Import Necessary Libraries

```
import pandas as pd
import numpy as np
```

11/22/24, 10:59 PM

import matplotlib.pyplot as plt

import seaborn as sns

from sklearn.model_selection import train_test_split from sklearn.preprocessing import StandardScaler

LOAD DATASET

dataset_path = '/content/COMP1801_Coursework_Dataset.csv' # Replace with actual path
df = pd.read_csv(dataset_path)

df.head()

n% Cobalt% Chromium% smal	l1D€
52 16.82 0.93	
38 6.14 4.26	
95 8.81 3.41	
33 16.86 2.78	
37 11.45 1.56	
11.	38 6.14 4.26 95 8.81 3.41 33 16.86 2.78

Next steps: Generate code with df

View recommended plots

New interactive sheet

df.info()
df.describe()

4

<</pre>
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1000 entries, 0 to 999
Data columns (total 16 columns):

Data	COTUMNIS (COCAT	TO COTUMNIS).		
#	Column	Non-Null Count	Dtype	
0	Lifespan	1000 non-null	float64	
1	partType	1000 non-null	object	
2	microstructure	1000 non-null	object	
3	coolingRate	1000 non-null	int64	
4	quenchTime	1000 non-null	float64	
5	forgeTime	1000 non-null	float64	
6	HeatTreatTime	1000 non-null	float64	
7	Nickel%	1000 non-null	float64	
8	Iron%	1000 non-null	float64	
9	Cobalt%	1000 non-null	float64	
10	Chromium%	1000 non-null	float64	
11	smallDefects	1000 non-null	int64	
12	largeDefects	1000 non-null	int64	
13	sliverDefects	1000 non-null	int64	
14	seedLocation	1000 non-null	object	
15	castType	1000 non-null	object	
dtypes: float64(8), int64(4), object(4)				
memory usage: 125 1+ KR				

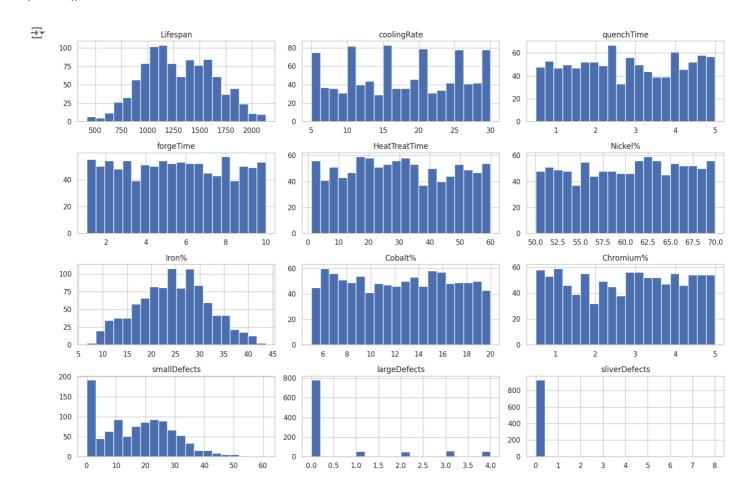
memory usage: 125.1+ KB

	Lifespan	coolingRate	quenchTime	forgeTime	HeatTreatTime	Nickel%	Iron%	Cobalt%	Chromium%	smallDefe
count	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000
mean	1298.556320	17.639000	2.764230	5.464600	30.194510	60.243080	24.553580	12.434690	2.768650	17.311
std	340.071434	7.491783	1.316979	2.604513	16.889415	5.790475	7.371737	4.333197	1.326496	12.268
min	417.990000	5.000000	0.500000	1.030000	1.030000	50.020000	6.660000	5.020000	0.510000	0.000
25%	1047.257500	11.000000	1.640000	3.170000	16.185000	55.287500	19.387500	8.597500	1.590000	7.000
50%	1266.040000	18.000000	2.755000	5.475000	29.365000	60.615000	24.690000	12.585000	2.865000	18.000
75%	1563.050000	24.000000	3.970000	7.740000	44.955000	65.220000	29.882500	16.080000	3.922500	26.000
max	2134.530000	30.000000	4.990000	10.000000	59.910000	69.950000	43.650000	19.990000	4.990000	61.000

print(df.columns)

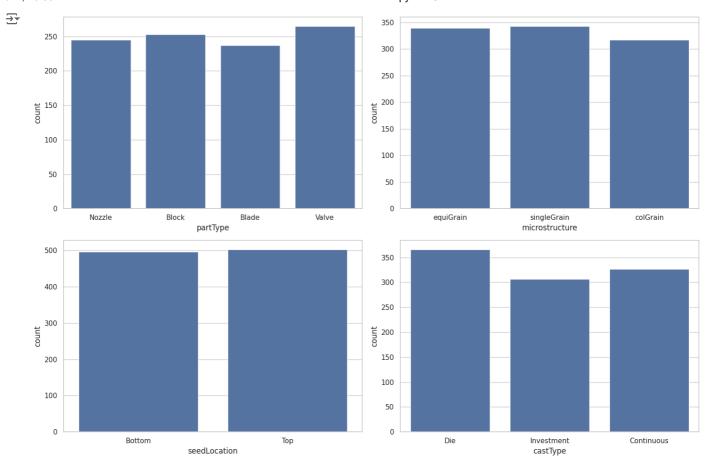
Data Exploration

```
#histograms for numerical columns
df.hist(figsize=(15, 10), bins=20)
plt.tight_layout()
plt.show()
```



```
# Import necessary visualization libraries
sns.set(style="whitegrid")

#categorical features
fig, axes = plt.subplots(2, 2, figsize=(15, 10))
sns.countplot(ax=axes[0, 0], x='partType', data=df)
sns.countplot(ax=axes[0, 1], x='microstructure', data=df)
sns.countplot(ax=axes[1, 0], x='seedLocation', data=df)
sns.countplot(ax=axes[1, 1], x='castType', data=df)
plt.tight_layout()
plt.show()
```



Preprocessing

```
from sklearn.preprocessing import LabelEncoder

# Creating copy of the original DataFrame to keep track of the original values
df_encoded = df.copy()

# Encoding categorical columns using LabelEncoder
label_encoders = {}
categorical_columns = ['partType', 'microstructure', 'seedLocation', 'castType']

for column in categorical_columns:
    le = LabelEncoder()
    df_encoded[column] = le.fit_transform(df_encoded[column])
    label_encoders[column] = le

# correlation heatmap including all columns
plt.figure(figsize=(12, 8))
sns.heatmap(df_encoded.corr(), annot=True, cmap='coolwarm')
plt.title('Correlation Heatmap')
plt.show()
```



```
Correlation Heatmap
                                                                                                                           1.0
                      Lifespan
                            0.0170.00480.032-0.0180.00840.0230.00550.0290.0360.00350.0180.0150.0029.011
     partType
               -0.075
                                                                                                                           0.8
                0.0160.017
                                  0.0001000940.0110.00410.0540.0150.0280.062-0.019<mark>-0.31 0.29</mark> -0.03-0.035
                0.0720.00480.000
                                        -0.0420.0140.00970.019.00910.0110.002<mark>80.81</mark> -0.030.043-0.0350.004
  coolingRate
                                                                                                                          - 0.6
                0.11 0.030.000940.042
                                              -0.0290.0070.0210.00230.0280.0150.0210.0160.0140.031-0.048
  quenchTime
                                                                                                                          - 0.4
                0.014-0.0180.0110.0140.029
                                                    0.0130.003<mark>60.033</mark>-0.0590.00940.01<del>7</del>0.00718.015-0.0590.031
    forgeTime
HeatTreatTime
                -0.110.0080.004-D.009-70.0070.013
                                                          0.0070.00410.02<mark>0.056</mark>-0.020.00920.0330.0870.023
                                                                                                                          - 0.2
      Nickel%
                0.32 0.023-0.0540.0190.0210.00360.007
                                                                -0.790.0016.00330.0350.022-0.0650.0220.0058
                -0.250.00550.0150.0090.00230.0330.004 -0.79
        Iron%
                                                                      -0.59 -0.19 0.024-0.01<del>6</del>0.057-0.0470.016
                                                                                                                          0.0
               -0.0360.0290.0280.011-0.0280.059-0.020.001<mark>6</mark>-0.59
                                                                        1
                                                                            0.0130.0160.00086.019<mark>0.055</mark>0.021
      Cobalt%
                0.075-0.0360.0620.00280.0150.009 D.0560.0033-0.19 0.013
                                                                                  0.0310.0060.03-0.0160.006
  Chromium%
                                                                                                                          -0.2
                 0.1-0.00350.019 0.81-0.0210.017-0.02-0.0350.0240.016-0.031
                                                                                        0.0450.0310.056-0.014
 smallDefects
 largeDefects -0.0520.018-0.31 -0.03-0.0160.0070300920.022-0.016.00086.0060.045
                                                                                               -0.12-0.029-0.03
                                                                                                                           -0.4
                -0.04-0.015<mark>0.29</mark> 0.0430.0140.015-0.0330.0650.057-0.0190.03 0.031-0.12
                                                                                                    0.0550.027
                                                                                                                           -0.6
 seedLocation 0.00480.00290.03-0.0350.031-0.0590.0870.022-0.0470.055-0.0160.056-0.0290.055
                                                                                                          -0.025
                -0.12\,0.011 -0.0350.004 -0.0480.0310.02 -0.0580.0160.021 -0.0060.014 -0.03 -0.0270.025
                                    coolingRate
                                         quenchTime
                                                            Nickel%
                                                                  Iron%
                                                                                          largeDefects
                                                                                                sliverDefects
                                                                                                      seedLocation
                              nicrostructure
                                                forgeTime
                                                      HeatTreatTime
                                                                                    smallDefects
                                                                              Chromium%
                                                                        Cobalt%
```

```
from sklearn.preprocessing import StandardScaler, OneHotEncoder
# Define categorical and numerical columns
categorical_cols = ['partType', 'microstructure', 'seedLocation', 'castType']
numerical_cols = ['coolingRate', 'quenchTime', 'forgeTime', 'HeatTreatTime',
                    'Nickel%', 'Iron%', 'Cobalt%', 'Chromium%'
                    'smallDefects', 'largeDefects', 'sliverDefects']
# ColumnTransformer to apply One-Hot Encoding and Scaling
preprocessor = ColumnTransformer(
    transformers=[
         ('num', StandardScaler(), numerical_cols),
         ('cat', OneHotEncoder(), categorical_cols)
)
# Fit and transform the data
X = df.drop(columns=['Lifespan'])
y = df['Lifespan']
X_processed = preprocessor.fit_transform(X)
import numpy as np
# Apply log transformation to skewed features
df['smallDefects'] = df['smallDefects'].apply(lambda x: np.log1p(x))
df['largeDefects'] = df['largeDefects'].apply(lambda x: np.log1p(x))
df['sliverDefects'] = df['sliverDefects'].apply(lambda x: np.log1p(x))
```

Splitting Train, Test and Validation set

from sklearn.compose import ColumnTransformer

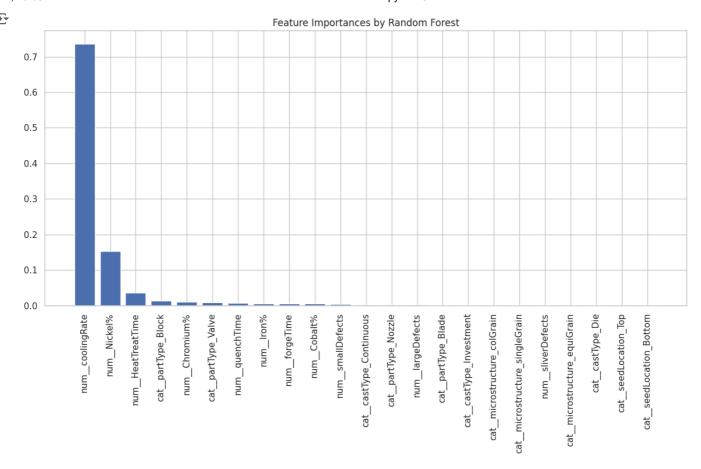
```
from sklearn.model_selection import train_test_split
# Split into train, validation, and test sets
```

X_train, X_temp, y_train, y_temp = train_test_split(X_processed, y, test_size=0.3, random_state=42)
X_val, X_test, y_val, y_test = train_test_split(X_temp, y_temp, test_size=0.5, random_state=42)

Model Building

```
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_score
# Train Linear Regression
lr_model = LinearRegression()
lr_model.fit(X_train, y_train)
# Predict on validation set
y_pred_val = lr_model.predict(X_val)
# Evaluate Linear Regression
rmse = np.sqrt(mean_squared_error(y_val, y_pred_val))
mae = mean_absolute_error(y_val, y_pred_val)
r2 = r2_score(y_val, y_pred_val)
print(f"Linear Regression - RMSE: {rmse}, MAE: {mae}, R<sup>2</sup>: {r2}")
→ Linear Regression - RMSE: 309.8211602317268, MAE: 263.239, R<sup>2</sup>: 0.17724324985936646
from sklearn.neural_network import MLPRegressor
# Train Neural Network
nn_model = MLPRegressor(hidden_layer_sizes=(64, 32), max_iter=1000, random_state=42)
nn_model.fit(X_train, y_train)
# Predict on validation set
y_pred_nn_val = nn_model.predict(X_val)
# Evaluate Neural Network
rmse_nn = np.sqrt(mean_squared_error(y_val, y_pred_nn_val))
mae_nn = mean_absolute_error(y_val, y_pred_nn_val)
r2_nn = r2_score(y_val, y_pred_nn_val)
print(f"Neural Network - RMSE: {rmse_nn}, MAE: {mae_nn}, R<sup>2</sup>: {r2_nn}")
Neural Network - RMSE: 312.2623518916146, MAE: 266.1946163482815, R<sup>2</sup>: 0.1642265805847657
# Predict on the test set using Linear Regression
y_pred_test_lr = lr_model.predict(X_test)
# Evaluate Linear Regression on the test set
rmse_test_lr = np.sqrt(mean_squared_error(y_test, y_pred_test_lr))
\label{eq:mae_test_lr} \verb| mae_test_lr = mean_absolute_error(y_test, y_pred_test_lr)| \\
r2_test_lr = r2_score(y_test, y_pred_test_lr)
print(f"Linear Regression - Test Set Evaluation: RMSE: \{rmse\_test\_lr\}, \ MAE: \{mae\_test\_lr\}, \ R^2: \{r^2\_test\_lr\}")
Fy Linear Regression - Test Set Evaluation: RMSE: 308.256251078006, MAE: 260.2119333333333, R<sup>2</sup>: 0.08548455298785684
from sklearn.ensemble import RandomForestRegressor
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_score
import numpy as np
# Train Random Forest Regressor
rf_model = RandomForestRegressor(n_estimators=100, random_state=42)
rf_model.fit(X_train, y_train)
# Predict on the validation set
y_pred_val_rf = rf_model.predict(X_val)
# Evaluate on the validation set
rmse_val_rf = np.sqrt(mean_squared_error(y_val, y_pred_val_rf))
mae_val_rf = mean_absolute_error(y_val, y_pred_val_rf)
r2_val_rf = r2_score(y_val, y_pred_val_rf)
print(f"Random Forest - Validation Set Evaluation: RMSE: {rmse_val_rf}, MAE: {mae_val_rf}, R<sup>2</sup>: {r<sup>2</sup>_val_rf}")
```

```
🔂 Random Forest - Validation Set Evaluation: RMSE: 79.84928373575096, MAE: 62.17729933333326, R²: 0.9453498508341751
# Predict on the test set using Random Forest
y_pred_test_rf = rf_model.predict(X_test)
# Evaluate Random Forest on the test set
rmse_test_rf = np.sqrt(mean_squared_error(y_test, y_pred_test_rf))
mae_test_rf = mean_absolute_error(y_test, y_pred_test_rf)
r2_test_rf = r2_score(y_test, y_pred_test_rf)
print(f"Random Forest - Test Set Evaluation: RMSE: {rmse_test_rf}, MAE: {mae_test_rf}, R<sup>2</sup>: {r2_test_rf}")
Random Forest - Test Set Evaluation: RMSE: 98.14016059182661, MAE: 76.21511799999993, R<sup>2</sup>: 0.9073040436541067
Hyper Parameter tuning Of Random Forest Refressor
from sklearn.model_selection import RandomizedSearchCV
# Define the parameter grid for Random Forest
param_grid = {
    'n_estimators': [100, 200, 300, 400],
    'max_depth': [10, 20, 30, None],
    'min_samples_split': [2, 5, 10],
    'min_samples_leaf': [1, 2, 4]
# Randomized Search with Cross-Validation
rf_random_search = RandomizedSearchCV(estimator=rf_model, param_distributions=param_grid,
                                      n_iter=20, cv=3, verbose=2, random_state=42, n_jobs=-1)
rf_random_search.fit(X_train, y_train)
# Best parameters from the random search
best_params = rf_random_search.best_params
print(f"Best Hyperparameters: {best params}")
# Use the best model found to evaluate on the test set
best_rf_model = rf_random_search.best_estimator_
y_pred_best_rf = best_rf_model.predict(X_test)
# Evaluate on the test set with the tuned model
rmse_best_rf = np.sqrt(mean_squared_error(y_test, y_pred_best_rf))
mae_best_rf = mean_absolute_error(y_test, y_pred_best_rf)
r2_best_rf = r2_score(y_test, y_pred_best_rf)
print(f"Tuned Random Forest - Test Set Evaluation: RMSE: {rmse_best_rf}, MAE: {mae_best_rf}, R<sup>2</sup>: {r2_best_rf}")
Fitting 3 folds for each of 20 candidates, totalling 60 fits
     Best Hyperparameters: {'n_estimators': 400, 'min_samples_split': 2, 'min_samples_leaf': 2, 'max_depth': 20}
     Tuned Random Forest - Test Set Evaluation: RMSE: 96.57878798902732, MAE: 74.57360168299249, R<sup>2</sup>: 0.9102300955960292
import matplotlib.pyplot as plt
importances = rf_model.feature_importances_
# Sort feature importance in descending order
indices = np.argsort(importances)[::-1]
feature_names = preprocessor.get_feature_names_out()
# Plot feature importance
plt.figure(figsize=(12, 8))
plt.title("Feature Importances by Random Forest")
plt.bar(range(len(importances)), importances[indices], align='center')
plt.xticks(range(len(importances)), [feature_names[i] for i in indices], rotation=90)
plt.tight_layout()
plt.show()
```



```
from sklearn.neural_network import MLPRegressor
from \ sklearn.metrics \ import \ mean\_squared\_error, \ mean\_absolute\_error, \ r2\_score
# Define the MLP Regressor
mlp_model = MLPRegressor(hidden_layer_sizes=(100, 50, 25), max_iter=5000, random_state=42)
# Fit the model to the training data
mlp_model.fit(X_train, y_train)
# Predict on validation set
y_pred_val_mlp = mlp_model.predict(X_val)
# Evaluate on the validation set
rmse_val_mlp = np.sqrt(mean_squared_error(y_val, y_pred_val_mlp))
mae_val_mlp = mean_absolute_error(y_val, y_pred_val_mlp)
r2_val_mlp = r2_score(y_val, y_pred_val_mlp)
print(f"MLP\ Regressor\ -\ Validation\ Set\ Evaluation:\ RMSE:\ \{rmse\_val\_mlp\},\ MAE:\ \{mae\_val\_mlp\},\ R^2:\ \{r2\_val\_mlp\}")
# Predict on test set
y_pred_test_mlp = mlp_model.predict(X_test)
# Evaluate on the test set
rmse_test_mlp = np.sqrt(mean_squared_error(y_test, y_pred_test_mlp))
mae_test_mlp = mean_absolute_error(y_test, y_pred_test_mlp)
r2_test_mlp = r2_score(y_test, y_pred_test_mlp)
print(f"MLP \ Regressor - Test \ Set \ Evaluation: \ RMSE: \{rmse\_test\_mlp\}, \ MAE: \{mae\_test\_mlp\}, \ R^2: \{r2\_test\_mlp\}"\}
    MLP Regressor - Validation Set Evaluation: RMSE: 155.9452112561726, MAE: 123.82929935698189, R<sup>2</sup>: 0.7915540851424223
     MLP Regressor - Test Set Evaluation: RMSE: 148.62509365702562, MAE: 121.86125532968974, R2: 0.7874057356254277
pip install shap
Requirement already satisfied: shap in /usr/local/lib/python3.10/dist-packages (0.46.0)
     Requirement already satisfied: numpy in /usr/local/lib/python3.10/dist-packages (from shap) (1.26.4)
     Requirement already satisfied: scipy in /usr/local/lib/python3.10/dist-packages (from shap) (1.13.1)
     Requirement already satisfied: scikit-learn in /usr/local/lib/python3.10/dist-packages (from shap) (1.5.2)
     Requirement already satisfied: pandas in /usr/local/lib/python3.10/dist-packages (from shap) (2.2.2)
```

```
Requirement already satisfied: tqdm>=4.27.0 in /usr/local/lib/python3.10/dist-packages (from shap) (4.66.6)
Requirement already satisfied: packaging>20.9 in /usr/local/lib/python3.10/dist-packages (from shap) (24.2)
Requirement already satisfied: slicer==0.0.8 in /usr/local/lib/python3.10/dist-packages (from shap) (0.0.8)
Requirement already satisfied: numba in /usr/local/lib/python3.10/dist-packages (from shap) (0.60.0)
Requirement already satisfied: cloudpickle in /usr/local/lib/python3.10/dist-packages (from shap) (3.1.0)
Requirement already satisfied: llvmlite<0.44,>=0.43.0dev0 in /usr/local/lib/python3.10/dist-packages (from numba->shap) (0.43.0)
Requirement already satisfied: python-dateutil>=2.8.2 in /usr/local/lib/python3.10/dist-packages (from pandas->shap) (2.8.2)
Requirement already satisfied: pytz>=2020.1 in /usr/local/lib/python3.10/dist-packages (from pandas->shap) (2024.2)
Requirement already satisfied: tzdata>=2022.7 in /usr/local/lib/python3.10/dist-packages (from scikit-learn->shap) (1.4.2)
Requirement already satisfied: joblib>=1.2.0 in /usr/local/lib/python3.10/dist-packages (from scikit-learn->shap) (3.5.0)
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.10/dist-packages (from python-dateutil>=2.8.2->pandas->shap) (1.16
```

Shap For Feature Importance of Neural network

```
import shap
import numpy as np

# Take a small sample of the training set for SHAP calculations to keep it feasible
X_sample = shap.sample(X_train, 100)  # Randomly sample 100 instances from X_train

# Create a KernelExplainer for the MLP Regressor
explainer = shap.KernelExplainer(mlp_model.predict, X_sample)

# Calculate SHAP values for a subset of the test set (to save on computation time)
X_test_sample = shap.sample(X_test, 50)  # Use a smaller sample from X_test
shap_values = explainer.shap_values(X_test_sample)

# Plot the summary of feature importance using SHAP values
shap.summary_plot(shap_values, X_test_sample, feature_names=preprocessor.get_feature_names_out())
```

₹ 100%

```
50/50 [01:50<00:00, 1.60s/it]
                                                                            High
             num_coolingRate
     cat seedLocation Bottom
     cat castType Continuous
           cat__partType_Block
         cat_seedLocation_Top
 cat__microstructure_equiGrain
cat_microstructure_singleGrain
             cat_castType_Die
     cat__castType_Investment
                                                                                Feature value
          cat__partType_Nozzle
  cat__microstructure_colGrain
           cat partType Blade
           cat__partType_Valve
                 num Nickel%
          num__HeatTreatTime
                   num__Iron%
                num__Cobalt%
             num quenchTime
            num largeDefects
            num_smallDefects
                                                                            Low
                                    -400
                                             -200
                                                             200
                                                                      400
                                   SHAP value (impact on model output)
```

```
import numpy as np
import pandas as pd
from sklearn.compose import ColumnTransformer
from \ sklearn.preprocessing \ import \ One HotEncoder, \ Standard Scaler
from sklearn.pipeline import Pipeline
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.neural_network import MLPRegressor
# Assuming df is your original dataset
X = df.drop(columns=['Lifespan'])
y = df['Lifespan']
\# Split the data into train, validation, and test sets (70/15/15 split)
X_train_full, X_test, y_train_full, y_test = train_test_split(X, y, test_size=0.15, random_state=42)
 X\_{train}, \ X\_{val}, \ y\_{train}, \ y\_{val} = train\_{test\_split} (X\_{train\_full}, \ y\_{train\_full}, \ test\_{size=0.1765}, \ random\_{state=42}) \\ \ \# \ 15\% \ of \ the \ 85\% \ train\_{train\_full}, \ y\_{train\_full}, \ y\_{train\_f
# Identifying categorical and numerical features
categorical_features = X.select_dtypes(include=['object', 'category']).columns
numerical_features = X.select_dtypes(include=['int64', 'float64']).columns
# Preprocessing for numerical and categorical features
preprocessor = ColumnTransformer(
           transformers=[
                       ('num', StandardScaler(), numerical_features),
                       ('cat', OneHotEncoder(), categorical_features)
)
\# Define the pipeline for the entire process
```

```
11/22/24, 10:59 PM
                                                                            task 1.ipynb - Colab
    pipeline = Pipeline(steps=[
        ('preprocessor', preprocessor),
        ('regressor', MLPRegressor(max_iter=3000, random_state=42))
    # Fit the preprocessor to the training data (transformations only)
    pipeline.fit(X_train, y_train)
    /usr/local/lib/python3.10/dist-packages/sklearn/neural_network/_multilayer_perceptron.py:690: ConvergenceWarning: Stochastic Optimia
           warnings.warn(
                                                            (i) (?
                                Pipeline
                     preprocessor: ColumnTransformer
                        num
                                                 cat
                  StandardScaler ?
                                         ▶ OneHotEncoder
                             MLPRegressor
    # Simplified hyperparameter grid
    param_grid = {
        'regressor__hidden_layer_sizes': [(50, 25), (100, 50)],
        'regressor__activation': ['relu'],
        'regressor__solver': ['adam'],
        'regressor__learning_rate': ['constant', 'adaptive'],
        'regressor__alpha': [0.0001, 0.001]
    Final Model of Task 1
    from sklearn.model_selection import RandomizedSearchCV
    # Randomized Search with a smaller number of iterations
    random_search = RandomizedSearchCV(
        estimator=pipeline.
        param_distributions=param_grid,
        n_iter=10, # Number of combinations to try
        cv=3.
        verbose=2,
        random state=42,
        n_jobs=-1
    # Fit the Randomized Search to the training data
    random_search.fit(X_train, y_train)
    # Get the best parameters from Random Search
    best params = random search.best params
    print(f"Best Parameters for Neural Network: {best_params}")
    # Use the best model to evaluate on the test set
    best_mlp_model = random_search.best_estimator_
    y_pred_test = best_mlp_model.predict(X_test)
    # Evaluate the tuned model on the test set
    rmse_test = np.sqrt(mean_squared_error(y_test, y_pred_test))
    mae_test = mean_absolute_error(y_test, y_pred_test)
    r2_test = r2_score(y_test, y_pred_test)
    print(f"Tuned \ Neural \ Network - Test \ Set \ Evaluation: \ RMSE: \{rmse\_test\}, \ MAE: \{mae\_test\}, \ R^2: \ \{r^2\_test\}")
    yusr/local/lib/python3.10/dist-packages/sklearn/model_selection/_search.py:320: UserWarning: The total space of parameters 8 is smal
           warnings.warn(
         Fitting 3 folds for each of 8 candidates, totalling 24 fits
```

Best Parameters for Neural Network: {'regressor__solver': 'adam', 'regressor__learning_rate': 'constant', 'regressor__hidden_layer_!

Tuned Neural Network - Test Set Evaluation: RMSE: 138.82320035823295, MAE: 108.10586101367554, R²: 0.8203236649837323

TASK 2

4

```
#Import Libraries
import pandas as pd
```

```
from sklearn.preprocessing import StandardScaler, OneHotEncoder
from sklearn.cluster import KMeans
from sklearn.model_selection import train_test_split, GridSearchCV, cross_val_score
from sklearn.compose import ColumnTransformer
from sklearn.pipeline import Pipeline
from sklearn.ensemble import RandomForestClassifier
from sklearn.neural_network import MLPClassifier
from sklearn.metrics import accuracy_score, classification_report, confusion_matrix
from sklearn.utils import shuffle
from imblearn.over_sampling import SMOTE
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns

#Load the Dataset
df = pd.read_csv('/content/COMP1801_Coursework_Dataset.csv')
```

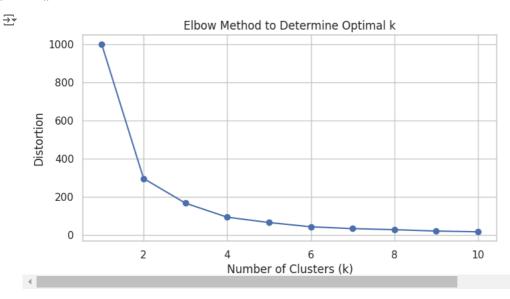
Scaling

```
# Normalizing the Lifespan feature to ensure K-Means is not affected by scale
scaler = StandardScaler()
df['normalized_Lifespan'] = scaler.fit_transform(df[['Lifespan']])
```

Clustering for Multi class Using Elbow Method

```
# Determine the Optimal Number of Clusters using the Elbow Method
# Use the Elbow Method to determine the optimal number of clusters
distortions = []
K = range(1, 11)
for k in K:
    kmeans = KMeans(n_clusters=k, random_state=42)
    kmeans.fit(df[['normalized_Lifespan']])
    distortions.append(kmeans.inertia_)

# Plot the Elbow Graph
plt.figure(figsize=(8, 4))
plt.plot(K, distortions, 'bo-')
plt.xlabel('Number of Clusters (k)')
plt.ylabel('Distortion')
plt.title('Elbow Method to Determine Optimal k')
plt.show()
```



```
optimal_k = 3  # Update this based on the Elbow graph
kmeans = KMeans(n_clusters=optimal_k, random_state=42)
df['Lifespan_group'] = kmeans.fit_predict(df[['normalized_Lifespan']])

# Assign 'Low', 'Medium', 'High' labels based on the cluster centers
cluster_centers = kmeans.cluster_centers_.flatten()
sorted_indices = cluster_centers.argsort()
lifespan_group_mapping = {sorted_indices[0]: 'Low', sorted_indices[1]: 'Medium', sorted_indices[2]: 'High'}
df['Lifespan_group'] = df['Lifespan_group'].map(lifespan_group_mapping)
```

```
df_with_lifespan = pd.read_csv('/content/COMP1801_Coursework_Dataset.csv')
df with lifespan['Lifespan group'] = kmeans.fit predict(scaler.fit transform(df with lifespan[['Lifespan']]))
df_with_lifespan['Lifespan_group'] = df_with_lifespan['Lifespan_group'].map(lifespan_group_mapping)
# Calculate min and max for each lifespan group
min_max_per_group = df_with_lifespan.groupby('Lifespan_group')['Lifespan'].agg(['min', 'max'])
print("\nMinimum and Maximum Lifespan for Each Class:")
print(min_max_per_group)
min_max_per_group.plot(kind='bar', figsize=(10, 6))
plt.xlabel('Lifespan Group')
plt.ylabel('Lifespan (Hours)')
plt.title('Minimum and Maximum Lifespan for Each Class')
plt.xticks(rotation=0)
plt.show()
     Minimum and Maximum Lifespan for Each Class:
                         min
                                  max
     Lifespan_group
                     1483.73 2134.53
     High
     Low
                      417.99 1085.01
     Medium
                     1085.23 1480.43
```

Minimum and Maximum Lifespan for Each Class min max 2000 1750 1500 Lifespan (Hours) 1250 1000 750 500 250 0 High Low Medium Lifespan Group

```
# Drop the Original Lifespan Feature to Avoid Data Leakage
# Drop the 'Lifespan' and 'normalized_Lifespan' columns now that clustering is complete
df = df.drop(columns=['Lifespan', 'normalized_Lifespan'])
# Split the Dataset into Training, Validation, and Test Sets (70/15/15 Split)
# Define features (X) and labels (y)
X = df.drop(columns=['Lifespan_group'])
y = df['Lifespan_group']
# Shuffle the dataset to ensure randomness
X, y = shuffle(X, y, random_state=42)
# Split the dataset into training, validation, and test sets
X_train, X_temp, y_train, y_temp = train_test_split(X, y, test_size=0.3, stratify=y, random_state=42)
X\_val, \ X\_test, \ y\_val, \ y\_test = train\_test\_split(X\_temp, \ y\_temp, \ test\_size=0.5, \ stratify=y\_temp, \ random\_state=42)
# Preprocessing - Feature Encoding and Scaling
# Identifying categorical and numerical features
categorical_features = [col for col in X.columns if df[col].dtype == 'object']
numerical_features = [col for col in X.columns if df[col].dtype != 'object']
# Preprocessing for numerical and categorical features
numerical_transformer = StandardScaler()
categorical_transformer = OneHotEncoder(handle_unknown='ignore')
# Combine transformers using ColumnTransformer
preprocessor = ColumnTransformer(
    transformers=[
```

```
('num', numerical_transformer, numerical_features),
        ('cat', categorical_transformer, categorical_features)
# Fit the preprocessor on the training data and transform training data
X_train = preprocessor.fit_transform(X_train)
# Applying SMOTE to Address Class Imbalance on Training Set Only
smote = SMOTE(random_state=42)
X_train, y_train = smote.fit_resample(X_train, y_train)
# Transform validation and test sets using the already fitted preprocessor
X val = preprocessor.transform(X val)
X_test = preprocessor.transform(X_test)
# Create Pipelines for Random Forest and Neural Network
# Random Forest Pipeline
rf_model = RandomForestClassifier(random_state=42, max_depth=10)
# Neural Network Pipeline
nn_model = MLPClassifier(max_iter=500, random_state=42, early_stopping=True)
# Train and Evaluate Random Forest Model
rf_model.fit(X_train, y_train)
# Evaluate the Random Forest Model on Validation Set
y_pred_rf_val = rf_model.predict(X_val)
print("\nValidation Set Evaluation - Random Forest Model:")
print(f"Accuracy: {accuracy_score(y_val, y_pred_rf_val):.4f}")
print("Classification Report:")
print(classification_report(y_val, y_pred_rf_val))
# Predict on the test set
y_pred_rf = rf_model.predict(X_test)
# Evaluate the Random Forest model
print("\nTest Set Evaluation - Random Forest Model:")
print(f"Accuracy: {accuracy_score(y_test, y_pred_rf):.4f}")
print("Classification Report:")
print(classification_report(y_test, y_pred_rf))
# Confusion matrix for Random Forest
conf_matrix_rf = confusion_matrix(y_test, y_pred_rf, labels=['Low', 'Medium', 'High'])
sns.heatmap(conf_matrix_rf, annot=True, cmap="Blues", fmt='g', xticklabels=['Low', 'Medium', 'High'], yticklabels=['Low', 'Medium', 'High']
plt.xlabel('Predicted')
plt.ylabel('Actual')
plt.title('Confusion Matrix - Random Forest Model')
plt.show()
# Feature Importance for Random Forest
feature\_names = numerical\_features + list(preprocessor.named\_transformers\_['cat'].get\_feature\_names\_out(categorical\_features))
feature_importances = rf_model.feature_importances_
feature importance df = pd.DataFrame({'Feature': feature names, 'Importance': feature importances})
feature_importance_df = feature_importance_df.sort_values(by='Importance', ascending=False)
print("\nFeature Importance - Random Forest:")
print(feature_importance_df)
```



Validation Set Evaluation - Random Forest Model: Accuracy: 0.7267

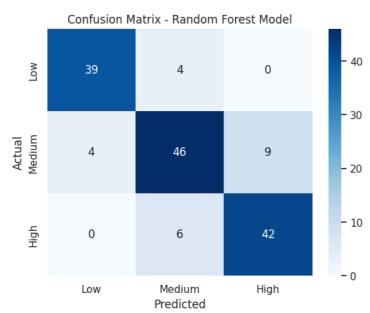
Classification	Report:
	precisio

010331.100010	precision	recall	f1-score	support
High	0.72	0.81	0.76	47
Low	0.80	0.80	0.80	44
Medium	0.68	0.61	0.64	59
accuracy			0.73	150
macro avg	0.73	0.74	0.73	150
weighted avg	0.73	0.73	0.72	150

Test Set Evaluation - Random Forest Model:

Accuracy: 0.8467 Classification Report:

Classificatio	precision	recall	f1-score	support
High	0.82	0.88	0.85	48
Low	0.91	0.91	0.91	43
Medium	0.82	0.78	0.80	59
accuracy			0.85	150
macro avg	0.85	0.85	0.85	150
weighted avg	0.85	0.85	0.85	150



Feature Importance - Random Forest:

	Feature	Importance
0	coolingRate	0.240113
8	smallDefects	0.113303
4	Nickel%	0.098745
5	Iron%	0.067173
7	Chromium%	0.066397
3	HeatTreatTime	0.063345
1	quenchTime	0.063331
6	Cobalt%	0.055193
2	forgeTime	0.049813
14	partType_Valve	0.026168
20	castType_Continuous	0.017395
9	largeDefects	0.017289
12	partType_Block	0.016060
22	castType_Investment	0.012381
21	castType_Die	0.012258
16	microstructure_equiGrain	0.012077
19	seedLocation_Top	0.012029
15	microstructure_colGrain	0.011609
18	seedLocation_Bottom	0.009852
11	partType_Blade	0.009513
13	partType_Nozzle	0.009333
17	microstructure_singleGrain	0.009108
10	sliverDefects	0.007516

[#] Hyperparameter Tuning for Neural Network

[#] Set up hyperparameter grid for tuning the Neural Network param_grid = {

^{&#}x27;hidden_layer_sizes': [(50,), (100, 50), (150, 100, 50)], 'activation': ['relu', 'tanh'],

^{&#}x27;learning_rate': ['constant', 'adaptive'],