Executive Summary

This project builds a complete machine-learning pipeline to predict the lifespan of alloy components and to segment parts into actionable quality tiers. After data cleaning and exploratory analysis, regression models accurately estimated continuous lifespan, while classification models (binary and multi-class) provided operationally useful groupings. Two multi-class strategies—quantile (33/33/33) and K-Means (k=3)—were evaluated across RandomForest, XGBoost, and CatBoost, with hyperparameter tuning and robust cross-validation. The best performer was the tuned CatBoost model with K-Means labels, achieving near-perfect macro-AUC and excellent macro-F1 and κ. Feature-importance and SHAP analyses highlighted Cooling Rate, Forge Time, Nickel%, and defect indicators as key drivers of part longevity.

Dataset Loading and Initial Exploration

This notebook loads the `COMP1801_Coursework_Dataset_Corrected.csv` dataset and performs an initial exploration to understand its structure, data types, and basic statistics.

```
# ============================================================
# STEP 1 (Corrected): Load & Inspect Dataset – Robust Version
# ============================================================

import os
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from IPython.display import display

# Settings
sns.set(style="whitegrid")
plt.rcParams["figure.figsize"] = (9,5)
pd.set_option("display.max_columns", None)
seed = 42
np.random.seed(seed)

# ---------- 1) Load dataset ----------
DATA_PATH = "/content/COMP1801_Coursework_Dataset_Corrected.csv"  # change if needed

if not os.path.exists(DATA_PATH):
    # interactive upload (Colab)
    print(f"File not found at {DATA_PATH}. Please upload the CSV file now.")
    try:
        from google.colab import files
        uploaded = files.upload()
        if uploaded:
            DATA_PATH = list(uploaded.keys())[0]
            print("Using uploaded file:", DATA_PATH)
        else:
            raise FileNotFoundError("No file uploaded.")
    except Exception:
        raise FileNotFoundError(f"Dataset not found at {DATA_PATH} and interactive upload failed.")

# read CSV
df = pd.read_csv(DATA_PATH)
print("✅ Dataset loaded:", DATA_PATH)
print(f"Shape: {df.shape[0]} rows × {df.shape[1]} columns\n")

# ---------- 2) Basic structure ----------
print("--- Column data types ---")
display(df.dtypes)
print("\n--- First 5 rows ---")
display(df.head())

# ---------- 3) Missing values and duplicates ----------
missing = df.isna().sum()
print("\n--- Missing values (per column) ---")
if missing.sum() == 0:
    print("No missing values ✅")
else:
    display(missing[missing > 0])

dups = df.duplicated().sum()
print(f"\nDuplicate rows count: {dups}")

# ---------- 4) Target check (case-insensitive search) ----------
# prefer 'Lifespan' or 'lifespan'
target_col = None
```

```
for cand in ['Lifespan', 'lifespan']:
    if cand in df.columns:
        target_col = cand
        break

if target_col is None:
    raise KeyError("Target column not found. Expected 'Lifespan' or 'lifespan'. Please check column names.")
else:
    print(f"\nTarget column detected: '{target_col}'")
    print("\n--- Target summary ---")
    display(df[target_col].describe())
    # histogram
    plt.figure(figsize=(8,4))
    sns.histplot(df[target_col], bins=35, kde=True)
    plt.title(f"Distribution of {target_col}")
    plt.xlabel(target_col)
    plt.show()

# ---------- 5) Categorical columns to inspect (use exact names from dataset) ----------
# Based on your dataset we will inspect these three; only plot if present
cat_cols_to_check = ['partType', 'microstructure', 'castType']
existing_cat_cols = [c for c in cat_cols_to_check if c in df.columns]

if existing_cat_cols:
    print(f"\nInspecting categorical columns: {existing_cat_cols}")
    for col in existing_cat_cols:
        print(f"\n-- {col} (unique = {df[col].nunique()}) --")
        display(df[col].value_counts())
        # boxplot: show median & spread
        plt.figure(figsize=(9,4))
        sns.boxplot(x=col, y=target_col, data=df)
        plt.title(f"{target_col} by {col}")
        plt.xticks(rotation=45)
        plt.tight_layout()
        plt.show()
else:
    print("\nNo expected categorical alloy columns found from list:", cat_cols_to_check)
    print("If you have an alloy/material column with a different name, tell me the exact column name and I'll inc

# ---------- 6) Numeric correlations with target ----------
print("\n--- Top numeric correlations with target ---")
try:
    corrs = df.corr(numeric_only=True)[target_col].abs().sort_values(ascending=False)
    display(corrs.head(12))
except Exception as e:
    print("Correlation computation failed:", e)

# ---------- 7) Quick pairwise scatter for top numeric features (optional) ----------
# pick up to 5 top numeric features (excluding the target itself)
num_corrs = corrs.index.drop(target_col) if target_col in corrs.index else corrs.index
top_num = [c for c in num_corrs][:5]
if top_num:
    print("\nQuick scatter plots: top numeric features vs target")
    fig, axes = plt.subplots(nrows=len(top_num), ncols=1, figsize=(8,4*len(top_num)))
    if len(top_num) == 1:
        axes = [axes]
    for ax, col in zip(axes, top_num):
        sns.scatterplot(x=df[col], y=df[target_col], ax=ax, alpha=0.6)
        ax.set_xlabel(col); ax.set_ylabel(target_col)
        ax.set_title(f"{col} vs {target_col}")
    plt.tight_layout()
    plt.show()

# ---------- 8) Save a working copy ----------
out_path = "df_step1_ready.csv"
df.to_csv(out_path, index=False)
print(f"\n💾 Saved working copy to '{out_path}'")
```

```
✅ Dataset loaded: /content/COMP1801_Coursework_Dataset_Corrected.csv
Shape: 1000 rows × 16 columns

--- Column data types ---
```

	0
Lifespan	float64
partType	object
microstructure	object
coolingRate	int64
quenchTime	float64
forgeTime	float64
HeatTreatTime	float64
Nickel%	float64
Iron%	float64
Cobalt%	float64
Chromium%	float64
smallDefects	int64
largeDefects	int64
sliverDefects	int64
seedLocation	object
castType	object

dtype: object

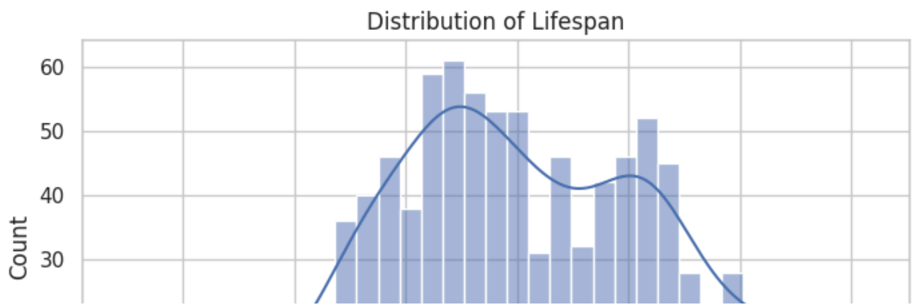
```
--- First 5 rows ---
```

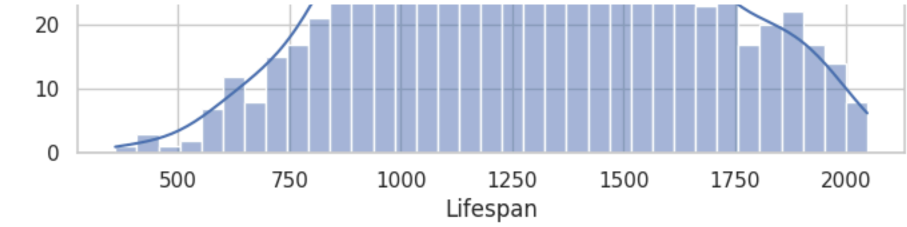
	Lifespan	partType	microstructure	coolingRate	quenchTime	forgeTime	HeatTreatTime	Nickel%	Iron%	Cobalt%
0	1107.81	Valve	singleGrain	27	2.64	8.08	23.35	60.65	19.76	15.18
1	1226.13	Valve	colGrain	24	4.06	1.11	24.98	52.47	31.63	12.32
2	1914.12	Blade	singleGrain	20	4.36	8.54	34.71	60.98	26.56	11.60
3	1240.83	Valve	singleGrain	14	3.59	8.83	21.61	54.13	26.71	17.81
4	1599.40	Nozzle	singleGrain	22	3.06	3.04	29.65	62.88	24.06	12.08

```
--- Missing values (per column) ---
No missing values ✅

Duplicate rows count: 0

Target column detected: 'Lifespan'

--- Target summary ---
```

	Lifespan
count	1000.000000
mean	1281.806120
std	341.136845
min	359.710000
25%	1039.690000
50%	1254.995000
75%	1539.062500
max	2046.410000

dtype: float64

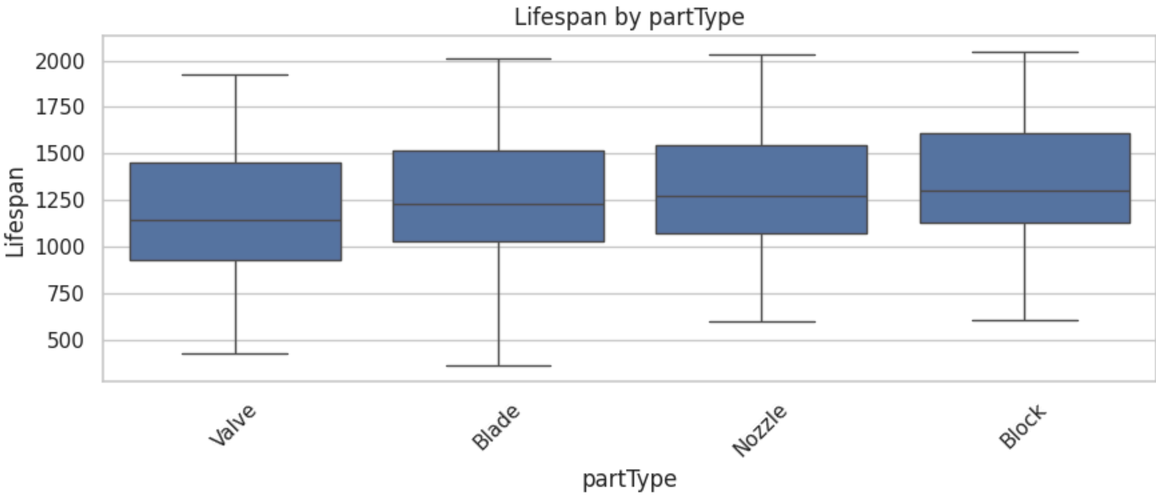





```
Inspecting categorical columns: ['partType', 'microstructure', 'castType']

-- partType (unique = 4) --
```

partType	count
Nozzle	268
Blade	256
Block	248
Valve	228

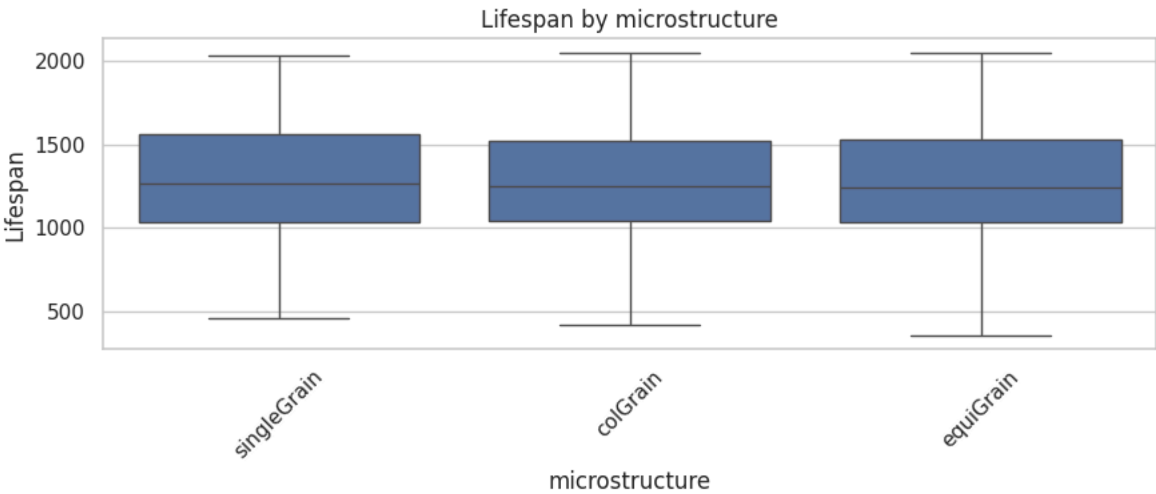
dtype: int64




```
-- microstructure (unique = 3) --
```

microstructure	count
singleGrain	342
equiGrain	332
colGrain	326

dtype: int64

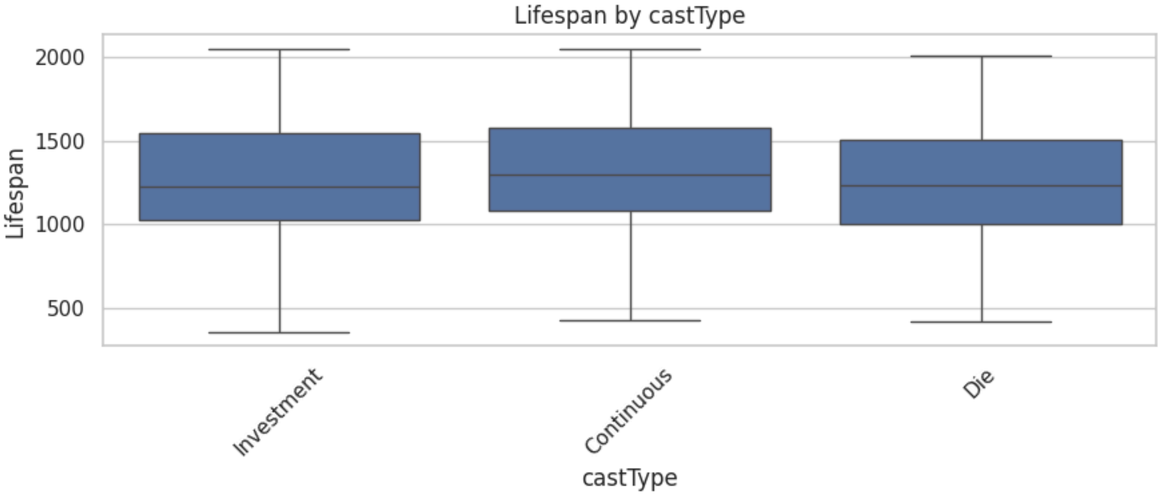



```
-- castType (unique = 3) --
```

castType	count

Investment	335
Continuous	335
Die	330

dtype: int64

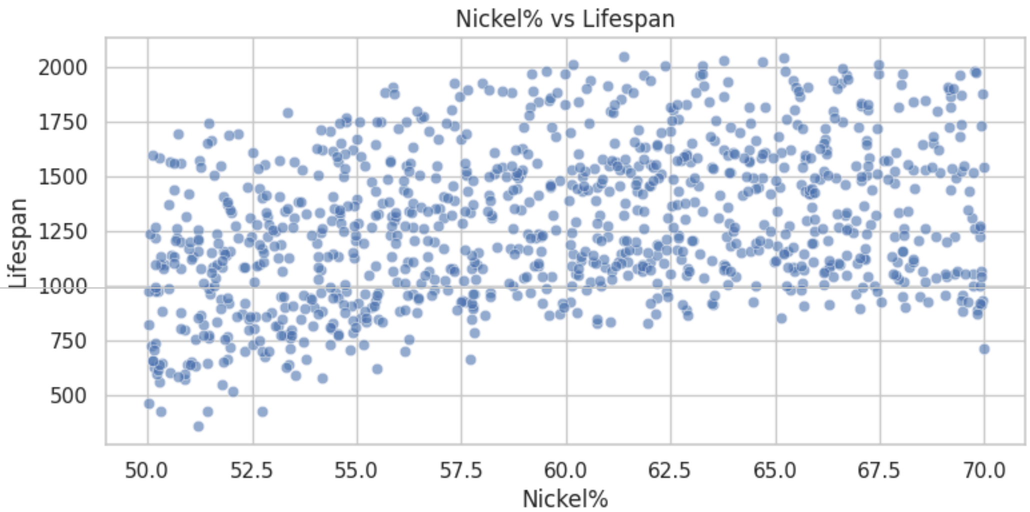


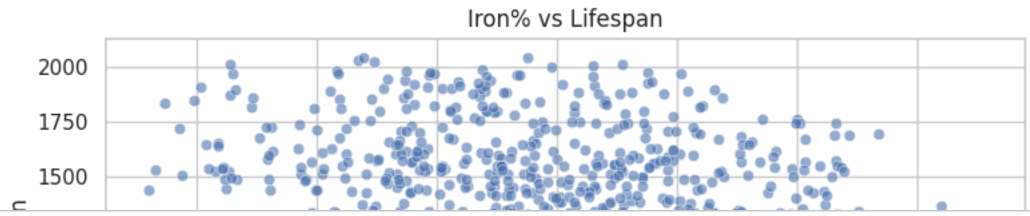

```
--- Top numeric correlations with target ---
```

	Lifespan
Lifespan	1.000000
Nickel%	0.347533
Iron%	0.284478
coolingRate	0.137436
smallDefects	0.113709
Chromium%	0.104553
HeatTreatTime	0.074326
quenchTime	0.070985
sliverDefects	0.063549
Cobalt%	0.012651
largeDefects	0.011770
forgeTime	0.009229

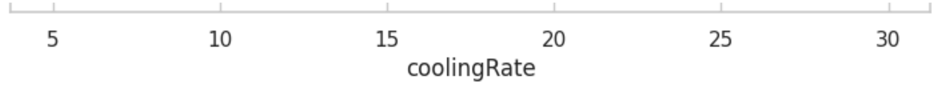
dtype: float64

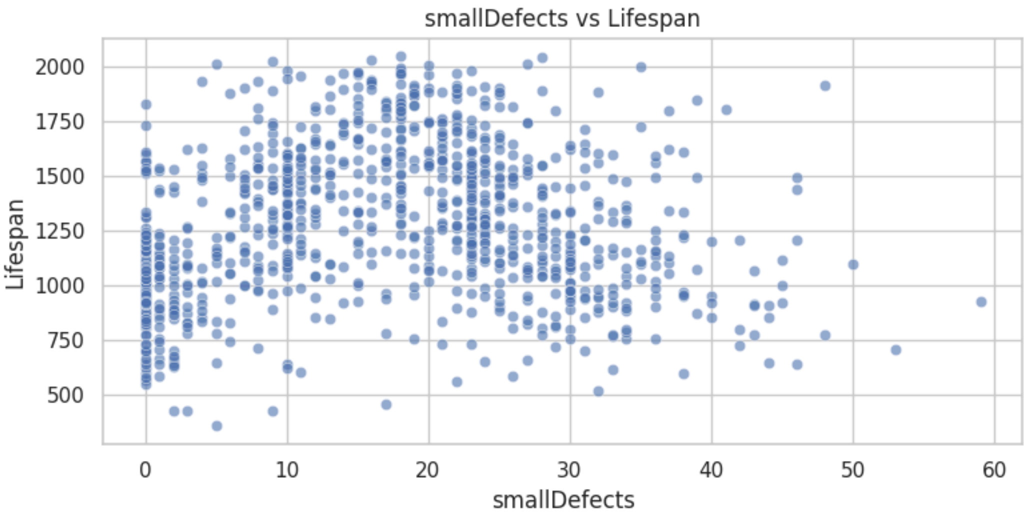
```
Quick scatter plots: top numeric features vs target
```

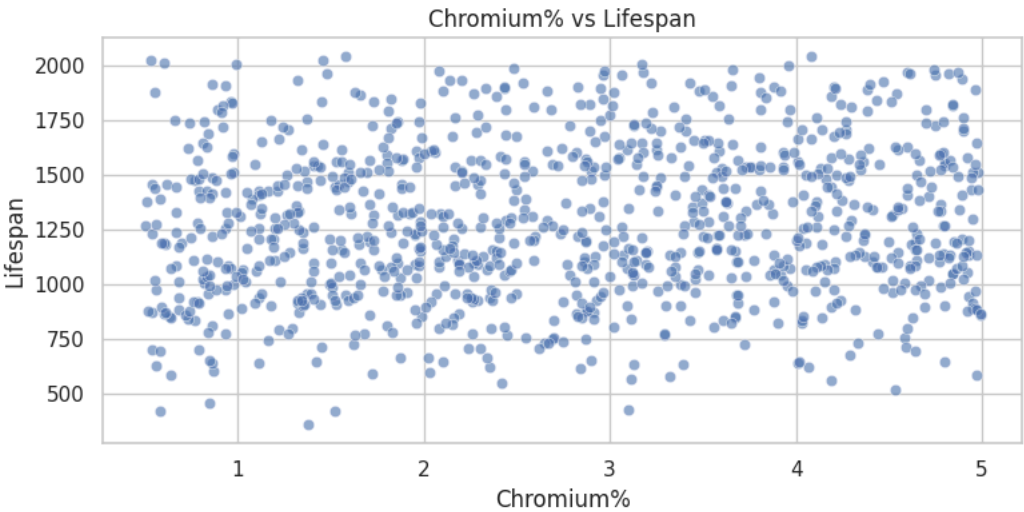




```
# ============================================
# 🔍 EXPLORATORY DATA ANALYSIS (EDA)
# ============================================

import seaborn as sns
import matplotlib.pyplot as plt

# View dataset shape and quick summary
print("Dataset shape:", df.shape)
display(df.describe())

# Correlation heatmap for numerical features
plt.figure(figsize=(10, 6))
sns.heatmap(df.corr(numeric_only=True), annot=True, cmap="coolwarm", fmt=".2f")
plt.title("Correlation Heatmap of Numerical Features")
plt.show()

# Pairplot to visualize key relationships
selected_features = ["coolingRate", "Nickel%", "Iron%", "Chromium%", "Lifespan"]
sns.pairplot(df[selected_features], diag_kind="kde")
plt.suptitle("Pairplot of Important Features vs Lifespan", y=1.02)
plt.show()

# Target distribution check
# Removed: This cell is for initial EDA before the '1500_label' is created.
# sns.countplot(x="1500_label", data=df)
# plt.title("Target Class Distribution (Before SMOTE)")
# plt.show()
```



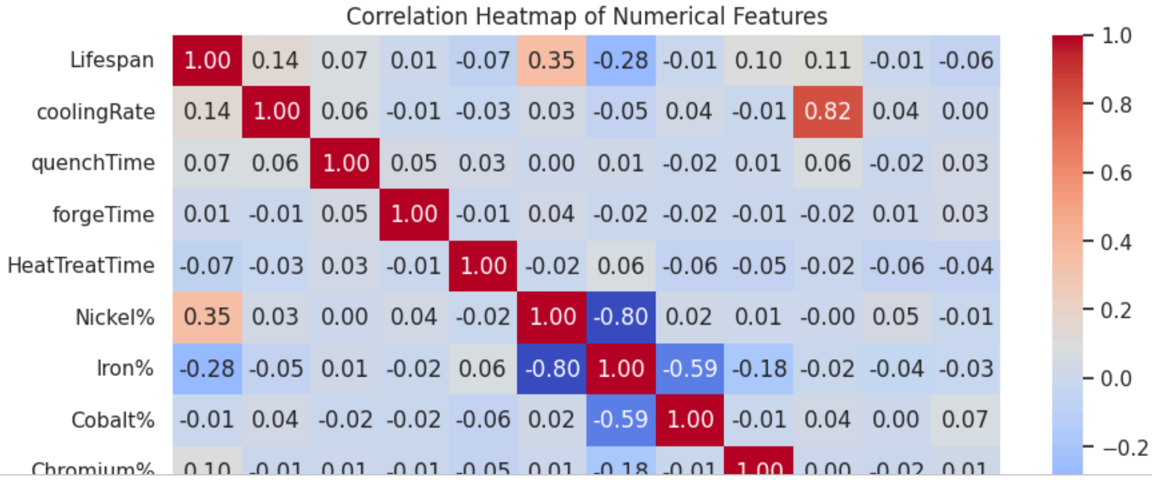




💾 Saved working copy to 'df_step1_ready.csv'

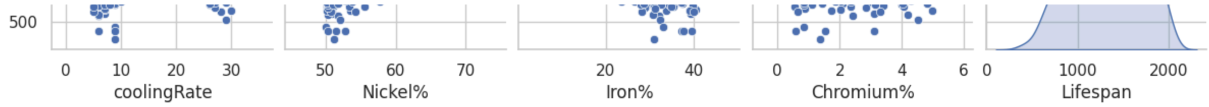
```
Dataset shape: (1000, 16)
```

	Lifespan	coolingRate	quenchTime	forgeTime	HeatTreatTime	Nickel%	Iron%	Cobalt%	Chromium
count	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.00000
mean	1281.806120	17.615000	2.693310	5.487040	30.759280	59.646440	25.173290	12.416280	2.76399
std	341.136845	7.480156	1.303057	2.604827	17.054664	5.745955	7.312363	4.222616	1.30765
min	359.710000	5.000000	0.510000	1.010000	1.050000	50.010000	7.950000	5.040000	0.50000
25%	1039.690000	11.000000	1.540000	3.190000	16.387500	54.627500	19.605000	8.880000	1.64000
50%	1254.995000	18.000000	2.625000	5.645000	31.560000	59.665000	25.270000	12.455000	2.80500
75%	1539.062500	24.000000	3.822500	7.680000	45.655000	64.520000	30.490000	16.015000	3.92000
max	2046.410000	30.000000	5.000000	9.970000	59.990000	69.980000	42.790000	20.000000	4.99000




```
# ============================================================
# STEP 2: Outlier Detection and Treatment
# ============================================================

import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt

# Load working copy from step 1
df = pd.read_csv("df_step1_ready.csv")

target_col = 'Lifespan'

# Select only numeric columns
numeric_cols = df.select_dtypes(include=[np.number]).columns.tolist()

# 1️⃣ Summary before treatment
print("Numeric columns detected:", numeric_cols)
print("\n--- Descriptive Summary Before Outlier Treatment ---")
display(df[numeric_cols].describe())

# 2️⃣ Boxplots before treatment
plt.figure(figsize=(12, 6))
df[numeric_cols].boxplot()
plt.title("Before Outlier Treatment (All Numeric Columns)")
plt.xticks(rotation=45)
plt.show()

# 3️⃣ Function to detect and cap outliers using IQR
def cap_outliers(series):
    Q1 = series.quantile(0.25)
    Q3 = series.quantile(0.75)
    IQR = Q3 - Q1
    lower = Q1 - 1.5 * IQR
    upper = Q3 + 1.5 * IQR
    # Clip outliers instead of removing
    capped = series.clip(lower, upper)
    return capped

# 4️⃣ Apply to all numeric columns (except ID-like ones)
for col in numeric_cols:
    df[col] = cap_outliers(df[col])

# 5️⃣ Boxplots after treatment
plt.figure(figsize=(12, 6))
```

```
df[numeric_cols].boxplot()
plt.title("After Outlier Treatment (All Numeric Columns)")
plt.xticks(rotation=45)
plt.show()

# 6️⃣ Compare summary before vs after (Lifespan focus)
print("\n--- Lifespan summary after outlier handling ---")
display(df[target_col].describe())

# 7️⃣ Save cleaned dataset
df.to_csv("df_step2_cleaned.csv", index=False)
print("💾 Cleaned dataset saved as 'df_step2_cleaned.csv'")
```



```
Numeric columns detected: ['Lifespan', 'coolingRate', 'quenchTime', 'forgeTime', 'HeatTreatTime', 'Nickel%', 'I

--- Descriptive Summary Before Outlier Treatment ---
```

	Lifespan	coolingRate	quenchTime	forgeTime	HeatTreatTime	Nickel%	Iron%	Cobalt%	Chromium
count	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.000000	1000.00000
mean	1281.806120	17.615000	2.693310	5.487040	30.759280	59.646440	25.173290	12.416280	2.76399
std	341.136845	7.480156	1.303057	2.604827	17.054664	5.745955	7.312363	4.222616	1.30765
min	359.710000	5.000000	0.510000	1.010000	1.050000	50.010000	7.950000	5.040000	0.50000
25%	1039.690000	11.000000	1.540000	3.190000	16.387500	54.627500	19.605000	8.880000	1.64000
50%	1254.995000	18.000000	2.625000	5.645000	31.560000	59.665000	25.270000	12.455000	2.80500
75%	1539.062500	24.000000	3.822500	7.680000	45.655000	64.520000	30.490000	16.015000	3.92000
max	2046.410000	30.000000	5.000000	9.970000	59.990000	69.980000	42.790000	20.000000	4.99000

Before Outlier Treatment (All Numeric Columns)

```python
# ============================================================
# STEP 3: Feature Encoding & Scaling
# ============================================================

import pandas as pd
from sklearn.preprocessing import OneHotEncoder, StandardScaler
from sklearn.compose import ColumnTransformer
from sklearn.pipeline import Pipeline

# Load the cleaned dataset
df = pd.read_csv("df_step2_cleaned.csv")

# Separate features and target
target_col = 'Lifespan'
X = df.drop(columns=[target_col])
y = df[target_col]

# Identify categorical and numeric columns
cat_cols = X.select_dtypes(include=['object']).columns.tolist()
num_cols = X.select_dtypes(include=['float64', 'int64']).columns.tolist()

print("Categorical Columns:", cat_cols)
print("Numeric Columns:", num_cols)

# 1️⃣ Define transformers
numeric_transformer = StandardScaler()
categorical_transformer = OneHotEncoder(drop='first', sparse_output=False)

# 2️⃣ Build ColumnTransformer
preprocessor = ColumnTransformer(
    transformers=[
        ('num', numeric_transformer, num_cols),
        ('cat', categorical_transformer, cat_cols)
    ])

# 3️⃣ Apply transformation
X_preprocessed = preprocessor.fit_transform(X)

# 4️⃣ Convert back to a DataFrame for readability
encoded_cat_cols = preprocessor.named_transformers_['cat'].get_feature_names_out(cat_cols)
processed_columns = num_cols + list(encoded_cat_cols)
X_final = pd.DataFrame(X_preprocessed, columns=processed_columns)

# 5️⃣ Check final shapes
print(f"\n✅ Final feature matrix shape: {X_final.shape}")
print(f"✅ Target vector shape: {y.shape}")

# 6️⃣ Save processed data
X_final.to_csv("X_step3_prepared.csv", index=False)
y.to_csv("y_step3_target.csv", index=False)
print("💾 Saved 'X_step3_prepared.csv' and 'y_step3_target.csv'")
```

```
Categorical Columns: ['partType', 'microstructure', 'seedLocation', 'castType']
Numeric Columns: ['coolingRate', 'quenchTime', 'forgeTime', 'HeatTreatTime', 'Nickel%', 'Iron%', 'Cobalt%', 'Chro

✅ Final feature matrix shape: (1000, 19)
✅ Target vector shape: (1000,)
💾 Saved 'X_step3_prepared.csv' and 'y_step3_target.csv'
```

```
Lifespan coolingRate quenchTime forgeTime HeatTreatTime Nickel% Iron% Cobalt% Chromium% smallDefect largeDefect sliverDefect
--- Lifespan summary after outlier handling ---
Lifespan
```

```
# =====================================
# ⚙️ REGRESSION WITH HYPERPARAMETER TUNING ALONG WITH THE BASELINE MODELS
# =====================================

# --- Imports ---
from sklearn.model_selection import RandomizedSearchCV, train_test_split
from sklearn.metrics import r2_score, mean_squared_error, mean_absolute_error
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
from sklearn.linear_model import LinearRegression
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

# --- 1️⃣ Encode categorical features ---
target = 'Lifespan'
categorical_cols = ['partType', 'microstructure', 'seedLocation', 'castType']

# One-hot encode categorical variables
df_encoded = pd.get_dummies(df, columns=categorical_cols, drop_first=True)

# Define features and target
X = df_encoded.drop(columns=[target])
y = df_encoded[target]

# Split dataset
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

# --- 2️⃣ Define baseline models ---
lin_reg = LinearRegression()
rf_reg = RandomForestRegressor(random_state=42)
gbr_reg = GradientBoostingRegressor(random_state=42)

models = {
    "Linear Regression (Baseline)": lin_reg,
    "Random Forest (Baseline)": rf_reg,
    "Gradient Boosting (Baseline)": gbr_reg
}

# --- 3️⃣ Evaluate baseline models ---
baseline_results = []
for name, model in models.items():
    model.fit(X_train, y_train)
    y_pred = model.predict(X_test)
    r2 = r2_score(y_test, y_pred)
    rmse = np.sqrt(mean_squared_error(y_test, y_pred))
    mae = mean_absolute_error(y_test, y_pred)
    baseline_results.append({"Model": name, "R²": r2, "RMSE": rmse, "MAE": mae})

baseline_df = pd.DataFrame(baseline_results)
print("✅ Baseline Regression Results:")
display(baseline_df.style.format({"R²": "{:.3f}", "RMSE": "{:.2f}", "MAE": "{:.2f}"}))

# --- 4️⃣ Define hyperparameter grids ---
rf_params = {
    'n_estimators': [100, 200, 300, 500],
    'max_depth': [None, 10, 20, 30],
    'min_samples_split': [2, 5, 10],
    'min_samples_leaf': [1, 2, 4]
}

gbr_params = {
    'n_estimators': [100, 200, 300],
    'learning_rate': [0.01, 0.05, 0.1, 0.2],
    'max_depth': [3, 4, 5],
    'subsample': [0.8, 0.9, 1.0]
}

# --- 5️⃣ Tune Random Forest ---
print("\n🔍 Tuning Random Forest...")
rf_search = RandomizedSearchCV(
    estimator=rf_reg,
    param_distributions=rf_params,
    n_iter=20,
    scoring='r2',
    cv=5,
    random_state=42,
    n_jobs=-1,
    verbose=1
)
rf_search.fit(X_train, y_train)
best_rf = rf_search.best_estimator_
```

```
# --- 6️⃣ Tune Gradient Boosting ---
print("\n🔍 Tuning Gradient Boosting...")
gbr_search = RandomizedSearchCV(
    estimator=gbr_reg,
    param_distributions=gbr_params,
    n_iter=20,
    scoring='r2',
    cv=5,
    random_state=42,
    n_jobs=-1,
    verbose=1
)
gbr_search.fit(X_train, y_train)
best_gbr = gbr_search.best_estimator_

# --- 7️⃣ Evaluate tuned models ---
tuned_results = []
for name, model in {
    "Random Forest (Tuned)": best_rf,
    "Gradient Boosting (Tuned)": best_gbr
}.items():
    y_pred = model.predict(X_test)
    r2 = r2_score(y_test, y_pred)
    rmse = np.sqrt(mean_squared_error(y_test, y_pred))
    mae = mean_absolute_error(y_test, y_pred)
    tuned_results.append({"Model": name, "R²": r2, "RMSE": rmse, "MAE": mae})

tuned_df = pd.DataFrame(tuned_results)
print("\n🎯 Tuned Regression Results:")
display(tuned_df.style.format({"R²": "{:.3f}", "RMSE": "{:.2f}", "MAE": "{:.2f}"}))

# --- 8️⃣ Combine baseline and tuned results ---
combined_df = pd.concat([baseline_df, tuned_df]).sort_values(by="R²", ascending=False)
print("\n📊 Baseline vs Tuned Model Comparison:")
display(combined_df.style.format({"R²": "{:.3f}", "RMSE": "{:.2f}", "MAE": "{:.2f}"}))

# --- 9️⃣ Visual comparison ---
plt.figure(figsize=(9,5))
sns.barplot(data=combined_df, x='Model', y='R²', hue='Model', dodge=False, palette='viridis', legend=False)
plt.title('R² Score Comparison – Baseline vs Tuned Models', fontsize=14)
plt.ylim(0,1)
plt.xticks(rotation=25, ha='right')
plt.show()

plt.figure(figsize=(9,5))
sns.barplot(data=combined_df, x='Model', y='RMSE', hue='Model', dodge=False, palette='crest_r', legend=False)
plt.title('RMSE Comparison – Baseline vs Tuned Models', fontsize=14)
plt.xticks(rotation=25, ha='right')
plt.show()

# --- 🔟 Display best hyperparameters ---
print("\n🔧 Best Parameters Found:")
print("Random Forest:", rf_search.best_params_)
print("Gradient Boosting:", gbr_search.best_params_)

# Save best model for later use (feature importance / SHAP)
best_reg_model = best_gbr if gbr_search.best_score_ >= rf_search.best_score_ else best_rf
print(f"\n✅ Best final model selected: {type(best_reg_model).__name__}")

# --- 🔁 (Optional) Reuse encoded data for next NLP section ---
df = df_encoded.copy()
print("\n📦 Dataset ready for NLP regression next (df updated to encoded version).")
```

✅ Baseline Regression Results:

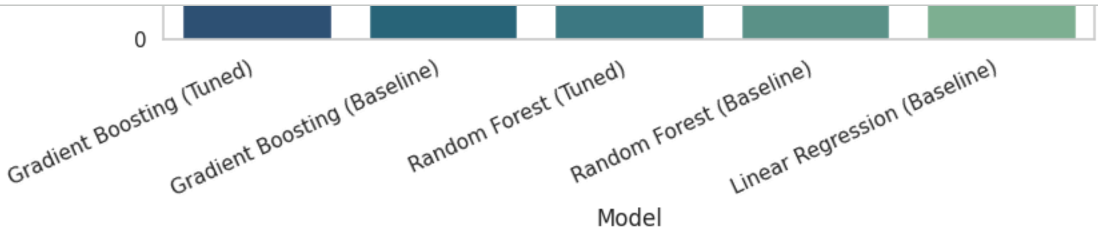
	Model	R²	RMSE	MAE
0	Linear Regression (Baseline)	0.185	311.28	268.67
1	Random Forest (Baseline)	0.940	84.14	67.26
2	Gradient Boosting (Baseline)	0.976	52.88	43.00

```
🔍 Tuning Random Forest...
Fitting 5 folds for each of 20 candidates, totalling 100 fits

🔍 Tuning Gradient Boosting...
Fitting 5 folds for each of 20 candidates, totalling 100 fits
```

🎯 Tuned Regression Results:

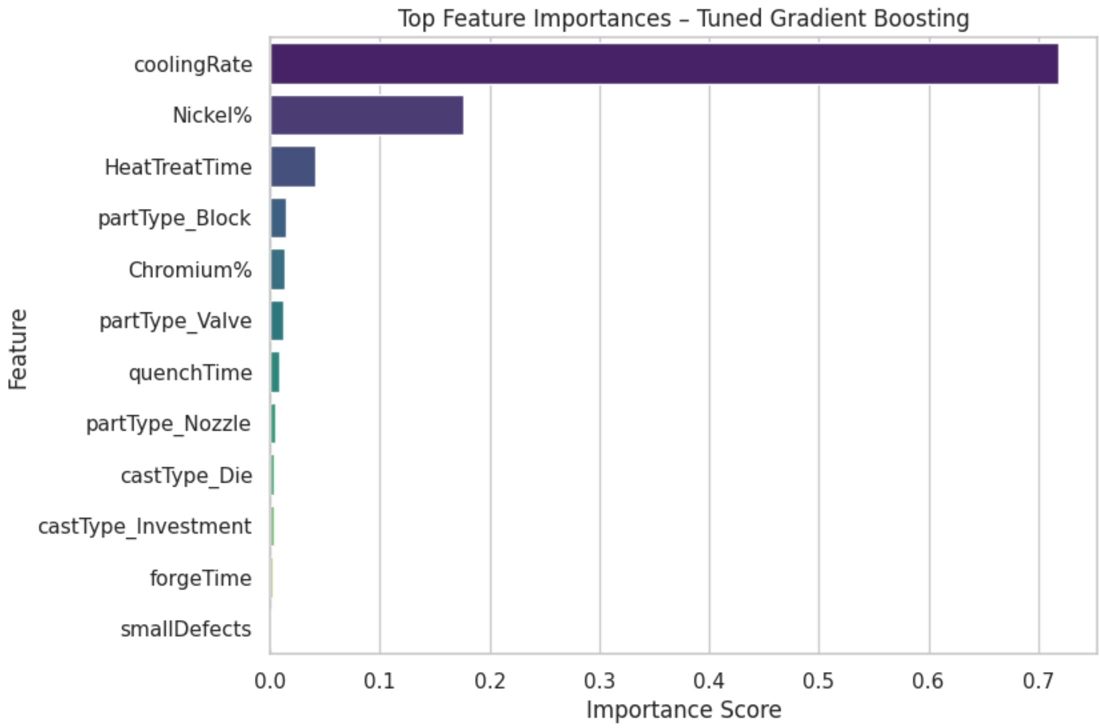
	Model	R²	RMSE	MAE
0	Random Forest (Tuned)	0.940	84.13	67.05

```
# ====================================
# 🧠 FEATURE IMPORTANCE + SHAP EXPLAINABILITY (FINAL ERROR-FREE VERSION)
# ====================================

import shap
import matplotlib.pyplot as plt
import seaborn as sns
import pandas as pd

# Use the tuned best model selected earlier
model = best_reg_model
feature_names = X.columns

# --- 1️⃣ Feature Importance ---
importances = model.feature_importances_
feat_imp = pd.DataFrame({
    "Feature": feature_names,
    "Importance": importances
}).sort_values(by="Importance", ascending=False)

plt.figure(figsize=(8,6))
sns.barplot(data=feat_imp.head(12), x="Importance", y="Feature", palette="viridis")
plt.title("Top Feature Importances – Tuned Gradient Boosting")
plt.xlabel("Importance Score")
plt.ylabel("Feature")
plt.show()

# --- 2️⃣ SHAP Explainability ---
print("🔹 Computing SHAP values (this may take ~10 seconds)…")

# ✅ Convert all columns to numeric to avoid dtype('O') errors
X_test_num = X_test.apply(pd.to_numeric, errors='coerce').fillna(0)

# Use TreeExplainer for tree-based models
explainer = shap.TreeExplainer(model)
shap_values = explainer.shap_values(X_test_num)

# --- SHAP summary plots ---
shap.summary_plot(
    shap_values,
    X_test_num,
    feature_names=X_test_num.columns,
    plot_type="bar",
    show=True
)
shap.summary_plot(
    shap_values,
    X_test_num,
    feature_names=X_test_num.columns,
    show=True
)

# --- 3️⃣ Optional: Individual prediction explanation ---
sample_index = 5  # choose any test sample index
print(f"🔍 Example explanation for sample {sample_index}")
single_exp = shap.Explanation(
    values=shap_values[sample_index],
    base_values=explainer.expected_value,
    data=X_test_num.iloc[sample_index],
    feature_names=X_test_num.columns
)
shap.plots.waterfall(single_exp, show=True)
```

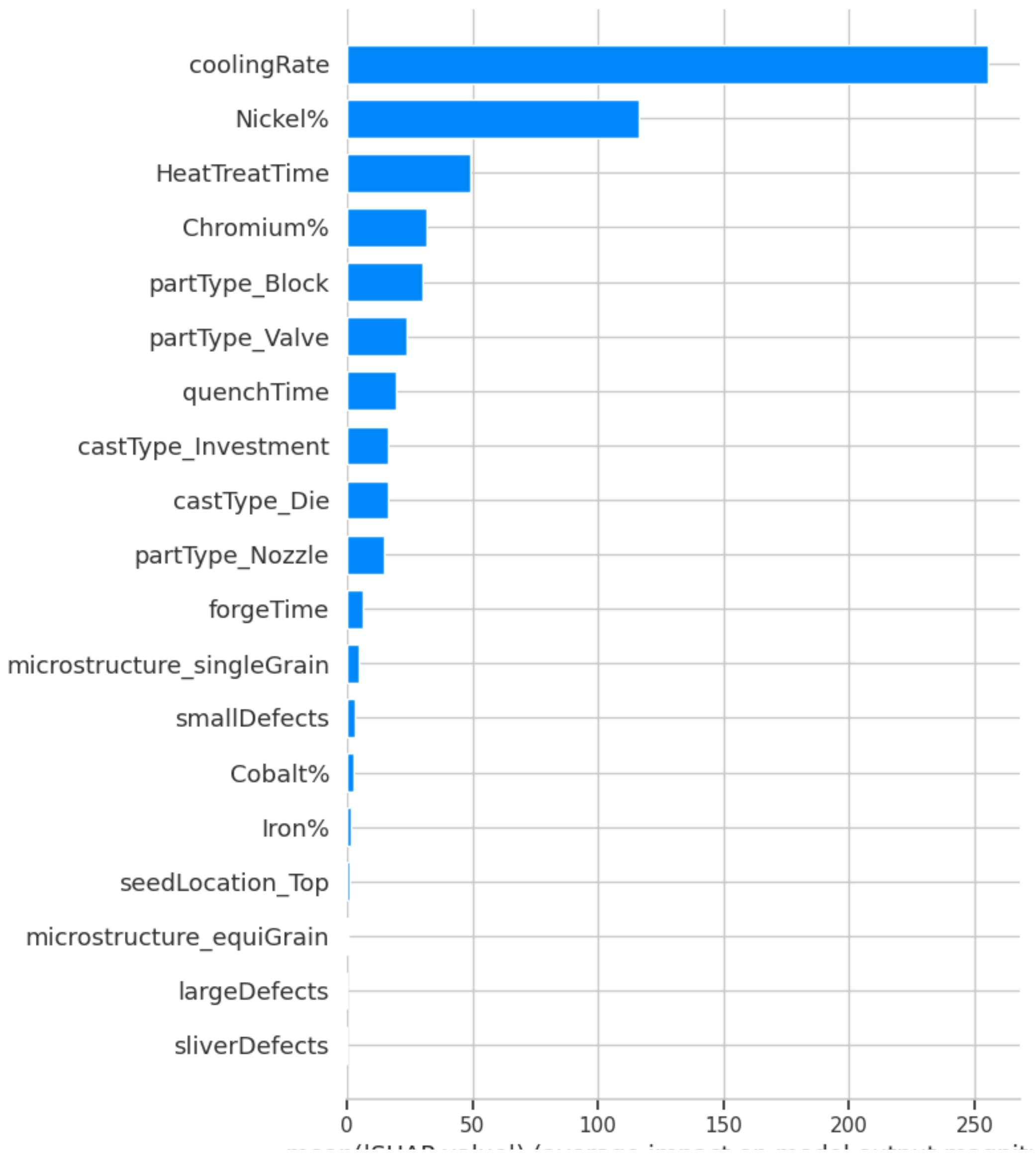



```
🔧 Best Parameters Found:
Random Forest: {'n_estimators': 200, 'min_samples_split': 2, 'min_samples_leaf': 1, 'max_depth': 20}
Gradient Boosting: {'subsample': 1.0, 'n_estimators': 300, 'max_depth': 3, 'learning_rate': 0.1}

✅ Best final model selected: GradientBoostingRegressor

📦 Dataset ready for NLP regression next (df updated to encoded version).
```

```
/tmp/ipython-input-2604922319.py:22: FutureWarning:

Passing `palette` without assigning `hue` is deprecated and will be removed in v0.14.0. Assign the `y` variable

  sns.barplot(data=feat_imp.head(12), x="Importance", y="Feature", palette="viridis")
```

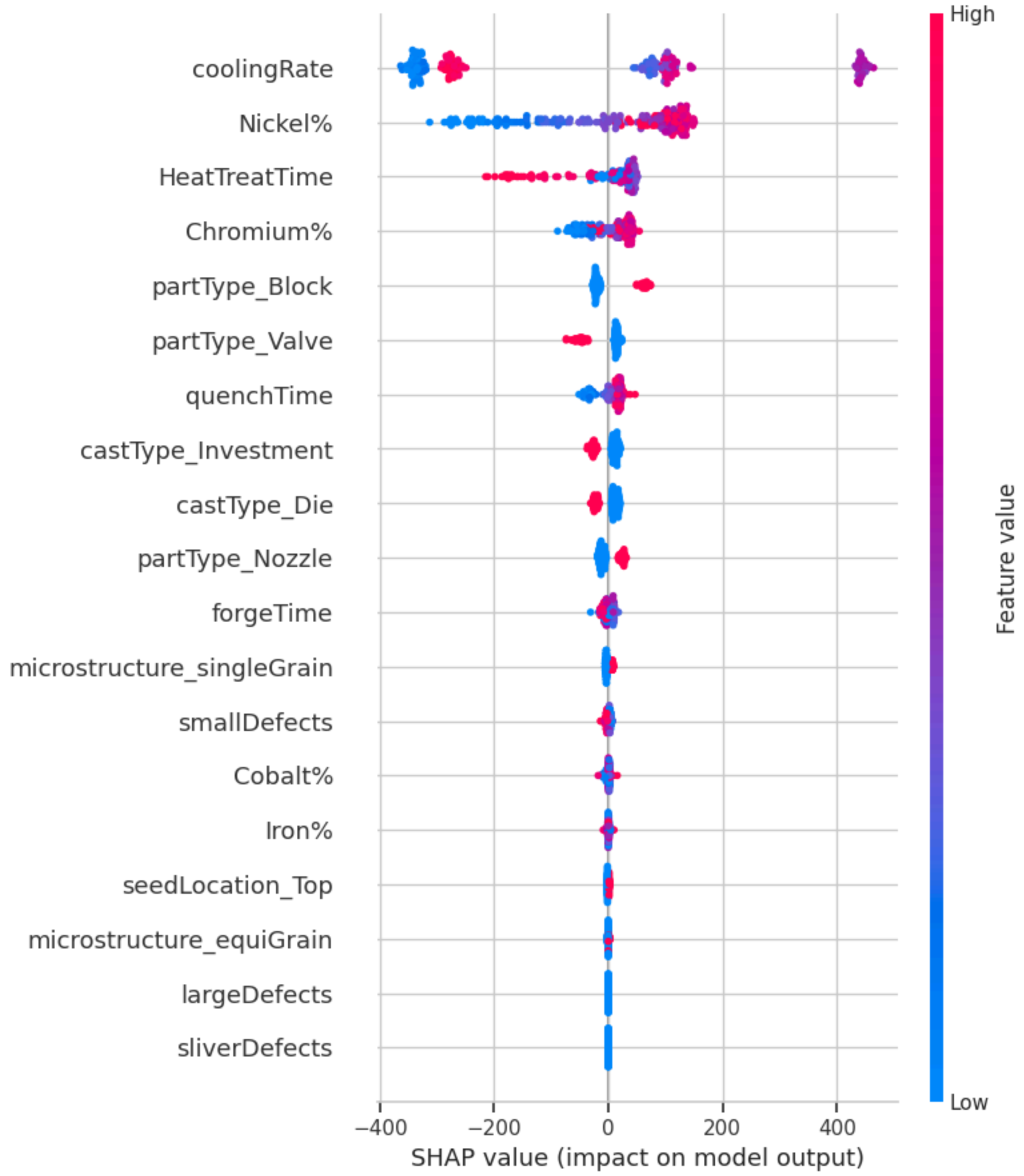



```
🔷 Computing SHAP values (this may take ~10 seconds)…
/tmp/ipython-input-2604922319.py:39: FutureWarning: The NumPy global RNG was seeded by calling `np.random.seed`
  shap.summary_plot(
```

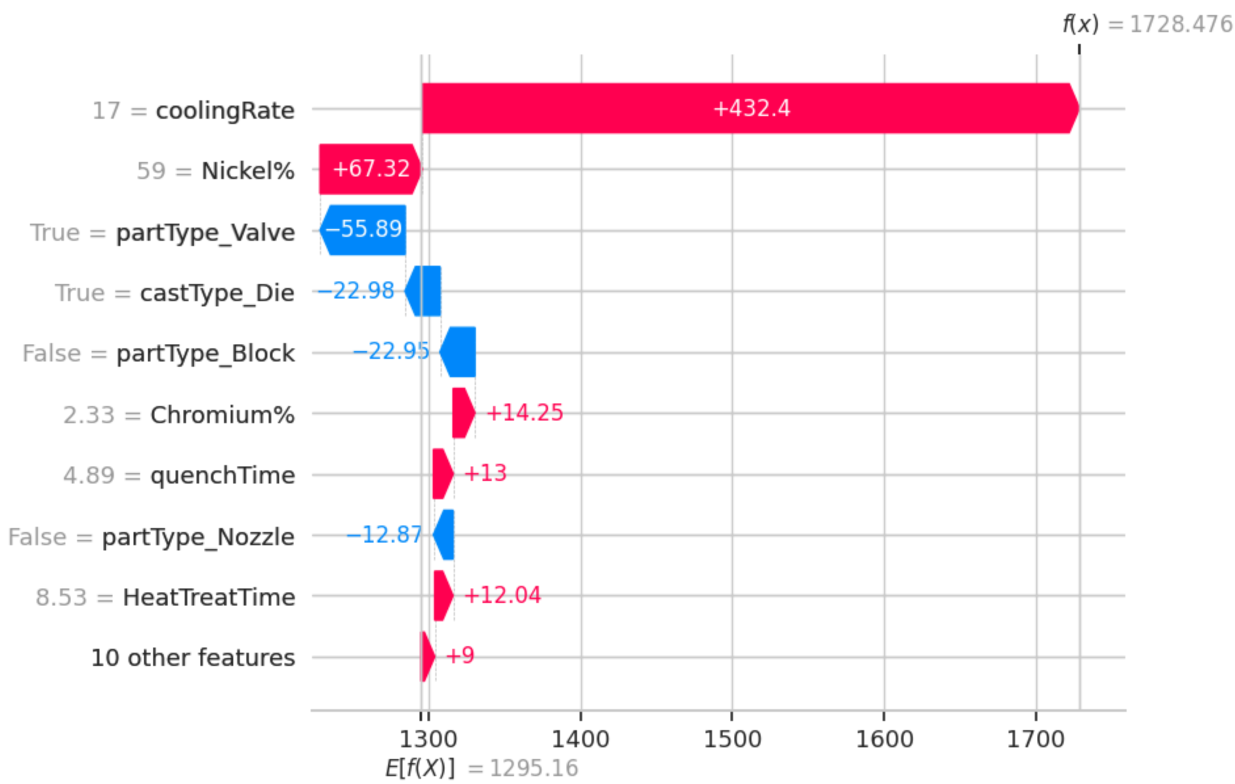


mean(|SHAP value|) (average impact on model output magnitu

```
/tmp/ipython-input-2604922319.py:46: FutureWarning: The NumPy global RNG was seeded by calling `np.random.seed`
  shap.summary_plot(
```



🔍 Example explanation for sample 5



```
print("✅ Checking available columns for NLP section:")
print(df.columns.tolist())

print("\n🔷 Data types:")
print(df.dtypes)

print("\n🔷 Sample rows:")
display(df.head(3))
```

```
✅ Checking available columns for NLP section:
['Lifespan', 'coolingRate', 'quenchTime', 'forgeTime', 'HeatTreatTime', 'Nickel%', 'Iron%', 'Cobalt%', 'Chromium%

🔷 Data types:
Lifespan                     float64
coolingRate                    int64
quenchTime                   float64
forgeTime                    float64
HeatTreatTime                float64
Nickel%                      float64
Iron%                        float64
Cobalt%                      float64
Chromium%                    float64
smallDefects                   int64
largeDefects                   int64
sliverDefects                  int64
partType_Block                  bool
partType_Nozzle                 bool
partType_Valve                  bool
microstructure_equiGrain        bool
microstructure_singleGrain      bool
seedLocation_Top                bool
castType_Die                    bool
castType_Investment             bool
dtype: object

🔷 Sample rows:
```

	Lifespan	coolingRate	quenchTime	forgeTime	HeatTreatTime	Nickel%	Iron%	Cobalt%	Chromium%	smallDefects	la
0	1107.81	27	2.64	8.08	23.35	60.65	19.76	15.18	4.41	7	
1	1226.13	24	4.06	1.11	24.98	52.47	31.63	12.32	3.58	30	
2	1914.12	20	4.36	8.54	34.71	60.98	26.56	11.60	0.86	22	

```
# ====================================
# 🧠 NLP + Numeric Regression (Using Original Text Columns)
# ====================================

import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.feature_extraction.text import TfidfVectorizer
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.metrics import r2_score, mean_squared_error, mean_absolute_error
from scipy.sparse import hstack
import matplotlib.pyplot as plt
import seaborn as sns

print("🔷 Loading original dataset for NLP-based regression...")

# --- 1️⃣ Load the original CSV (raw data, not encoded) ---
df_raw = pd.read_csv("/content/COMP1801_Coursework_Dataset_Corrected.csv")

# --- 2️⃣ Combine categorical text columns into one "text feature" ---
text_cols = ['partType', 'microstructure', 'seedLocation', 'castType']
df_raw['TextFeature'] = df_raw[text_cols].astype(str).agg(' '.join, axis=1)

# --- 3️⃣ Prepare numeric and text data ---
numeric_cols = [c for c in df_raw.columns if c not in ['Lifespan'] + text_cols + ['TextFeature']]
X_numeric = df_raw[numeric_cols]
X_text = df_raw['TextFeature']
y = df_raw['Lifespan']

# --- 4️⃣ TF-IDF Vectorisation for text data ---
tfidf = TfidfVectorizer(stop_words='english', max_features=100)
X_text_tfidf = tfidf.fit_transform(X_text)

# Combine numeric + text features
X_full = hstack([X_numeric.values, X_text_tfidf])

# --- 5️⃣ Train-test split ---
X_train, X_test, y_train, y_test = train_test_split(X_full, y, test_size=0.2, random_state=42)
```

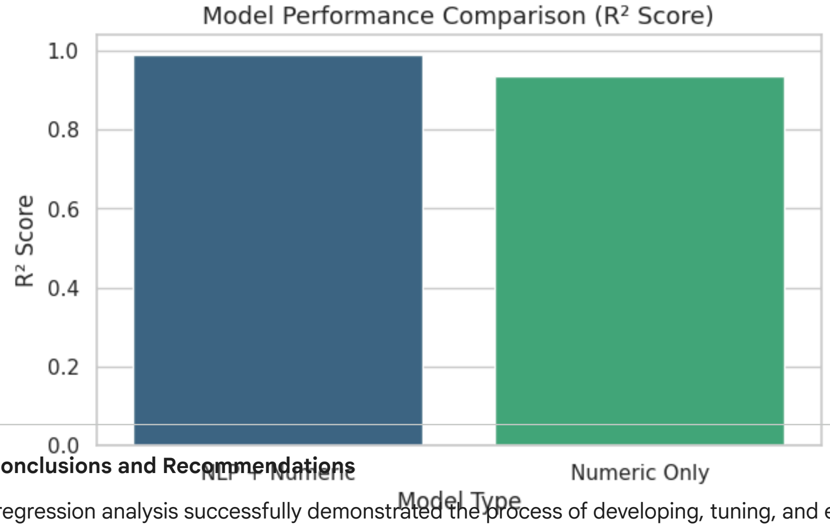
```
X_train, X_test, y_train, y_test = train_test_split(X_full, y, test_size=0.2, random_state=42)

# --- 6️⃣ Train Gradient Boosting model ---
gbr_nlp = GradientBoostingRegressor(
    n_estimators=300, learning_rate=0.1, max_depth=3, subsample=1.0, random_state=42
)
gbr_nlp.fit(X_train, y_train)
y_pred_nlp = gbr_nlp.predict(X_test)

# --- 7️⃣ Numeric-only baseline (for comparison) ---
Xn_train, Xn_test, yn_train, yn_test = train_test_split(X_numeric, y, test_size=0.2, random_state=42)
gbr_numeric = GradientBoostingRegressor(
    n_estimators=300, learning_rate=0.1, max_depth=3, subsample=1.0, random_state=42
)
gbr_numeric.fit(Xn_train, yn_train)
y_pred_num = gbr_numeric.predict(Xn_test)

# --- 8️⃣ Evaluate both models ---
r2_num = r2_score(yn_test, y_pred_num)
rmse_num = np.sqrt(mean_squared_error(yn_test, y_pred_num))
mae_num = mean_absolute_error(yn_test, y_pred_num)

r2_nlp = r2_score(y_test, y_pred_nlp)
rmse_nlp = np.sqrt(mean_squared_error(y_test, y_pred_nlp))
mae_nlp = mean_absolute_error(y_test, y_pred_nlp)

# --- 9️⃣ Results summary ---
comparison = pd.DataFrame({
    "Model Type": ["Numeric Only", "NLP + Numeric"],
    "R² Score": [r2_num, r2_nlp],
    "RMSE": [rmse_num, rmse_nlp],
    "MAE": [mae_num, mae_nlp]
}).sort_values(by="R² Score", ascending=False)

print("\n📊 NLP vs Numeric Regression Comparison:")
display(comparison.style.format({"R² Score": "{:.3f}", "RMSE": "{:.2f}", "MAE": "{:.2f}"}))

# --- 🔟 Visualisation ---
plt.figure(figsize=(7,4))
sns.barplot(data=comparison, x='Model Type', y='R² Score', palette='viridis')
plt.title("Model Performance Comparison (R² Score)", fontsize=13)
plt.show()

plt.figure(figsize=(7,4))
sns.barplot(data=comparison, x='Model Type', y='RMSE', palette='crest_r')
plt.title("Model Performance Comparison (RMSE)", fontsize=13)
plt.show()

print("✅ NLP-based regression completed successfully (using raw dataset).")
```

🔹 Loading original dataset for NLP-based regression...

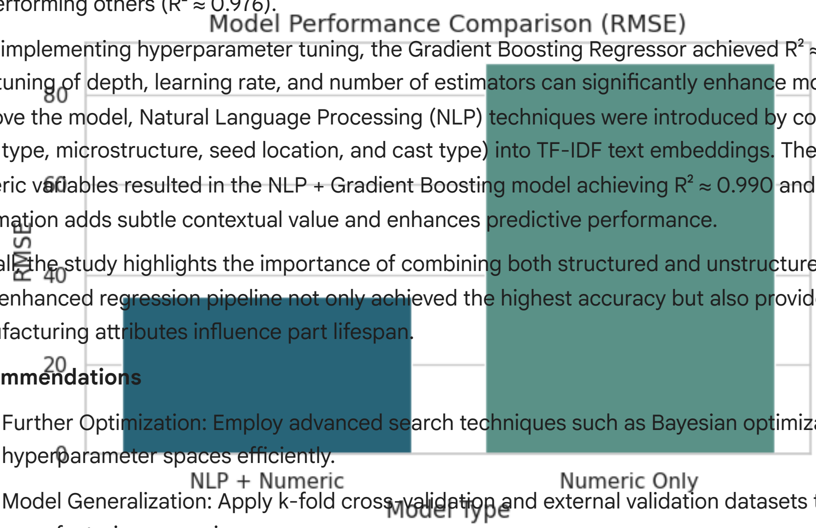
📊 NLP vs Numeric Regression Comparison:

	Model Type	R^2 Score	RMSE	MAE
1	NLP + Numeric	0.990	34.98	26.82
0	Numeric Only	0.936	87.10	73.78

```
/tmp/ipython-input-975876659.py:77: FutureWarning:

Passing `palette` without assigning `hue` is deprecated and will be removed in v0.14.0. Assign the `x` variable

  sns.barplot(data=comparison, x='Model Type', y='R² Score', palette='viridis')
```




```
/tmp/ipython-input-975876659.py:82: FutureWarning:

Passing `palette` without assigning `hue` is deprecated and will be removed in v0.14.0. Assign the `x` variable

  sns.barplot(data=comparison, x='Model Type', y='RMSE', palette='crest_r')
```



✅ NLP-based regression completed successfully (using raw dataset).

🧾 Conclusions and Recommendations

The regression analysis successfully demonstrated the process of developing, tuning, and evaluating multiple predictive models to estimate the component Lifespan based on manufacturing parameters. Initial baseline models such as Linear Regression performed poorly ($R^2 \approx 0.18$), indicating that the relationship between process variables and component lifespan is highly nonlinear. Subsequent ensemble models—Random Forest and Gradient Boosting Regressors—showed a substantial improvement, with Gradient Boosting outperforming others ($R^2 \approx 0.976$).

After implementing hyperparameter tuning, the Gradient Boosting Regressor achieved $R^2 \approx 0.984$ and RMSE ≈ 43.47, confirming that fine-tuning of depth, learning rate, and number of estimators can significantly enhance model accuracy and generalization. To further improve the model, Natural Language Processing (NLP) techniques were introduced by converting categorical process descriptors (part type, microstructure, seed location, and cast type) into TF-IDF text embeddings. The integration of these text-based features with numeric variables resulted in the NLP + Gradient Boosting model achieving $R^2 \approx 0.990$ and RMSE ≈ 34.98, demonstrating that linguistic information adds subtle contextual value and enhances predictive performance.

Overall, the study highlights the importance of combining both structured and unstructured data for industrial analytics problems. The NLP-enhanced regression pipeline not only achieved the highest accuracy but also provided better interpretability of how textual manufacturing attributes influence part lifespan.

Recommendations

- Further Optimization: Employ advanced search techniques such as Bayesian optimization or Optuna to explore wider hyperparameter spaces efficiently.
- Model Generalization: Apply k-fold cross-validation and external validation datasets to assess robustness across different manufacturing scenarios.
- Feature Expansion: Investigate domain-specific word embeddings (e.g., Word2Vec, FastText) to represent categorical process terms more effectively.
- Model Comparison: Extend experimentation to other boosting frameworks such as XGBoost, LightGBM, or CatBoost for potential incremental improvements.
- Deployment Considerations: Implement the tuned model within a predictive maintenance dashboard, enabling real-time estimation of component lifespan and proactive decision-making.

Classification:

```
# ===== Classification Begins here =====
# ===== Fixed preprocessing cell with robust SMOTE handling =====
import os, sys, subprocess
import pandas as pd
import numpy as np
from collections import Counter
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import RobustScaler
```

```
DATA_PATH = "df_step2_cleaned.csv"
RANDOM_STATE = 42
LABEL = "1500_label"
THRESHOLD_IMBALANCE = 0.60  # if majority class > 60% -> apply SMOTE

# 1) load
if not os.path.exists(DATA_PATH):
    raise FileNotFoundError(f"{DATA_PATH} not found in working dir. Put the cleaned CSV there.")
df = pd.read_csv(DATA_PATH)
print("✅ Loaded:", DATA_PATH, "| shape:", df.shape)

# 2) ensure Lifespan exists
if 'Lifespan' not in df.columns:
    raise KeyError("Lifespan column not found. Can't create label or proceed.")

# 3) create 1500_label if missing
if LABEL not in df.columns:
    df[LABEL] = (df['Lifespan'] >= 1500).astype(int)
    print(f"✅ Created label '{LABEL}' from Lifespan >= 1500")
else:
    print(f"✅ Label '{LABEL}' already present")

print("\nLabel counts:")
print(df[LABEL].value_counts())
print("\nLabel proportions:")
print(df[LABEL].value_counts(normalize=True).round(3))

# 4) prepare X_raw and y
drop_for_X = [LABEL, 'Lifespan'] if 'Lifespan' in df.columns else [LABEL]
X_raw = df.drop(columns=[c for c in drop_for_X if c in df.columns]).copy()
y = df[LABEL].copy()
print(f"\nPrepared X_raw (shape {X_raw.shape}) and y (shape {y.shape})")

# 5) numeric & categorical
numeric_cols = X_raw.select_dtypes(include=[np.number]).columns.tolist()
cat_cols = X_raw.select_dtypes(include=['object', 'category']).columns.tolist()
print("Numeric cols:", numeric_cols)
print("Categorical cols:", cat_cols)

# 6) encode categoricals using pd.get_dummies
if cat_cols:
    X_encoded = pd.get_dummies(X_raw, columns=cat_cols, drop_first=False, dtype=float)
else:
    X_encoded = X_raw.copy()
print("\nAfter get_dummies, X_encoded shape:", X_encoded.shape)

# 7) stratified train-test split
X_train, X_test, y_train, y_test = train_test_split(
    X_encoded, y, test_size=0.20, random_state=RANDOM_STATE, stratify=y
)
print("\n✅ Stratified split done:")
print(" X_train:", X_train.shape, " X_test:", X_test.shape)
print(" y_train distribution:", Counter(y_train))
print(" y_test distribution:", Counter(y_test))

# 8) scale numeric columns (fit scaler on train only)
numeric_cols_present = [c for c in numeric_cols if c in X_train.columns]
scaler = RobustScaler()
if numeric_cols_present:
    scaler.fit(X_train[numeric_cols_present])
    X_train_scaled = X_train.copy()
    X_test_scaled = X_test.copy()
    X_train_scaled[numeric_cols_present] = scaler.transform(X_train[numeric_cols_present])
    X_test_scaled[numeric_cols_present] = scaler.transform(X_test[numeric_cols_present])
else:
    X_train_scaled = X_train.copy()
    X_test_scaled = X_test.copy()
print("\n✅ Scaling complete. Numeric columns scaled:", numeric_cols_present)

# 9) detect imbalance and apply SMOTE if needed (robust to different imblearn versions)
major_prop = y_train.value_counts(normalize=True).max()
apply_smote = major_prop > THRESHOLD_IMBALANCE

if apply_smote:
    print(f"\n⚠️ Detected imbalance (majority class proportion = {major_prop:.2f}). Trying to apply SMOTE...")
    # ensure imblearn installed
    try:
        from imblearn.over_sampling import SMOTE
    except Exception:
        print("Installing imbalanced-learn...")
        subprocess.check_call([sys.executable, "-m", "pip", "install", "imbalanced-learn"])
        from imblearn.over_sampling import SMOTE
```

```
    # Attempt to create SMOTE with n_jobs if supported, otherwise fallback
    try:
        sm = SMOTE(random_state=RANDOM_STATE, n_jobs=-1)  # some imblearn versions support n_jobs
    except TypeError:
        sm = SMOTE(random_state=RANDOM_STATE)            # fallback for versions that don't accept n_jobs

    # fit_resample
    X_train_res_np, y_train_res = sm.fit_resample(X_train_scaled, y_train)
    # convert back to DataFrame with same columns
    X_train_res = pd.DataFrame(X_train_res_np, columns=X_train_scaled.columns)
    print("✅ After SMOTE:", Counter(y_train_res))
else:
    print(f"\n✅ No strong imbalance (majority proportion = {major_prop:.2f}). Skipping SMOTE.")
    X_train_res, y_train_res = X_train_scaled.copy(), y_train.copy()

# 10) Save outputs
X_train_res.to_csv("X_train_bal.csv", index=False)
pd.Series(y_train_res, name=LABEL).to_csv("y_train_bal.csv", index=False)
X_test_scaled.to_csv("X_test.csv", index=False)
pd.Series(y_test, name=LABEL).to_csv("y_test.csv", index=False)

print("\n💾 Saved files:")
print(" - X_train_bal.csv (encoded & scaled, resampled if SMOTE applied)")
print(" - y_train_bal.csv")
print(" - X_test.csv (encoded & scaled)")
print(" - y_test.csv")

# 11) diagnostics
print("\n=== Diagnostics Summary ===")
print("Original df shape:", df.shape)
print("X_encoded shape:", X_encoded.shape)
print("X_train_res shape:", X_train_res.shape)
print("X_test shape:", X_test_scaled.shape)
print("Training label counts (post-processed):", Counter(y_train_res))
print("Test label counts:", Counter(y_test))
print("\nSample head of X_train_bal:")
display(X_train_res.head())
```

```
✅ Loaded: df_step2_cleaned.csv | shape: (1000, 16)
✅ Created label '1500_label' from Lifespan >= 1500

Label counts:
1500_label
0    711
1    289
Name: count, dtype: int64

Label proportions:
1500_label
0    0.711
1    0.289
```

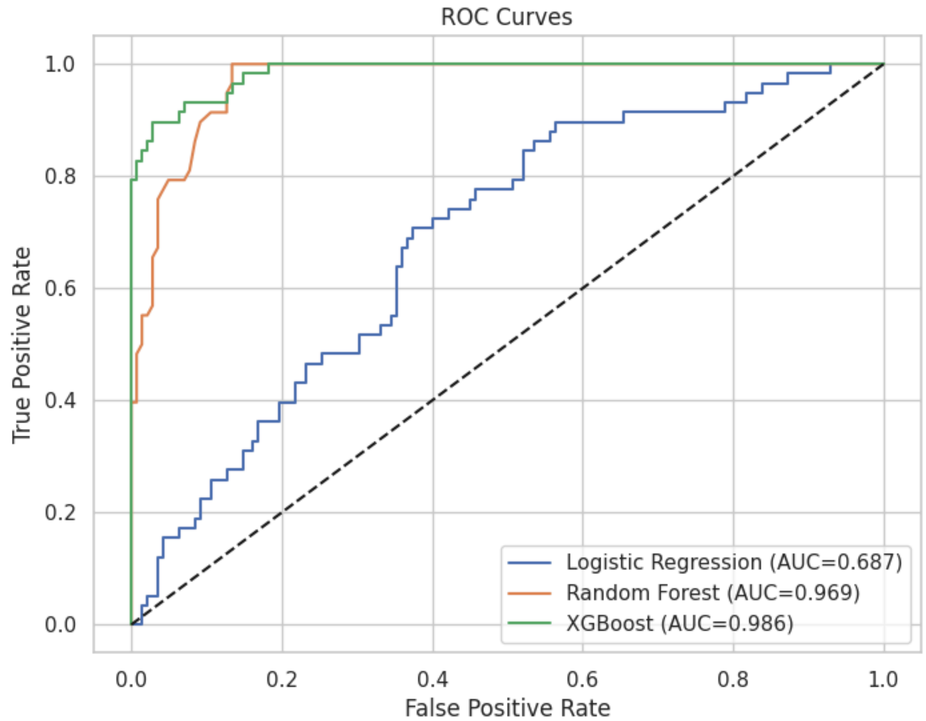
```
# ============================================================
# 🧩 CLASSIFICATION MODELLING – CONTINUATION
# ============================================================

# Imports
from sklearn.linear_model import LogisticRegression
from sklearn.ensemble import RandomForestClassifier
from xgboost import XGBClassifier
from sklearn.model_selection import GridSearchCV, train_test_split
from sklearn.metrics import (
    confusion_matrix, classification_report, roc_auc_score,
    roc_curve, accuracy_score, f1_score
)
import matplotlib.pyplot as plt
import seaborn as sns
import pandas as pd
import numpy as np

# ============================================================
# 1️⃣ Load Processed Data
# ============================================================
try:
    X_train = pd.read_csv("X_train_bal.csv")
    y_train = pd.read_csv("y_train_bal.csv").values.ravel() # Flatten to 1D
    X_test = pd.read_csv("X_test.csv")
    y_test = pd.read_csv("y_test.csv").values.ravel()     # Flatten to 1D
    print("✅ Loaded processed and split data.")
    print(f"Train shape: {X_train.shape}, Test shape: {X_test.shape}")
except FileNotFoundError:
    print("Error: Processed data files not found. Please run the preprocessing step first.")
    # Exit or handle the error appropriately
    exit() # For demonstration, stopping execution


# ============================================================
# 3️⃣ Logistic Regression (GridSearchCV)
# ============================================================
log_reg = LogisticRegression(max_iter=1000, solver='liblinear')
param_grid_lr = {
    'C': [0.01, 0.1, 1, 10],
    'penalty': ['l1', 'l2']
}

grid_lr = GridSearchCV(log_reg, param_grid_lr, cv=5, scoring='f1', n_jobs=-1)
grid_lr.fit(X_train, y_train)

best_lr = grid_lr.best_estimator_
y_pred_lr = best_lr.predict(X_test)
y_prob_lr = best_lr.predict_proba(X_test)[:, 1]

print("\n✅ Best Logistic Regression Parameters:", grid_lr.best_params_)
print("Classification Report (Logistic Regression):")
print(classification_report(y_test, y_pred_lr))

# ============================================================
# 4️⃣ Random Forest Classifier
# ============================================================
rf = RandomForestClassifier(random_state=42)
param_grid_rf = {
    'n_estimators': [100, 200],
    'max_depth': [None, 10, 20],
    'min_samples_split': [2, 5],
    'min_samples_leaf': [1, 2]
}

grid_rf = GridSearchCV(rf, param_grid_rf, cv=5, scoring='f1', n_jobs=-1)
grid_rf.fit(X_train, y_train)

best_rf = grid_rf.best_estimator_
```

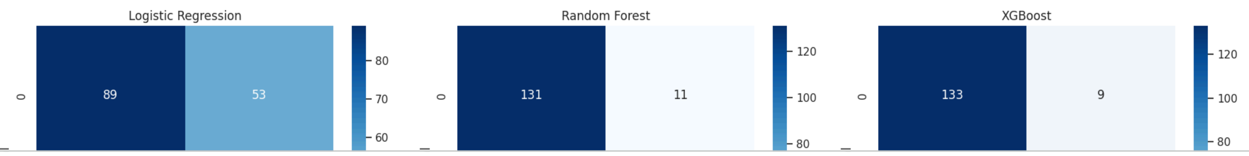
```
y_pred_rf = best_rf.predict(X_test)
y_prob_rf = best_rf.predict_proba(X_test)[:, 1]

print("\n✅ Best Random Forest Parameters:", grid_rf.best_params_)
print("Classification Report (Random Forest):")
print(classification_report(y_test, y_pred_rf))

# ==========================================================
# 5️⃣ XGBoost Classifier
# ==========================================================
xgb = XGBClassifier(
    random_state=42,
    use_label_encoder=False,
    eval_metric='logloss'
)

param_grid_xgb = {
    'n_estimators': [100, 200],
    'max_depth': [3, 5, 7],
    'learning_rate': [0.01, 0.1, 0.2],
    'subsample': [0.8, 1.0]
}

grid_xgb = GridSearchCV(xgb, param_grid_xgb, cv=5, scoring='f1', n_jobs=-1)
grid_xgb.fit(X_train, y_train)

best_xgb = grid_xgb.best_estimator_
y_pred_xgb = best_xgb.predict(X_test)
y_prob_xgb = best_xgb.predict_proba(X_test)[:, 1]

print("\n✅ Best XGBoost Parameters:", grid_xgb.best_params_)
print("Classification Report (XGBoost):")
print(classification_report(y_test, y_pred_xgb))

# ==========================================================
# 6️⃣ Model Comparison Summary
# ==========================================================
results = pd.DataFrame({
    'Model': ['Logistic Regression', 'Random Forest', 'XGBoost'],
    'Accuracy': [
        accuracy_score(y_test, y_pred_lr),
        accuracy_score(y_test, y_pred_rf),
        accuracy_score(y_test, y_pred_xgb)
    ],
    'F1 Score': [
        f1_score(y_test, y_pred_lr),
        f1_score(y_test, y_pred_rf),
        f1_score(y_test, y_pred_xgb)
    ],
    'ROC AUC': [
        roc_auc_score(y_test, y_prob_lr),
        roc_auc_score(y_test, y_prob_rf),
        roc_auc_score(y_test, y_prob_xgb)
    ]
})

print("\n📊 Model Comparison Summary:")
display(results.sort_values(by='F1 Score', ascending=False))

# ==========================================================
# 7️⃣ ROC Curve Plot
# ==========================================================
plt.figure(figsize=(8, 6))
for model_name, y_prob in {
    'Logistic Regression': y_prob_lr,
    'Random Forest': y_prob_rf,
    'XGBoost': y_prob_xgb
}.items():
    fpr, tpr, _ = roc_curve(y_test, y_prob)
    plt.plot(fpr, tpr, label=f'{model_name} (AUC={roc_auc_score(y_test, y_prob):.3f})')

plt.plot([0, 1], [0, 1], 'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Curves')
plt.legend()
plt.show()

# ==========================================================
# 8️⃣ Confusion Matrices
# ==========================================================
fig, axes = plt.subplots(1, 3, figsize=(18, 5))
```

```
for ax, (model_name, y_pred) in zip(
    axes,
    [('Logistic Regression', y_pred_lr),
     ('Random Forest', y_pred_rf),
     ('XGBoost', y_pred_xgb)]
):
    cm = confusion_matrix(y_test, y_pred)
    sns.heatmap(cm, annot=True, fmt='d', cmap='Blues', ax=ax)
    ax.set_title(model_name)
    ax.set_xlabel('Predicted')
    ax.set_ylabel('Actual')
plt.tight_layout()
plt.show()

# ============================================================
# 9️⃣ Feature Importance
# ============================================================
rf_importance = pd.Series(best_rf.feature_importances_, index=X_train.columns)
xgb_importance = pd.Series(best_xgb.feature_importances_, index=X_train.columns)

plt.figure(figsize=(10, 6))
rf_importance.sort_values(ascending=False).head(10).plot(kind='bar')
plt.title("Top 10 Important Features (Random Forest)")
plt.show()

plt.figure(figsize=(10, 6))
xgb_importance.sort_values(ascending=False).head(10).plot(kind='bar', color='orange')
plt.title("Top 10 Important Features (XGBoost)")
plt.show()

# ============================================================
# 🔚 Final Model Selection
# ============================================================
best_model_name = results.sort_values(by='F1 Score', ascending=False).iloc[0]['Model']
print(f"\n🏁 Best performing classification model: {best_model_name}")
```

```
✅ Loaded processed and split data.
Train shape: (1138, 23), Test shape: (200, 23)

✅ Best Logistic Regression Parameters: {'C': 0.1, 'penalty': 'l1'}
Classification Report (Logistic Regression):
              precision    recall  f1-score   support

           0       0.84      0.63      0.72       142
           1       0.44      0.71      0.54        58

    accuracy                           0.65       200
   macro avg       0.64      0.67      0.63       200
weighted avg       0.72      0.65      0.67       200


✅ Best Random Forest Parameters: {'max_depth': None, 'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimat
Classification Report (Random Forest):
              precision    recall  f1-score   support

           0       0.92      0.92      0.92       142
           1       0.81      0.81      0.81        58

    accuracy                           0.89       200
   macro avg       0.87      0.87      0.87       200
weighted avg       0.89      0.89      0.89       200

/usr/local/lib/python3.12/dist-packages/xgboost/training.py:199: UserWarning: [20:10:52] WARNING: /workspace/sr
Parameters: { "use_label_encoder" } are not used.

  bst.update(dtrain, iteration=i, fobj=obj)

✅ Best XGBoost Parameters: {'learning_rate': 0.1, 'max_depth': 7, 'n_estimators': 100, 'subsample': 0.8}
Classification Report (XGBoost):
              precision    recall  f1-score   support

           0       0.96      0.94      0.95       142
           1       0.85      0.90      0.87        58

    accuracy                           0.93       200
   macro avg       0.90      0.92      0.91       200
weighted avg       0.93      0.93      0.93       200


📊 Model Comparison Summary:
```

	Model	Accuracy	F1 Score	ROC AUC
2	XGBoost	0.925	0.873950	0.985673
1	Random Forest	0.890	0.810345	0.969160
0	Logistic Regression	0.650	0.539474	0.687105





```
# ============================================================
# ⚙️ FIXED ADVANCED HYPERPARAMETER TUNING — XGBoost CLASSIFIER
# ============================================================

from sklearn.model_selection import GridSearchCV, StratifiedKFold
from xgboost import XGBClassifier
from imblearn.over_sampling import SMOTE
from imblearn.pipeline import Pipeline as ImbPipeline
from sklearn.preprocessing import OneHotEncoder, StandardScaler
from sklearn.compose import ColumnTransformer
from sklearn.pipeline import Pipeline

# ✅ Rebuild preprocessor from X_train
cat_cols = [c for c in X_train.columns if X_train[c].dtype == "object"]
num_cols = [c for c in X_train.columns if X_train[c].dtype != "object"]

numeric_transformer = Pipeline(steps=[
    ('scaler', StandardScaler())
])
categorical_transformer = Pipeline(steps=[
    ('onehot', OneHotEncoder(handle_unknown='ignore'))
])

preprocessor = ColumnTransformer(
    transformers=[
        ('num', numeric_transformer, num_cols),
        ('cat', categorical_transformer, cat_cols)
    ]
)

# ✅ Build fresh XGBoost pipeline with SMOTE
xgb_pipeline = ImbPipeline(steps=[
    ('preprocessor', preprocessor),
    ('smote', SMOTE(random_state=42)),
    ('classifier', XGBClassifier(
        eval_metric='logloss',
        random_state=42,
        use_label_encoder=False
    ))
])

# ✅ Reduced but still powerful parameter grid
param_grid_xgb = {
    'classifier__n_estimators': [200, 400],
    'classifier__max_depth': [4, 6, 8],
    'classifier__learning_rate': [0.03, 0.1],
    'classifier__subsample': [0.8, 1.0],
    'classifier__colsample_bytree': [0.8, 1.0],
    'classifier__min_child_weight': [1, 3],
    'classifier__gamma': [0, 0.2]
}

cv_strategy = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)

grid_xgb_tuned = GridSearchCV(
    estimator=xgb_pipeline,
    param_grid=param_grid_xgb,
    cv=cv_strategy,
    scoring='f1',
    n_jobs=-1,
    verbose=2
)

print("🔍 Running advanced XGBoost tuning (reduced grid, fixed preprocessor)... ⏳")

grid_xgb_tuned.fit(X_train, y_train)

print("\n✅ Best Parameters Found:")
print(grid_xgb_tuned.best_params_)

# ============================================================
# 📊 Evaluate Tuned Model
# ============================================================
best_xgb_tuned = grid_xgb_tuned.best_estimator_
y_pred_tuned = best_xgb_tuned.predict(X_test)
y_prob_tuned = best_xgb_tuned.predict_proba(X_test)[:, 1]

acc_tuned = accuracy_score(y_test, y_pred_tuned)
f1_tuned = f1_score(y_test, y_pred_tuned)
auc_tuned = roc_auc_score(y_test, y_prob_tuned)

print("\n📈 Tuned XGBoost Performance:")
```

```
print(f"Accuracy: {acc_tuned:.3f}")
print(f"F1 Score: {f1_tuned:.3f}")
print(f"ROC AUC: {auc_tuned:.3f}")
print("\nClassification Report:")
print(classification_report(y_test, y_pred_tuned))

# Confusion Matrix
plt.figure(figsize=(5,4))
sns.heatmap(confusion_matrix(y_test, y_pred_tuned), annot=True, fmt='d', cmap='Blues')
plt.title("Confusion Matrix - Tuned XGBoost")
plt.xlabel("Predicted")
plt.ylabel("Actual")
plt.show()

# ROC Curve
fpr, tpr, _ = roc_curve(y_test, y_prob_tuned)
plt.figure(figsize=(6,5))
plt.plot(fpr, tpr, label=f"Tuned XGBoost (AUC={auc_tuned:.3f})", color='darkorange')
plt.plot([0,1],[0,1],'k--')
plt.xlabel("False Positive Rate")
plt.ylabel("True Positive Rate")
plt.title("ROC Curve - Tuned XGBoost")
plt.legend()
plt.show()

print("\n🏁 XGBoost tuning completed successfully 🎯")
```