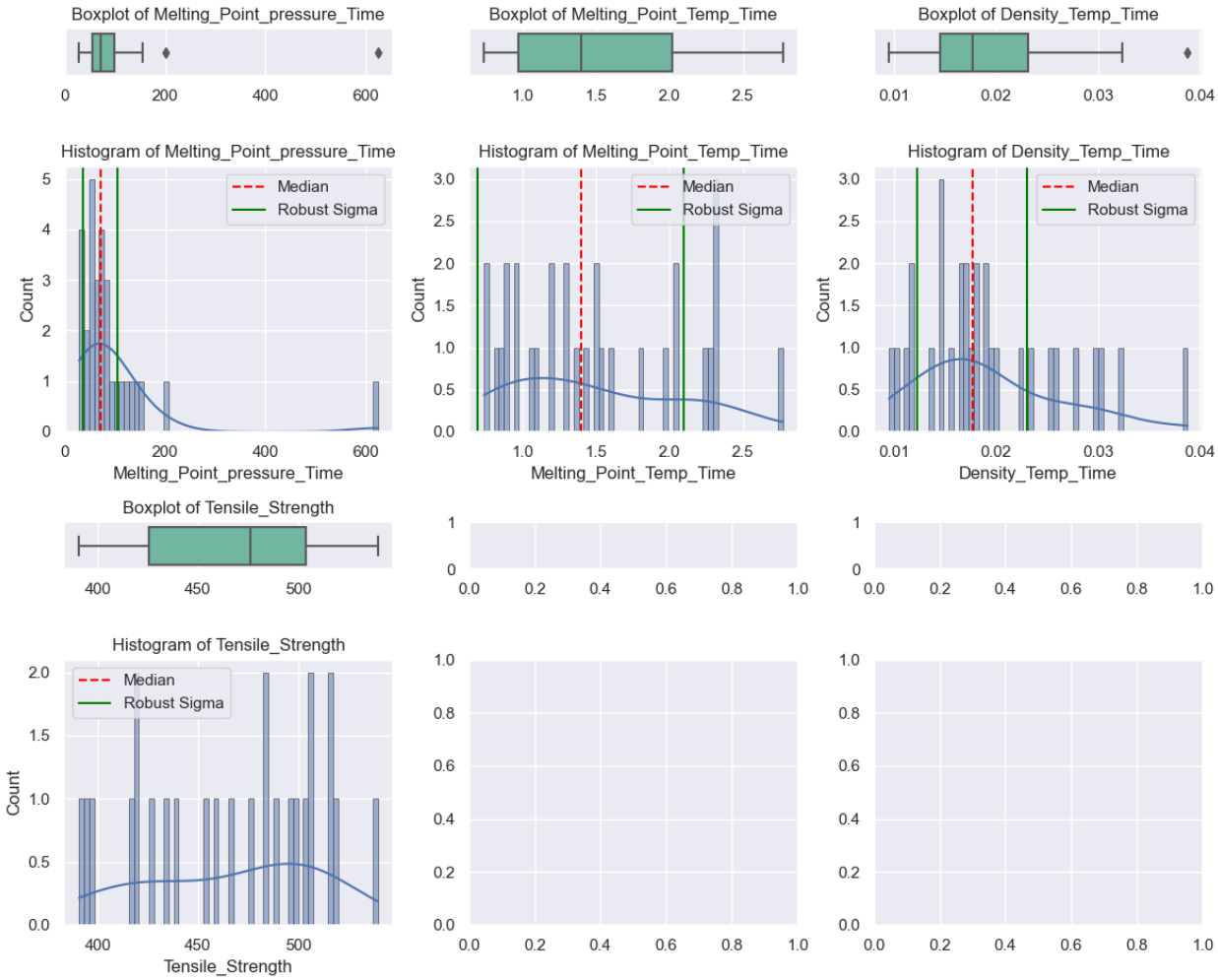
```
scaler = StandardScaler()
# Fitting the scaler to the features
features_normalized = scaler.fit_transform(modeling_df)

normalized_df = pd.DataFrame(features_normalized,
columns=modeling_df.columns, index=modeling_df.index)

# Adding the non-normalized 'Tensile_Strength' column back into the
DataFrame
modeling_df['Tensile_Strength'] = Target
normalized_df['Tensile_Strength'] = Target

normalized_df.describe()
```

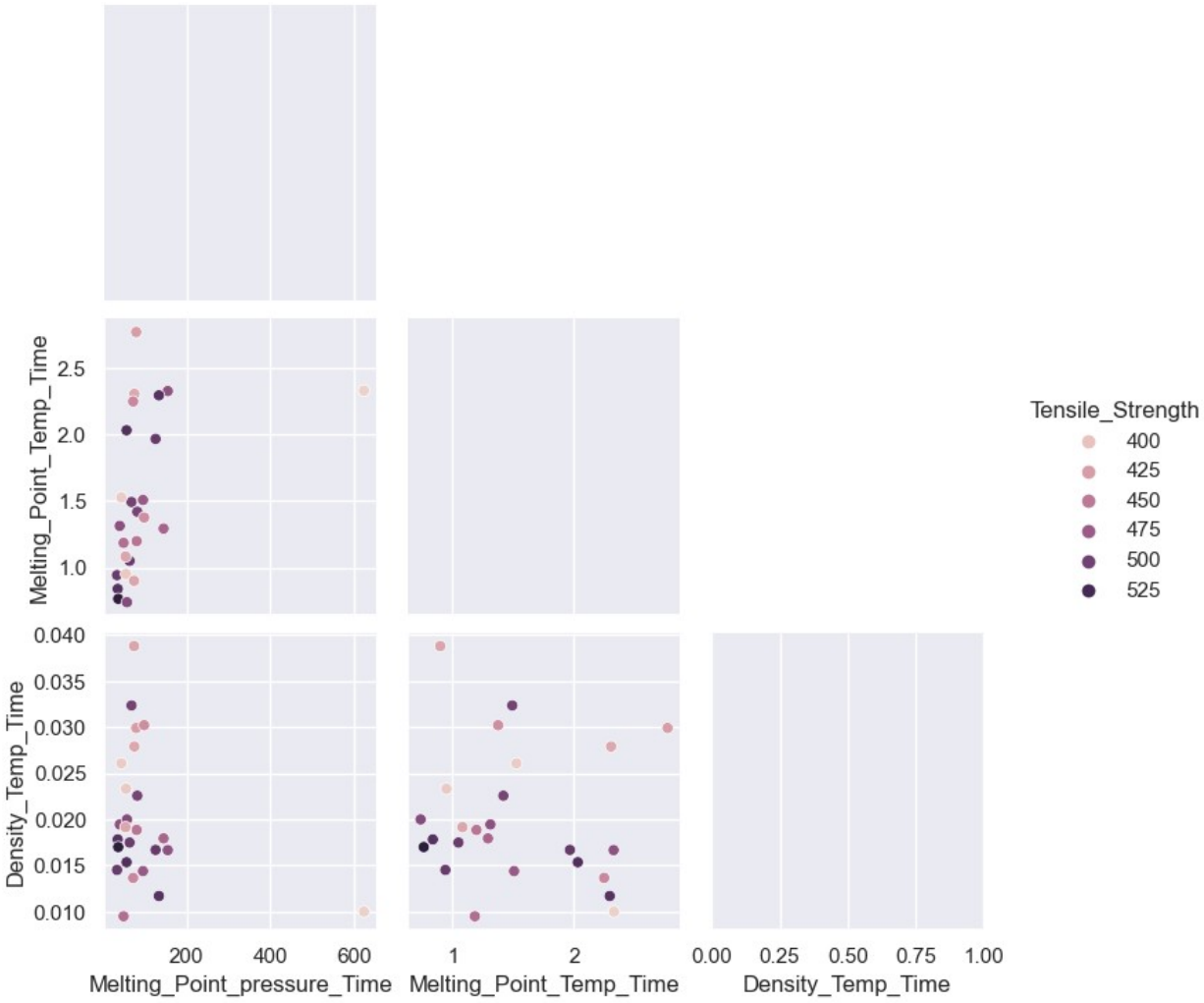
```
       Melting_Point_pressure_Time  Melting_Point_Temp_Time  \
count                 3.000000e+01             3.000000e+01
mean                 -8.141636e-17            -5.773160e-16
std                   1.017095e+00             1.017095e+00
min                  -6.483562e-01            -1.340902e+00
25%                  -4.060089e-01            -9.240472e-01
```

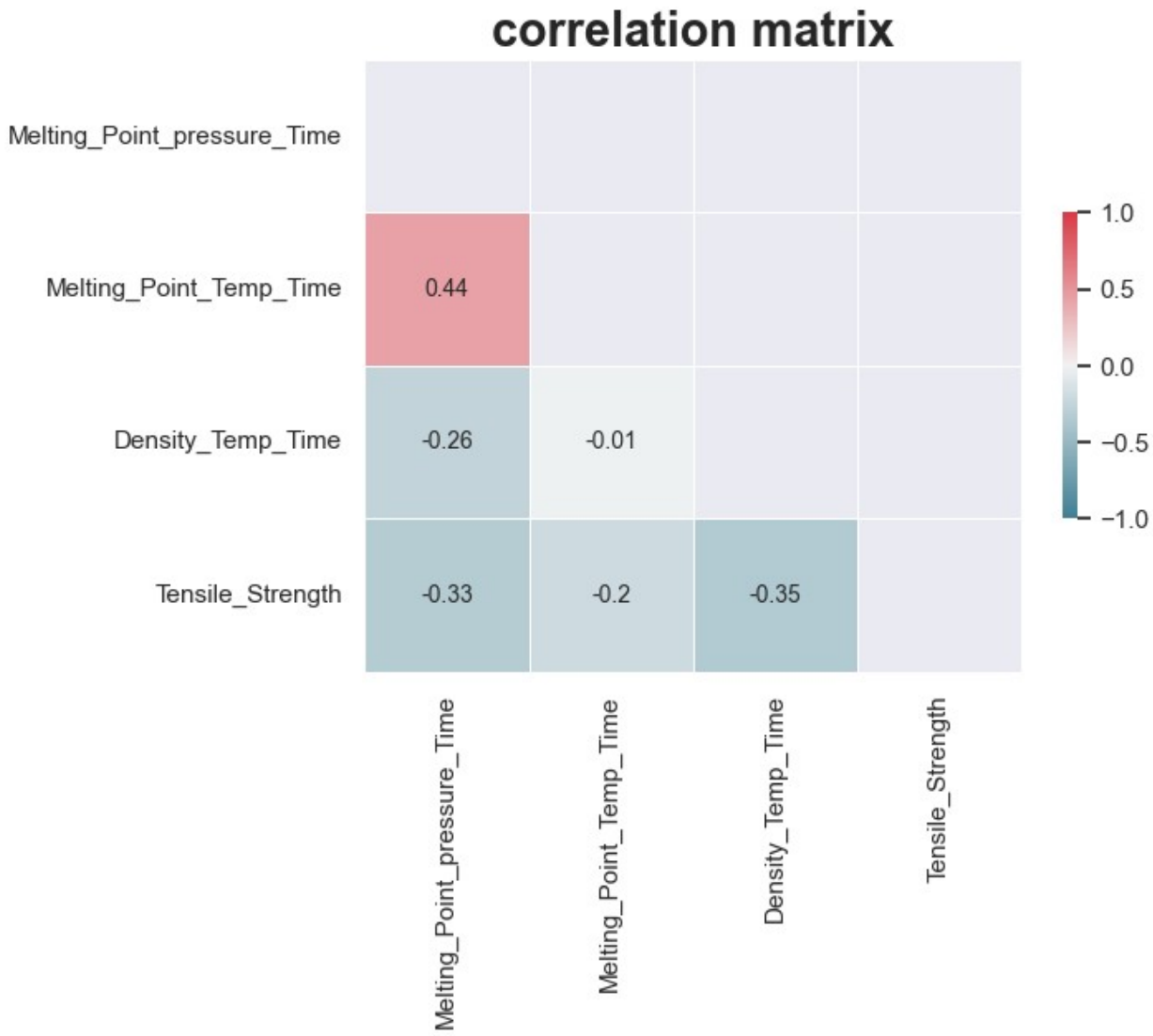
```
50%                   -2.451428e-01             -1.834459e-01
75%                    1.537411e-02              9.024096e-01
max                    4.987889e+00              2.228235e+00
```

```
       Density_Temp_Time  Tensile_Strength
count       3.000000e+01         25.000000
mean        8.067621e-16        465.809200
std         1.017095e+00         44.129447
min        -1.408704e+00        390.670000
25%        -6.856874e-01        425.430000
50%        -2.455149e-01        476.080000
75%         5.338695e-01        503.710000
max         2.765233e+00        539.570000
```

```
vis_raw_materials_df = Visualization(df = modeling_df)
vis_raw_materials_df.plot_histograms(bins = 60,rows= 4,cols = 3)

vis_raw_materials_df.pairplot_histograms(plot_features =
modeling_df.columns,hue_column="Tensile_Strength")

vis_raw_materials_df.plot_correlation_matrix()
```


Boxplot of Melting_Point_pressure_Time
Boxplot of Melting_Point_Temp_Time
Boxplot of Density_Temp_Time
Histogram of Melting_Point_pressure_Time
Median
Robust Sigma
Count
Melting_Point_pressure_Time
Histogram of Melting_Point_Temp_Time
Melting_Point_Temp_Time
Histogram of Density_Temp_Time
Density_Temp_Time
Boxplot of Tensile_Strength
Histogram of Tensile_Strength
Tensile_Strength


Melting_Point_Temp_Time
2.5
2.0
1.5
1.0
Density_Temp_Time
0.040
0.035
0.030
0.025
0.020
0.015
0.010
200
400
600
Melting_Point_pressure_Time
1
2
Melting_Point_Temp_Time
0.00
0.25
0.50
0.75
1.00
Density_Temp_Time
Tensile_Strength
400
425
450
475
500
525



Insights on Tensile Strength and Recommendations for Experiments

Overview

Tensile strength has been extensively documented and experimented on for over 200 years. Many raw materials have well-known "pure" tensile strength values, which can be incorporated as features in our modeling process. Ductile materials like steel exhibit well-defined elastic behavior characterized by a linear stress-strain relationship.

Key Recommendations

1. **Incorporate Pure Tensile Strength Data**:
   - Utilize existing literature to incorporate the pure tensile strength values of raw materials as additional features in the model. This will help in understanding the baseline behavior of each material.

2. **Scrap Redundant Data**:
   - Eliminate redundant data on raw materials with well-established properties to streamline the dataset and focus on more variable factors.
3. **Feature Engineering**:
   - **Melting Point and Purity**:
     - Pure substances have a higher and more precise melting point compared to impure substances or mixtures. Feature engineering based on the relationship between melting point and purity can provide valuable insights.
   - **Label Encoding**:
     - Consider label encoding the real data of raw materials and sensor types used for strain and stress measurements to capture more nuanced relationships.

Experimentation Recommendations

Based on the model's findings, the following specific experiments are recommended for the R&D team to optimize tensile strength using the existing raw materials:

1. **Adjust Raw Material Compositions**:
   - Experiment with varying the compositions of existing raw materials to understand their impact on tensile strength. This includes testing different alloys or composite materials.
2. **Processing Temperature**:
   - Conduct experiments at different processing temperatures to determine the optimal temperature that maximizes tensile strength for each raw material.
3. **Processing Time**:
   - Investigate the effects of different processing times on tensile strength. Shorter or longer processing times may influence the material's microstructure and, consequently, its tensile properties.
4. **Processing Pressure**:
   - Test the impact of varying pressures during processing. Higher or lower pressures could affect the density and internal structure of the material, influencing its tensile strength.

Insights from Initial Models

- **Cosine Distance**:
  - Although the idea of using cosine distance was explored, the results were not significant. However, it remains a potential feature if combined with label encoding of raw material or sensor type data.

Conclusion

These insights and recommendations are aimed at helping the R&D team design targeted experiments to optimize tensile strength. By incorporating pure tensile strength data, refining feature engineering techniques, and systematically varying processing parameters, we can achieve a deeper understanding and enhancement of the materials' tensile properties.

Modeling

```
class ModelComparison:
    def __init__(self, X_train, y_train, X_test, y_test,random_state):
        self.X_train = X_train
        self.y_train = y_train
        self.X_test = X_test
        self.y_test = y_test
        self.best_model = None
        self.models = {
            'Linear Regression': LinearRegression(),
            'Lasso Regression': Lasso(alpha=0.01),
            'Ridge Regression': Ridge(alpha=0.05),
            'ElasticNet': ElasticNet(alpha=0.01, l1_ratio=0.7),
            'Random Forest Regressor':
RandomForestRegressor(random_state=random_state),
            'SVR': SVR(),
            'XGBoost Regressor':
xgb.XGBRegressor(objective='reg:squarederror',
random_state=random_state),
            'CatBoost Regressor': CatBoostRegressor(verbose=0,
random_state=random_state),
            'Bayesian Ridge Regression': BayesianRidge()  # Adding
Bayesian Ridge Regression

        }
        self.results = pd.DataFrame()
        self.predictions = {}  # To store model predictions for later
use in plotting

    def train(self,fit_best = False,X = None,y = None):

        if fit_best:
            self.fittest_model = self.models[self.best_model]
            self.fittest_model.fit(X, y)
            print(f"Best model {self.best_model} trained
successfully.")
        else:
            # Train each model on the training set
            for name, model in self.models.items():
                model.fit(self.X_train, self.y_train)
                print(f"Model {name} retrained successfully.")

    def calculate_regression_metrics(self, name, actual, y_pred):
        mae = mean_absolute_error(actual, y_pred)
        mse = mean_squared_error(actual, y_pred)
        rmse = np.sqrt(mse)
        mape = np.mean(np.abs((actual - y_pred) / actual)) * 100
        r2 = r2_score(actual, y_pred)
```

```
        metrics_df = pd.DataFrame({
            '#': ['MAE', 'MSE', 'RMSE', 'MAPE', 'R^2'],
            name: [mae, mse, rmse, mape, r2]
        })

        metrics_df_indexed = metrics_df.set_index('#').T
        return metrics_df_indexed

    def evaluate(self):
        # Evaluate each model on the test set
        for name, model in self.models.items():
            y_pred = model.predict(self.X_test)
            self.predictions[name] = y_pred  # Store predictions
            # Calculate metrics and concatenate to the results
DataFrame
            metrics_df = self.calculate_regression_metrics(name,
self.y_test, y_pred)
            self.results = pd.concat([self.results, metrics_df],
ignore_index=True)

        # Add model names to the results DataFrame and sort by MAPE
        self.results["Model"] = self.models.keys()
        self.results = self.results.sort_values(by=('MAPE'),
ascending=True)
        self.best_model = self.results["Model"].iloc[0]
        return self.results

    def plot_evaluation(self,model_name, best_model = False):

        if model_name in self.models and model_name in
self.predictions:
            model = self.models[model_name]
            y_pred = self.predictions[model_name]
            if best_model:
                y_pred = self.fittest_model.predict(self.X_test)
            residuals = y_pred - self.y_test
            fig, axs = plt.subplots(2, 2, figsize=(15, 10))

            sns.scatterplot(x=y_pred, y=self.y_test, ax=axs[0, 0],
label='Data Points')
            axs[0, 0].plot(y_pred, y_pred, color='red', label=f'Line:
$R^2$ = {r2_score(self.y_test, y_pred):.2f}')
            axs[0, 0].set_xlabel('Actual Values')
            axs[0, 0].set_ylabel('Predicted Values')
            axs[0, 0].set_title(f'{model_name} - Scatter Plot of
Predicted vs. Actual Values')
            axs[0, 0].legend()

            if hasattr(model, 'feature_importances_'):
                feature_importances = model.feature_importances_
```

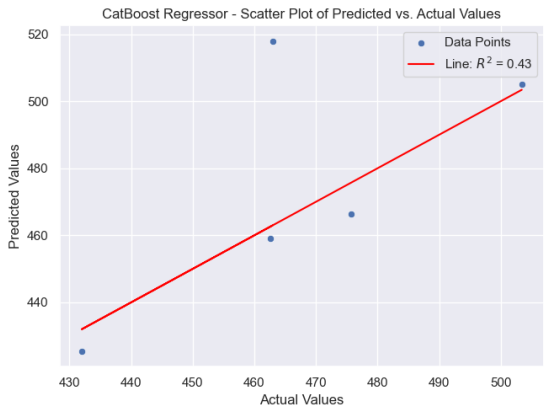
```
                sorted_indices = np.argsort(feature_importances)[::-1]
                sorted_feature_names = np.array(self.X_test.columns)
[sorted_indices]
                feature_importance_df = pd.DataFrame({'Feature':
sorted_feature_names, 'Importance':
feature_importances[sorted_indices]})
                axs[0, 1].barh(feature_importance_df['Feature'],
feature_importance_df['Importance'])
                axs[0, 1].set_xlabel('Importance')
                axs[0, 1].set_ylabel('Feature')
                axs[0, 1].set_title(f'{model_name} - Feature
Importance')
                axs[0, 1].invert_yaxis()

            sm.qqplot(residuals, line='s', ax=axs[1, 0])
            axs[1, 0].set_title(f'{model_name} - Q-Q Plot')

            n = len(y_pred)
            k = 1  # Number of predictors
            threshold = 4 / (n - k - 1)
            model_influence = OLSInfluence(sm.OLS(y_pred,
sm.add_constant(self.X_test)).fit())
            cooks = model_influence.cooks_distance[0]

            axs[1, 1].vlines(x=np.arange(len(cooks)), ymin=0,
ymax=cooks, color='tab:blue')
            axs[1, 1].axhline(y=threshold, color='red',
linestyle='--', label=f'Threshold: 4/(n-k-1) = {threshold:.2f}')
            axs[1, 1].set_xlabel('Observation Index')
            axs[1, 1].set_ylabel("Cook's Distance")
            axs[1, 1].set_title("Cook's Distance Plot")
            axs[1, 1].legend()

            plt.tight_layout()
            plt.show()
        else:
            print(f"Model {model_name} not found or no predictions
available.")

    def predict_new_samples(self, new_X):
        # Select the best model based on the lowest MAPE value
        best_model_name = self.results.iloc[0]['Model']  # Assuming
the results are sorted by MAPE, ascending
        best_model = self.models[best_model_name]

        # Predict using the best model
        new_predictions = best_model.predict(new_X)

        return new_predictions
```

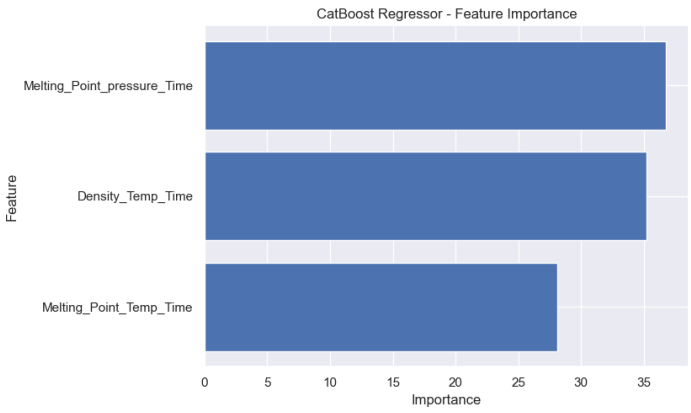
```
test_rows = 5
random_state = 902010

Train_df = normalized_df.iloc[:-test_rows]
Test_df = normalized_df.iloc[-test_rows:]
X = Train_df.drop('Tensile_Strength', axis=1)  # excluding test rows
and target variable
y = Train_df['Tensile_Strength']

# Split data into training and validation
X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.2,
random_state=random_state)

# Creating a ModelComparison instance
comparison_instance = ModelComparison(X_train, y_train, X_val,
y_val,random_state)

# Training the models and evaluating them
comparison_instance.train()
comparison_instance.evaluate()
```

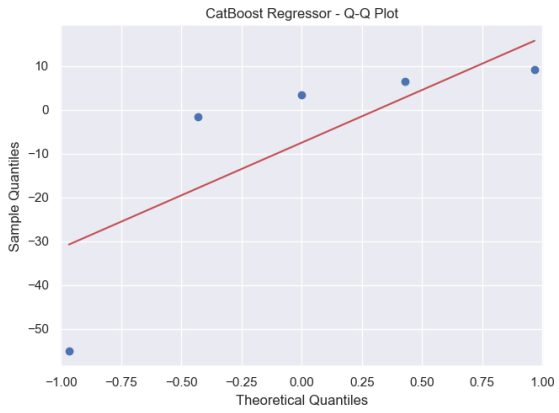
```
Model Linear Regression retrained successfully.
Model Lasso Regression retrained successfully.
Model Ridge Regression retrained successfully.
Model ElasticNet retrained successfully.
Model Random Forest Regressor retrained successfully.
Model SVR retrained successfully.
Model XGBoost Regressor retrained successfully.
Model CatBoost Regressor retrained successfully.
Model Bayesian Ridge Regression retrained successfully.
```

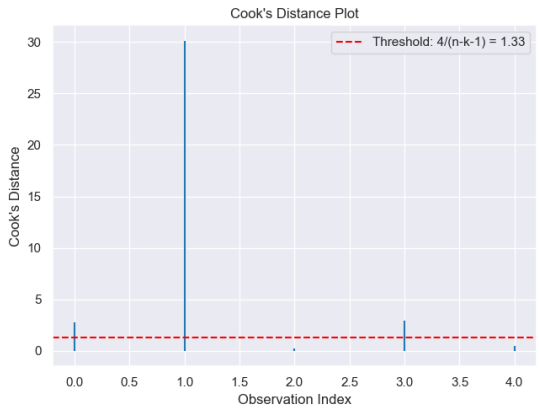
```
#         MAE          MSE       RMSE      MAPE       R^2  \
7  15.169454   633.385154  25.167144  3.041672  0.427068
4  17.462700   677.587500  26.030511  3.511689  0.387084
0  18.689687   780.371931  27.935138  3.886364  0.294110
1  18.697429   779.758134  27.924150  3.888062  0.294665
2  18.716280   778.359605  27.899097  3.891677  0.295930
3  18.726832   777.549192  27.884569  3.893887  0.296663
8  22.605007   717.183753  26.780287  4.681163  0.351267
5  29.884366  1090.092146  33.016544  6.390464  0.013950
6  34.635198  2120.171812  46.045323  7.048325 -0.917815

#                      Model
7         CatBoost Regressor
4    Random Forest Regressor
0          Linear Regression
1           Lasso Regression
2           Ridge Regression
3                 ElasticNet
8  Bayesian Ridge Regression
```

```
5                             SVR
6          XGBoost Regressor

comparison_instance.plot_evaluation(comparison_instance.best_model)
```









Recommendations:

Model Selection:

- The CatBoost Regressor is recommended as the best-performing model for predicting tensile strength due to its superior accuracy and higher R^2 value.

Hyperparameter Tuning:

- While the CatBoost Regressor performed well, further hyperparameter tuning could potentially improve its performance even more.

Feature Engineering:

- The moderate R^2 values across most models suggest that additional feature engineering or the inclusion of new relevant features could enhance the model's performance.

Model Validation:

- Given the limited data, consider using cross-validation to ensure the robustness of the model's performance.

Additional Data:

- Collecting more data points could improve the model's generalizability and provide more reliable performance estimates.

Model Interpretability:

- Investigate the feature importances and partial dependence plots from the CatBoost model to gain insights into how different features impact tensile strength predictions.

Hyperparameter tuning

```
class HyperparameterTuner:
    def __init__(self, metric: Callable = mean_absolute_error,
early_stopping_rounds: int = 100, random_state: int = 902010):
        self.metric = metric
        self.early_stopping_rounds = early_stopping_rounds
        self.random_state = random_state

    def hyperparameter_tuning(self, space: Dict[str, Union[float,
int]],
                              X_train: pd.DataFrame, y_train:
pd.Series,
                              X_val: pd.DataFrame, y_val: pd.Series) -
> Dict[str, Any]:

        model = CatBoostRegressor(**space,
random_seed=self.random_state,

early_stopping_rounds=self.early_stopping_rounds, verbose=False)
        model.fit(X_train, y_train, eval_set=(X_val, y_val))

        pred = model.predict(X_val)
        score = self.metric(y_val, pred)
        return {'loss': score, 'status': STATUS_OK, 'model': model}

    def tune_and_train(self, space, X_train, y_train, X_val, y_val):
        trials = Trials()
        best = fmin(fn=lambda space: self.hyperparameter_tuning(space,
X_train, y_train,
                                                                X_val,
y_val),
                    space=space,
                    algo=tpe.suggest,
                    max_evals=50,
                    trials=trials)
```

```
        best_model = CatBoostRegressor(**best,
random_seed=self.random_state)
        best_model.fit(X_train, y_train, eval_set=(X_val, y_val),
verbose=100)
        return best_model, trials

# Define the complete search space here
space = {
    'depth': hp.choice('depth', range(1, 11)),
    'l2_leaf_reg': hp.uniform('l2_leaf_reg', 1, 10),
    'learning_rate': hp.loguniform('learning_rate', -5, 0),
    # 'random_strength': hp.uniform('random_strength', 1, 20),
    'subsample': hp.uniform('subsample', 0.5, 1),
    'colsample_bylevel': hp.uniform('colsample_bylevel', 0.5, 1)
}

# Assuming your data is already prepared
tuner = HyperparameterTuner(random_state = random_state)
best_model, all_trials = tuner.tune_and_train(space, X_train, y_train,
X_val, y_val)

comparison_instance.calculate_regression_metrics(comparison_instance.b
est_model + " - Hypertuned",
                                                 actual =
y_val,y_pred = best_model.predict(X_val))

  0%|          | 0/50 [00:00<?, ?trial/s, best loss=?]

100%|██████████| 50/50 [00:18<00:00,  2.65trial/s, best loss:
13.208486398352544]
0:    learn: 44.7945966     test: 34.5134164 best: 34.5134164 (0)
      total: 324us    remaining: 324ms
100:  learn: 27.9732509     test: 22.7812837 best: 22.1675425 (91)
      total: 28.6ms   remaining: 255ms
200:  learn: 18.7518803     test: 24.8797891 best: 22.1675425 (91)
      total: 63ms     remaining: 250ms
300:  learn: 13.1031409     test: 26.6211073 best: 22.1675425 (91)
      total: 93.7ms   remaining: 218ms
400:  learn: 9.3271215 test: 27.8226283 best: 22.1675425 (91) total:
129ms remaining: 193ms
500:  learn: 6.8784745 test: 28.8030922 best: 22.1675425 (91) total:
158ms remaining: 158ms
600:  learn: 5.1254311 test: 30.3784649 best: 22.1675425 (91) total:
200ms remaining: 133ms
700:  learn: 3.8627198 test: 31.4040851 best: 22.1675425 (91) total:
232ms remaining: 98.9ms
800:  learn: 2.8648560 test: 32.0818781 best: 22.1675425 (91) total:
260ms remaining: 64.7ms
900:  learn: 2.1173506 test: 32.4215799 best: 22.1675425 (91) total:
292ms remaining: 32.1ms
```

```
999:  learn: 1.5796716 test: 32.5245018 best: 22.1675425 (91) total:
322ms remaining: 0us

bestTest = 22.1675425
bestIteration = 91

Shrink model to first 92 iterations.

#                                          MAE          MSE        RMSE
MAPE  \
CatBoost Regressor - Hypertuned  18.245115  491.400013  22.167544
3.746112

#                                         R^2
CatBoost Regressor - Hypertuned  0.555501
```

Results

```
comparison_instance.fittest_model = best_model
comparison_instance.train(fit_best = True,X =
pd.concat([X_train,X_val]), y = pd.concat([y_train,y_val]))

X_Test = Test_df.drop('Tensile_Strength', axis=1)
Test_results = comparison_instance.fittest_model.predict(X_Test)

num_rows = len(formulations_df_final)
formulations_df_final.loc[num_rows-5:num_rows, 'Tensile_Strength'] =
Test_results

formulations_df_final

Best model CatBoost Regressor trained successfully.

   Formulation_ID Formulation_Name  Processing_Temperature
Processing_Time  \
0              F1   Formulation_01                   213.0
4.43
1              F2   Formulation_02                   250.8
2.30
2              F3   Formulation_03                   249.4
1.88
3              F4   Formulation_04                   339.3
3.84
4              F5   Formulation_05                   342.5
4.24
5              F6   Formulation_06                   229.6
2.39
6              F7   Formulation_07                   399.5
1.38
7              F8   Formulation_08                   253.4
```

```
4.76
8              F9   Formulation_09                    395.3
2.59
9             F10   Formulation_10                    282.2
3.07
10            F11   Formulation_11                    206.6
4.35
11            F12   Formulation_12                    269.0
3.70
12            F13   Formulation_13                    326.9
3.94
13            F14   Formulation_14                    336.1
1.84
14            F15   Formulation_15                    306.2
3.17
15            F16   Formulation_16                    289.6
3.78
16            F17   Formulation_17                    310.6
1.91
17            F18   Formulation_18                    318.5
1.70
18            F19   Formulation_19                    216.2
4.93
19            F20   Formulation_20                    273.9
3.07
20            F21   Formulation_21                    248.4
2.04
21            F22   Formulation_22                    360.6
4.99
22            F23   Formulation_23                    294.1
4.86
23            F24   Formulation_24                    396.7
3.23
24            F25   Formulation_25                    279.8
4.53
25            F26   Formulation_26                    363.3
1.75
26            F27   Formulation_27                    359.7
2.12
27            F28   Formulation_28                    230.1
3.80
28            F29   Formulation_29                    301.6
4.39
29            F30   Formulation_30                    339.2
4.43

    Processing_Pressure   RM1   RM2   RM3   RM4   RM5  ...  RM24  RM25
RM26  \
0                  4.64   0.0   0.0   0.0   0.0   0.0  ...   0.0   0.0
```

```
0.0
1                  8.99   0.0   0.0   0.0   0.0   0.0  ...  12.0   0.0
0.0
2                  8.66   0.0   0.0  24.0   0.0   0.0  ...   0.0   3.0
0.0
3                  9.42   0.0   0.0  27.0   8.0   0.0  ...   0.0   0.0
0.0
4                  8.07   0.0   0.0   0.0   0.0   0.0  ...   0.0   0.0
0.0
5                  7.02   0.0   0.0   0.0  27.0   0.0  ...   0.0   0.0
16.0
6                  6.23   0.0   0.0   0.0   0.0   0.0  ...   0.0   0.0
0.0
7                  4.35   0.0   9.0   0.0   0.0   0.0  ...   0.0   0.0
0.0
8                  9.46   0.0   0.0   0.0   0.0   0.0  ...   0.0  15.0
0.0
9                  9.76   0.0   3.0   0.0   0.0   0.0  ...   6.0   0.0
1.0
10                 3.56   0.0   0.0   0.0   0.0   0.0  ...   0.0   0.0
45.0
11                 3.75   0.0   0.0   0.0  35.0   0.0  ...   0.0   0.0
0.0
12                 5.37   0.0   0.0   0.0   0.0   0.0  ...  23.0   0.0
47.0
13                 5.04  25.0   0.0   0.0   0.0   0.0  ...  12.0   0.0
0.0
14                 9.95   0.0   0.0   0.0   0.0   0.0  ...   0.0  14.0
71.0
15                 2.58   0.0   0.0   0.0  51.0   0.0  ...   0.0   0.0
0.0
16                 1.16   0.0   0.0   0.0   4.0  65.0  ...   0.0   0.0
0.0
17                 5.45   0.0   0.0   0.0   0.0   0.0  ...   0.0   0.0
19.0
18                 2.61   0.0   0.0   0.0   0.0   0.0  ...   0.0   0.0
0.0
19                 4.30   0.0   0.0   0.0   0.0   0.0  ...   0.0   0.0
0.0
20                 7.70   0.0   0.0   0.0   0.0   0.0  ...   7.0   0.0
0.0
21                 7.49   0.0   0.0   0.0  51.0   0.0  ...   4.0   0.0
0.0
22                 3.77   0.0   0.0  42.0   0.0   0.0  ...   0.0   0.0
0.0
23                 5.88   0.0   0.0   2.0   0.0   0.0  ...   2.0   0.0
0.0
24                 5.58   0.0   0.0   0.0   0.0   0.0  ...   0.0   0.0
0.0
```

```
25                 6.73   0.0  82.0   0.0   0.0   0.0  ...   0.0   0.0
0.0
26                 3.25   0.0   0.0   0.0   0.0   0.0  ...   0.0   0.0
0.0
27                 6.31   0.0   0.0   0.0   0.0   0.0  ...   0.0   0.0
0.0
28                 9.81   0.0   0.0   0.0   0.0   0.0  ...   0.0  10.0
0.0
29                 5.38   0.0   0.0  88.0   0.0   0.0  ...   0.0   0.0
0.0

    RM27  RM28  RM29  RM30  Number_of_Materials  Percentage_Sum  \
0    0.0  10.0   7.0   0.0                    5           100.0
1    0.0   4.0   0.0   0.0                    4           100.0
2    0.0   0.0   0.0   0.0                    4           100.0
3    0.0  11.0   0.0   0.0                    4           100.0
4    0.0   0.0   0.0   0.0                    3           100.0
5    0.0   0.0   0.0   0.0                    4           100.0
6    0.0   0.0   0.0   0.0                    4           100.0
7    0.0   0.0   0.0   0.0                    5           100.0
8   28.0   0.0   0.0   0.0                    5           100.0
9    0.0   0.0   0.0   0.0                    5           100.0
10   0.0   0.0   0.0   0.0                    4           100.0
11   0.0   0.0   0.0   0.0                    3           100.0
12   0.0   0.0   0.0   0.0                    5           100.0
13   0.0   0.0   0.0   0.0                    5           100.0
14   0.0  12.0   0.0   0.0                    4           100.0
15   0.0   0.0   0.0   0.0                    3           100.0
16   0.0  12.0   0.0   0.0                    5           100.0
17   0.0   0.0   0.0   0.0                    3           100.0
18   0.0   0.0   0.0   0.0                    4           100.0
19   0.0   0.0   0.0  25.0                    3           100.0
20   0.0   0.0   0.0   9.0                    4           100.0
21   0.0   0.0  28.0   0.0                    4           100.0
22   0.0   0.0   0.0   0.0                    3           100.0
23   0.0   0.0   0.0   0.0                    5           100.0
24   0.0   0.0   0.0   0.0                    3           100.0
25   0.0   0.0   0.0   0.0                    3           100.0
26  21.0   0.0   0.0   0.0                    5           100.0
27   0.0   0.0   0.0   0.0                    3           100.0
28   0.0   0.0   0.0   0.0                    5           100.0
29   0.0   0.0   0.0   0.0                    3           100.0

    Tensile_Strength
0         498.050000
1         517.930000
2         425.430000
3         505.060000
4         515.620000
```

```
5          416.850000
6          506.260000
7          395.900000
8          459.150000
9          394.190000
10         496.100000
11         435.290000
12         503.710000
13         483.130000
14         483.550000
15         466.470000
16         390.670000
17         515.580000
18         419.600000
19         476.080000
20         439.630000
21         539.570000
22         488.670000
23         453.530000
24         419.210000
25         503.664059
26         489.106580
27         445.363854
28         490.945905
29         474.062405

[30 rows x 38 columns]
```

Appendix: Design Of Experiment (DOE)

With only 25 samples, traditional machine learning might struggle to generalize well.

Design of Experiments (DOE) can be very useful in such cases as it focuses on systematically planning experiments to understand the factors affecting your outcomes.

There are software tools like JMP for DOE, offering features like factorial designs, response surface methodologies, and more.

However, in this section, I will use `statsmodels` and `pyDOE2` in Python to perform DOE, as they provide robust functionalities for exploring the relationships between variables efficiently, especially with small datasets.

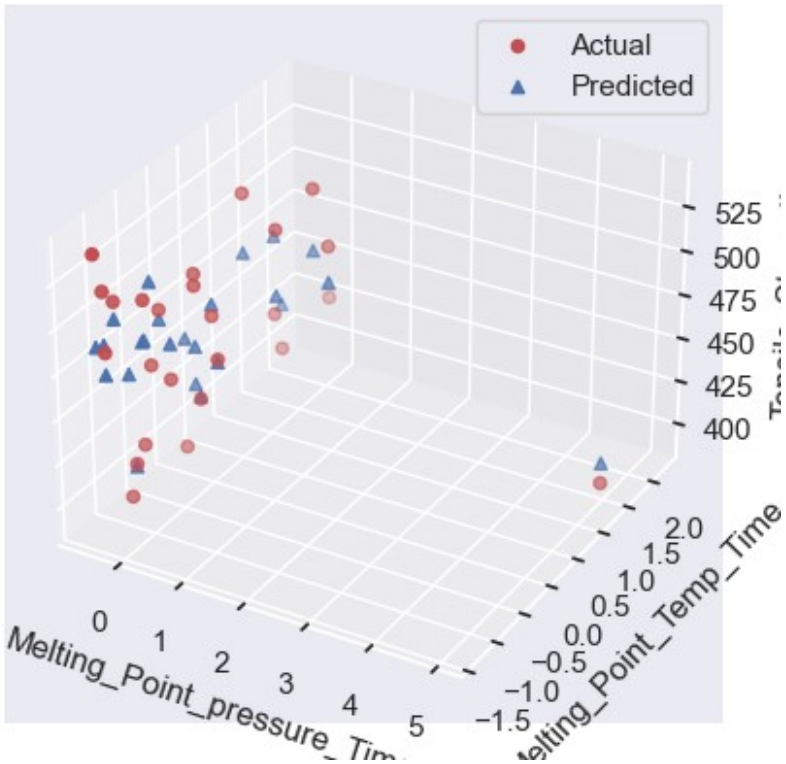
```
from statsmodels.sandbox.regression.predstd import wls_prediction_std
import statsmodels.api as sm
from statsmodels.formula.api import ols
from pyDOE2 import lhs

# Generate mixture design using Latin Hypercube Sampling
def generate_mixture_design(n_samples, n_factors):
    # Generate samples from a Latin Hypercube Sampling
```

```
    samples = lhs(n_factors, samples=n_samples, criterion='center')
    # Normalize the samples to make sure they sum to 1 (for mixture
design)
    samples /= samples.sum(axis=1, keepdims=True)
    return samples

df_mixture = Train_df.copy()

# Fit the mixture model using ordinary least squares (OLS)
model = ols('Tensile_Strength ~ Melting_Point_pressure_Time +
Melting_Point_Temp_Time + Density_Temp_Time', data=df_mixture).fit()

# Summary of the model
print(model.summary())

# Predicting and plotting the response surface
df_mixture['PredictedStrength'] = model.predict(df_mixture)

# Visualizing the response surface
from mpl_toolkits.mplot3d import Axes3D

fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.scatter(df_mixture['Melting_Point_pressure_Time'],
df_mixture['Melting_Point_Temp_Time'], df_mixture['Tensile_Strength'],
c='r', marker='o', label='Actual')
ax.scatter(df_mixture['Melting_Point_pressure_Time'],
df_mixture['Melting_Point_Temp_Time'],
df_mixture['PredictedStrength'], c='b', marker='^', label='Predicted')
ax.set_xlabel('Melting_Point_pressure_Time')
ax.set_ylabel('Melting_Point_Temp_Time')
ax.set_zlabel('Tensile_Strength')
plt.legend()
plt.show()

mae = np.mean(np.abs(df_mixture['Tensile_Strength'] -
df_mixture['PredictedStrength']))
print(f'Mean Absolute Error: {mae:.2f}')

# Predict on new data
new_data = X_Test.copy()

# Ensure the proportions sum to 1
new_data = new_data.apply(lambda row: row / row.sum(), axis=1)

# Predict tensile strength for the new formulations
new_data['PredictedStrength'] = model.predict(new_data)
print(new_data)

# Optional: plotting the response surface over a grid (useful for 2D
```

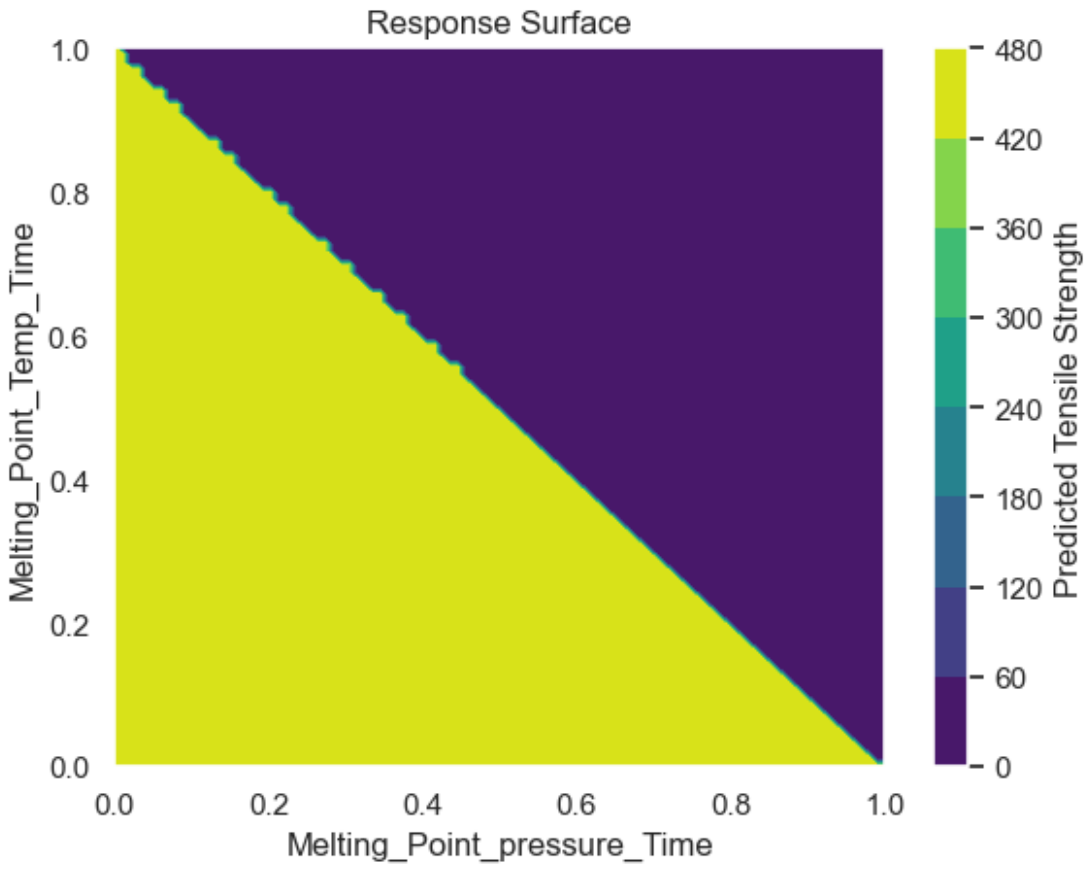
```
visualizations)
def plot_response_surface_2d(model, factor1, factor2, n_points=100):
    factor1_range = np.linspace(0, 1, n_points)
    factor2_range = np.linspace(0, 1, n_points)
    factor1_mesh, factor2_mesh = np.meshgrid(factor1_range,
factor2_range)

    response_values = np.zeros_like(factor1_mesh)

    for i in range(factor1_mesh.shape[0]):
        for j in range(factor1_mesh.shape[1]):
            # Proportions must sum to 1, so the third factor is 1 -
sum of the first two
            factor3_value = 1 - factor1_mesh[i, j] - factor2_mesh[i,
j]
            if factor3_value >= 0:
                response_values[i, j] = model.predict(pd.DataFrame({
                    factor1: [factor1_mesh[i, j]],
                    factor2: [factor2_mesh[i, j]],
                    'Density_Temp_Time': [factor3_value]
                }))[0]

    plt.contourf(factor1_mesh, factor2_mesh, response_values,
cmap='viridis')
    plt.colorbar(label='Predicted Tensile Strength')
    plt.xlabel(factor1)
    plt.ylabel(factor2)
    plt.title('Response Surface')
    plt.show()

# Plot response surface for the first two raw materials
plot_response_surface_2d(model, 'Melting_Point_pressure_Time',
'Melting_Point_Temp_Time')
```

```
                            OLS Regression Results

==============================================================================
========
Dep. Variable:       Tensile_Strength   R-squared:
0.322
Model:                             OLS   Adj. R-squared:
0.226
Method:                  Least Squares   F-statistic:
3.331
Date:                 Sun, 19 May 2024   Prob (F-statistic):
0.0392
Time:                         21:42:02   Log-Likelihood:
-124.78
No. Observations:                   25   AIC:
257.6
```

```
Df Residuals:                          21   BIC:
262.4
Df Model:                               3

Covariance Type:            nonrobust

==============================================================================
==========================
                                   coef    std err          t      P>|
t|      [0.025      0.975]
------------------------------------------------------------------------------
-------------------------
Intercept                       468.0242      7.808     59.943
0.000     451.787     484.261
Melting_Point_pressure_Time     -17.8706      8.384     -2.132
0.045     -35.306      -0.435
Melting_Point_Temp_Time          -2.7013      8.347     -0.324
0.749     -20.060      14.657
Density_Temp_Time               -20.4166      7.984     -2.557
0.018     -37.020      -3.814
==============================================================================
========
Omnibus:                        1.171   Durbin-Watson:
1.678
Prob(Omnibus):                  0.557   Jarque-Bera (JB):
1.088
Skew:                          -0.368   Prob(JB):
0.580
Kurtosis:                       2.291   Cond. No.
1.72
==============================================================================
========

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is
correctly specified.
```




```
Mean Absolute Error: 28.72
                Melting_Point_pressure_Time
Melting_Point_Temp_Time  \
Formulation_ID

F26                                0.171766                  1.233060

F27                                1.112987                  0.628941

F28                               -0.564432                  0.230688

F29                                0.228313                  0.368507

F30                                0.151898                  0.430195


                Density_Temp_Time  PredictedStrength
Formulation_ID
F26                     -0.404825         469.888960
F27                     -0.741928         461.583185
F28                      1.333744         450.257286
F29                      0.403180         454.717131
F30                      0.417907         455.615397
```



Conclusions and Recommendations for DOE

- The model shows that `Melting_Point_pressure_Time` and `Density_Temp_Time` are significant predictors of tensile strength, both having a negative impact.
- `Melting_Point_Temp_Time` does not significantly affect tensile strength, and it might be considered for removal in future model iterations to simplify the model.
- The R-squared value indicates a modest fit, suggesting that there may be other important predictors not included in the model. Further feature engineering or the inclusion of additional variables may improve the model's performance.
- Given the limited number of observations (25), the model may benefit from additional data to provide more robust estimates and improve generalizability.
- Consider cross-validation or bootstrapping techniques to validate the stability of the model with the current dataset size.
- The CatBoost Regressor achieved better metrics (MAE: 18.245115, MSE: 491.400013, RMSE: 22.167544, MAPE: 3.746112, R^2: 0.555501). However, due to the low number of samples, we should be cautious about these results. Only with more data can we validate the model's performance and reliability.

In summary, while the model has identified significant predictors of tensile strength, its explanatory power is limited, and further refinement and additional data collection are recommended to improve the model's performance.

Productization Proposal Design

Overview

This proposal outlines a theoretical design for a product that guides researchers in optimizing tensile strength through user-friendly interfaces and real-time data analysis.

Key Components

1. **Dashboard**
   - **Features**: Key metrics, recent experiments, material performance overview.
   - **UI Elements**: Summary tiles, recent activity feed, performance charts.
2. **Data Input Forms**
   - **Features**: Input for raw material properties, processing parameters, experimental results.
   - **UI Elements**: Dropdown menus, text fields, file upload options.
3. **Visualization Tools**
   - **Features**: Visual representation of data relationships.
   - **UI Elements**: Interactive graphs, charts, heatmaps.
4. **Recommendation Engine**
   - **Features**: Suggests new experiments based on data.
   - **UI Elements**: Suggestion box, actionable insights.
5. **Real-Time Analytics**
   - **Features**: Processes data in real-time, provides immediate feedback.
   - **UI Elements**: Live data feed, instant analysis results.
6. **Data Engineering Pipeline (Data as a Service - DaaS)**
   - **Features**: Ensures seamless data flow and transformation, integrates with various data sources and sinks.
   - **Components**: Data ingestion, data processing, data storage, and data delivery mechanisms.

Data Flow Diagram

1. **API Integration**:
   - **Purpose**: Connects to external databases, research tools, and laboratory equipment.
   - **Function**: Ensures seamless data exchange and real-time updates.
2. **User Interface**:

- **Purpose**: Collects input data from researchers and displays analyzed results.
- **Function**: Facilitates easy interaction and visualization.

3. **Data Input/Output**:
   - **Purpose**: Allows for easy input of experimental data, material properties, and processing parameters.
   - **Function**: Outputs visualizations and experiment recommendations.
4. **Data Engineering Pipeline (DaaS)**:
   - **Purpose**: Manages data ingestion, processing, storage, and delivery.
   - **Function**: Ensures efficient data flow and transformation, supports real-time interaction and analysis.
5. **Real-Time Interaction**:
   - **Purpose**: Processes and analyzes data in real-time.
   - **Function**: Provides immediate feedback and adjusts recommendations based on new data.

Mockup (Wireframe Example)

```plaintext
+-----------------------------------------------------------+
| Dashboard |
|-----------------------------------------------------------|
| Key Metrics | Recent Experiments | Material Overview |
|-----------------------------------------------------------|
| Metric 1 | Experiment 1 | Performance Chart |
| Metric 2 | Experiment 2 | |
|-----------------------------------------------------------|
| Data Input Forms |
|-----------------------------------------------------------|
| Raw Material Properties | |
| [Dropdown | Text Field | Upload] | |
|-----------------------------------------------------------|
| Processing Parameters | |
| [Dropdown | Text Field | Upload] |
|-----------------------------------------------------------|
| Visualization Tools |
|-----------------------------------------------------------|
| [Interactive Graph | Chart | Heatmap] | |
|-----------------------------------------------------------|
| Recommendation Engine | |
|-----------------------------------------------------------|
| Suggestions: | |
| 1. Adjust material composition |
| 2. Change processing temperature |
|-----------------------------------------------------------|
| Real-Time Analytics |
|-----------------------------------------------------------|
| [Live Data Feed | Instant Analysis Results] |
+-----------------------------------------------------------+
| Data Engineering Pipeline (DaaS) |
|-----------------------------------------------------------|
| Data Ingestion | Data Processing | Data Storage | Data Delivery |
+-----------------------------------------------------------+
```

This theoretical design provides a comprehensive framework for productizing the tensile strength optimization capability.

By integrating APIs, designing an intuitive UI, implementing a robust data engineering pipeline, and supporting real-time interaction, this product can significantly enhance the research and development process, guiding researchers, accelerating experimentation, and improving material development.