

task

June 18, 2025

1 Data loading and EDA

```
[1]: import pandas as pd
import numpy as np
import torch
import seaborn as sns
import matplotlib.pyplot as plt
```

```
[2]: # load the dataset
df = pd.read_csv('./data_ML.csv')
df
```

```
[2]:
```

	asset_price	maturity	rate	div	ivol	american_op
0	113.935171	0.285741	0.008467	0.023575	0.538127	6.612107
1	98.305405	0.813916	0.019547	0.018027	0.048863	2.626842
2	109.189731	0.713558	0.022951	0.015280	0.303538	6.430745
3	83.402084	2.879962	0.042272	0.058719	0.163288	20.903553
4	127.549831	0.907992	0.026664	0.017533	0.562713	12.156191
...
100450	76.042759	0.102861	0.025629	0.034502	0.171373	23.964726
100451	102.305683	0.832775	0.028396	0.005028	0.315285	9.583641
100452	75.284271	2.685636	0.053380	0.023887	0.298182	27.715600
100453	122.245305	4.843896	0.003533	0.034317	0.287358	22.513776
100454	104.543032	0.648455	0.049105	0.069530	0.415862	11.625611

[100455 rows x 6 columns]

```
[3]: # check for missing values (if any)
df.isnull().sum()
```

```
[3]: asset_price    0
maturity          0
rate              0
div              0
ivol             0
american_op       0
dtype: int64
```

```
[4]: # Check the data types and basic information
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 100455 entries, 0 to 100454
Data columns (total 6 columns):
#   Column          Non-Null Count  Dtype
---  -
0   asset_price     100455 non-null float64
1   maturity        100455 non-null float64
2   rate            100455 non-null float64
3   div             100455 non-null float64
4   ivol            100455 non-null float64
5   american_op     100455 non-null float64
dtypes: float64(6)
memory usage: 4.6 MB
```

```
[5]: # Generate descriptive statistics
df.describe().T
```

```
[5]:
```

	count	mean	std	min	25%	\
asset_price	100455.0	98.141144	16.859969	7.000066e+01	83.673626	
maturity	100455.0	1.214371	1.256565	1.000099e-01	0.423637	
rate	100455.0	0.034799	0.024509	5.430000e-07	0.015554	
div	100455.0	0.035258	0.024718	5.430000e-07	0.015851	
ivol	100455.0	0.339526	0.156516	1.500000e-05	0.213415	
american_op	100455.0	15.961782	10.663400	5.001207e-01	6.905906	

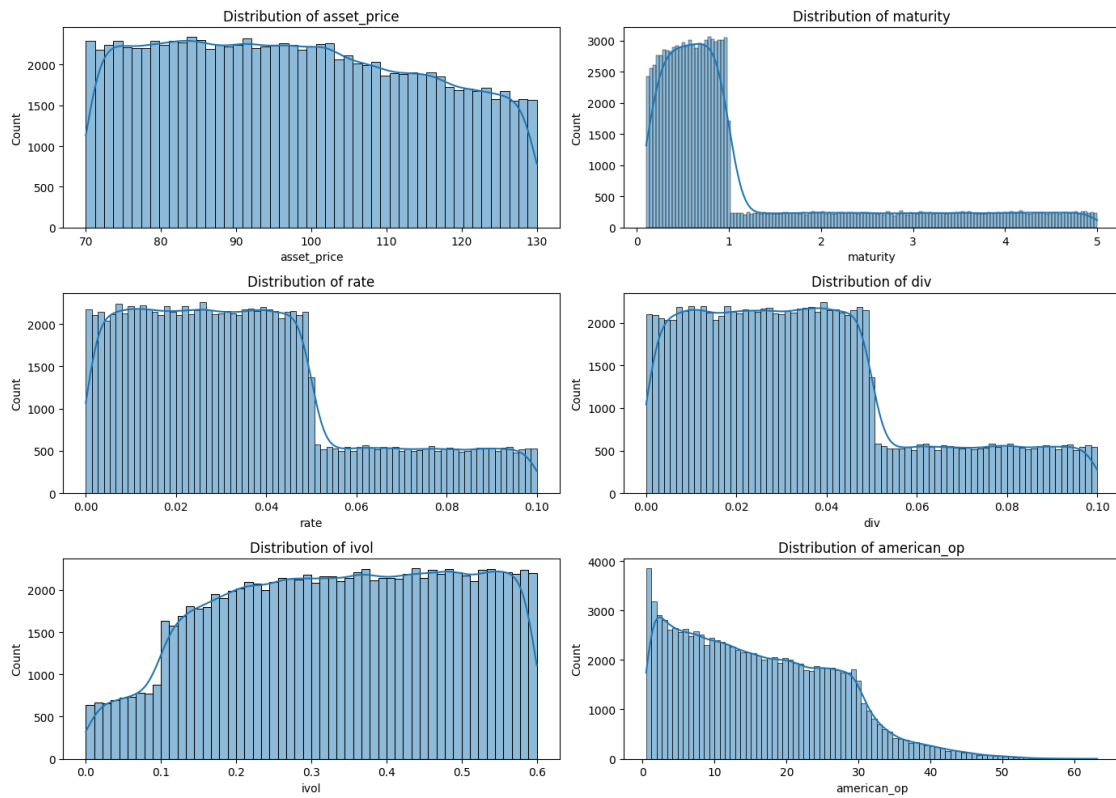
	50%	75%	max
asset_price	97.373486	112.142653	129.999578
maturity	0.725755	1.246729	4.999891
rate	0.031079	0.046666	0.099998
div	0.031543	0.047077	0.099993
ivol	0.345592	0.473691	0.599988
american_op	14.696291	23.921224	63.146473

1.1 Data Visualization - Distributions and Relationships

```
[6]: # Create histograms for all numerical features
plt.figure(figsize=(14, 10))

for i, column in enumerate(df.columns):
    plt.subplot(3, 2, i+1)
    sns.histplot(df[column], kde=True)
    plt.title(f'Distribution of {column}')
    plt.tight_layout()
```

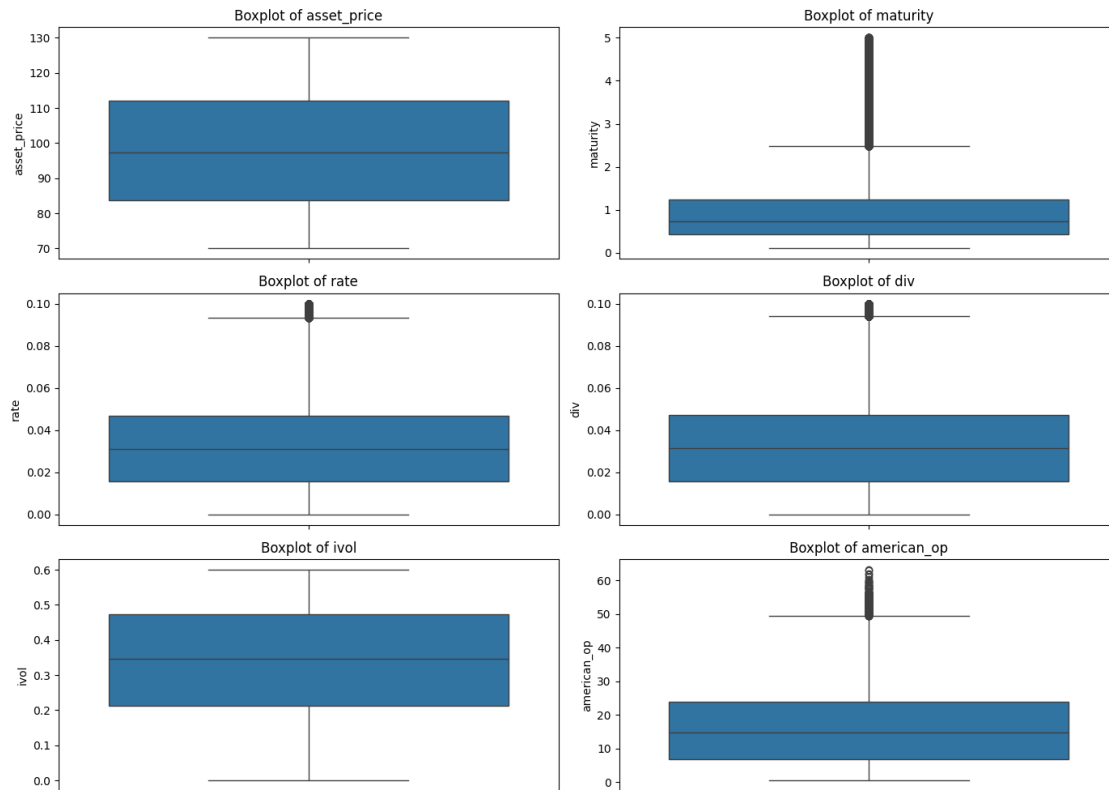
```
plt.show()
```



```
[7]: # Create boxplots for all numerical features
plt.figure(figsize=(14, 10))

for i, column in enumerate(df.columns):
    plt.subplot(3, 2, i+1)
    sns.boxplot(y=df[column])
    plt.title(f'Boxplot of {column}')
    plt.tight_layout()

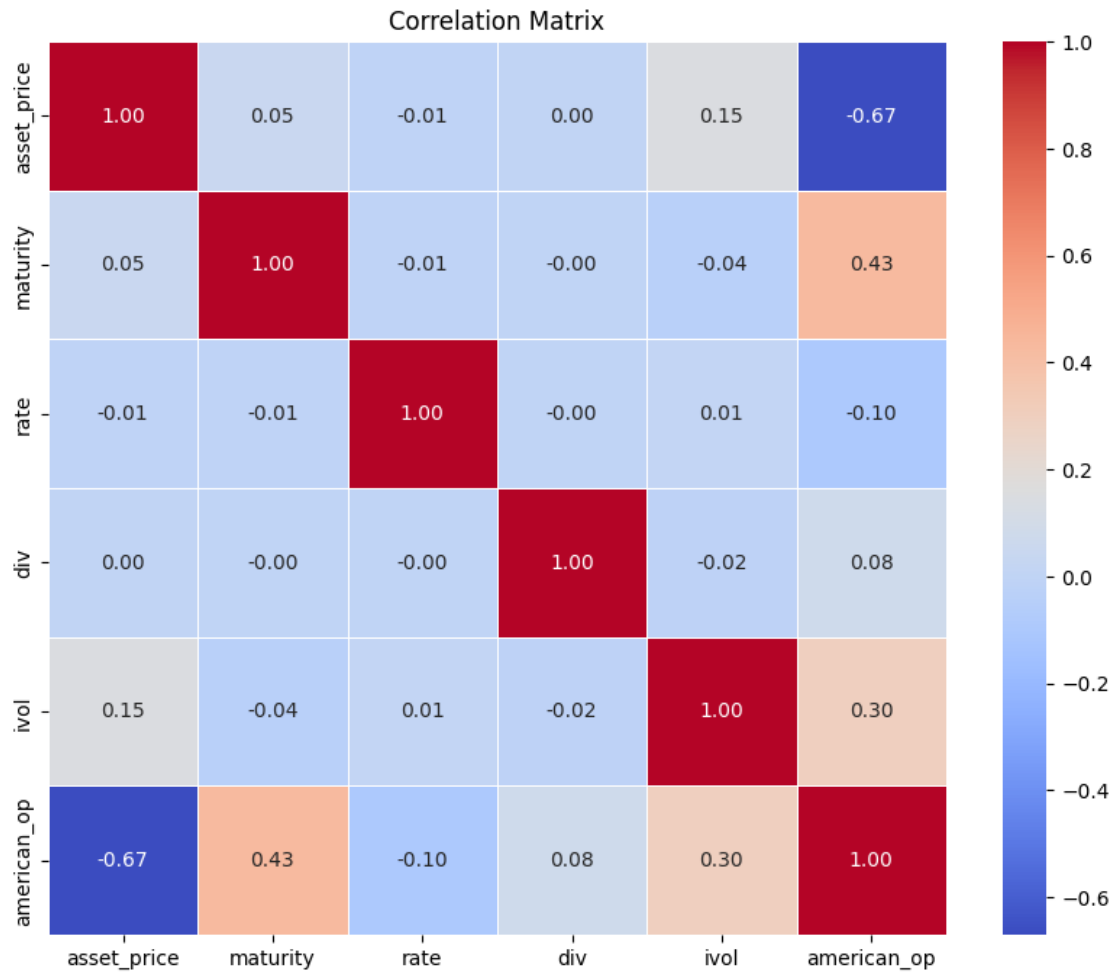
plt.show()
```



1.2 Correlation Analysis

```
[8]: # Calculate and visualize the correlation matrix
corr_matrix = df.corr()
plt.figure(figsize=(10, 8))
sns.heatmap(corr_matrix, annot=True, cmap='coolwarm', fmt='.2f', linewidths=0.5)
plt.title('Correlation Matrix')
plt.show()

# Print the correlations with american_op (target variable)
print("\nCorrelations with american_op:")
corr_with_target = corr_matrix['american_op'].sort_values(ascending=False)
print(corr_with_target)
```



```
Correlations with american_op:
american_op    1.000000
maturity        0.427901
ivol            0.296504
div             0.078785
rate            -0.097986
asset_price     -0.670509
Name: american_op, dtype: float64
```

1.3 Feature Relationships with Target Variable

```
[9]: # Scatter plots of features vs target variable
plt.figure(figsize=(14, 10))

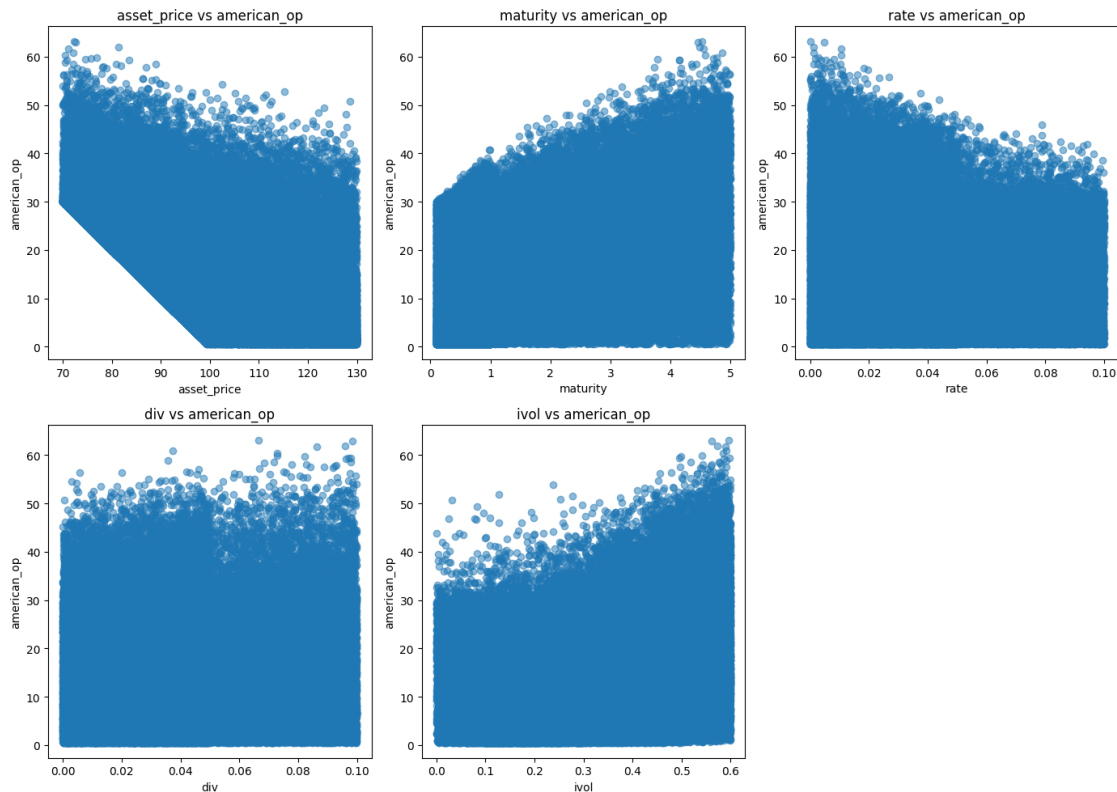
features = [col for col in df.columns if col != 'american_op']
```

```

for i, feature in enumerate(features):
    plt.subplot(2, 3, i+1)
    plt.scatter(df[feature], df['american_op'], alpha=0.5)
    plt.title(f'{feature} vs american_op')
    plt.xlabel(feature)
    plt.ylabel('american_op')
    plt.tight_layout()

plt.show()

```



1.4 Outlier Analysis and Treatment

```

[10]: # Function to detect outliers using IQR method
def detect_outliers_iqr(df, column):
    Q1 = df[column].quantile(0.25)
    Q3 = df[column].quantile(0.75)
    IQR = Q3 - Q1
    lower_bound = Q1 - 1.5 * IQR
    upper_bound = Q3 + 1.5 * IQR
    outliers = df[(df[column] < lower_bound) | (df[column] > upper_bound)]
    return outliers, lower_bound, upper_bound

```

```

# Check outliers for each feature
for column in df.columns:
    outliers, lower_bound, upper_bound = detect_outliers_iqr(df, column)
    outlier_percentage = len(outliers) / len(df) * 100
    print(f"Feature: {column}")
    print(f"Number of outliers: {len(outliers)} ({outlier_percentage:.2f}%)")
    print(f"Lower bound: {lower_bound:.4f}, Upper bound: {upper_bound:.4f}\n")

```

```

Feature: asset_price
Number of outliers: 0 (0.00%)
Lower bound: 40.9701, Upper bound: 154.8462

```

```

Feature: maturity
Number of outliers: 16904 (16.83%)
Lower bound: -0.8110, Upper bound: 2.4814

```

```

Feature: rate
Number of outliers: 2600 (2.59%)
Lower bound: -0.0311, Upper bound: 0.0933

```

```

Feature: div
Number of outliers: 2495 (2.48%)
Lower bound: -0.0310, Upper bound: 0.0939

```

```

Feature: ivol
Number of outliers: 0 (0.00%)
Lower bound: -0.1770, Upper bound: 0.8641

```

```

Feature: american_op
Number of outliers: 281 (0.28%)
Lower bound: -18.6171, Upper bound: 49.4442

```

```

[11]: # Using modified Z-score method to detect outliers
def modified_z_score(df, column):
    median = df[column].median()
    mad = np.median(np.abs(df[column] - median))
    modified_z_scores = 0.6745 * (df[column] - median) / mad
    return modified_z_scores
# Check outliers using modified Z-score
for column in df.columns:
    z_scores = modified_z_score(df, column)
    outliers = df[np.abs(z_scores) > 3.5]
    outlier_percentage = len(outliers) / len(df) * 100
    print(f"Feature: {column}")

```

```
print(f"Number of outliers (modified Z-score): {len(outliers)}\n")
↳({outlier_percentage:.2f}%)\n")
```

Feature: asset_price

Number of outliers (modified Z-score): 0 (0.00%)

Feature: maturity

Number of outliers (modified Z-score): 17618 (17.54%)

Feature: rate

Number of outliers (modified Z-score): 0 (0.00%)

Feature: div

Number of outliers (modified Z-score): 0 (0.00%)

Feature: ivol

Number of outliers (modified Z-score): 0 (0.00%)

Feature: american_op

Number of outliers (modified Z-score): 15 (0.01%)

we can see that the ‘maturity’ column column has the most amount of outliers and they make up to 17% of the total number of data

Since in this case the outliers isn’t indicated to be a form of measure error it’s a valid measure and thus I will keep them in the data

1.5 Machine Learning Model Preparation

```
[12]: from sklearn.model_selection import train_test_split
      from sklearn.preprocessing import StandardScaler
      from sklearn.pipeline import Pipeline

      # Prepare the data for machine learning
      X = df.drop('american_op', axis=1)
      y = df['american_op']

      # Split the data into training and testing sets
      X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
↳random_state=42)
      X_test, X_validation, y_test, y_validation = train_test_split(X_test, y_test,
↳test_size=0.5, random_state=42)
      print(f"Training data shape: {X_train.shape}")
      print(f"Testing data shape: {X_test.shape}")
      print(f"Validation data shape: {X_validation.shape}")
      print(f"Training labels shape: {y_train.shape}")
      print(f"Testing labels shape: {y_test.shape}")
```



```
print(f"Validation labels shape: {y_validation.shape}")
```

```
Training data shape: (80364, 5)
Testing data shape: (10045, 5)
Validation data shape: (10046, 5)
Training labels shape: (80364,)
Testing labels shape: (10045,)
Validation labels shape: (10046,)
```

2 Models

```
[13]: def mean_relative_error(y_true, y_pred):
        return np.mean(np.abs((y_true - y_pred) / y_true))
```

```
[54]: from sklearn.model_selection import KFold
        from sklearn.svm import SVR
        from sklearn.linear_model import Ridge
        import optuna

        def objective_ridge(trial):
            params = {
                'alpha' : trial.suggest_float('alpha', 1e-4, 1e2, log=True)
            }

            pipeline = Pipeline([
                ('scaler', StandardScaler()),
                ('ridge', Ridge(**params))
            ])

            # Manual cross-validation loop to use custom metric
            kf = KFold(n_splits=2, shuffle=True, random_state=42)
            errors = []

            for train_idx, val_idx in kf.split(X_train):
                X_fold_train, X_fold_val = X_train.iloc[train_idx], X_train.
↪iloc[val_idx]
                y_fold_train, y_fold_val = y_train.iloc[train_idx], y_train.
↪iloc[val_idx]

                pipeline.fit(X_fold_train, y_fold_train)
                y_pred = pipeline.predict(X_fold_val)

                error = mean_relative_error(y_fold_val, y_pred)
                errors.append(error)
```

```

    print(f"Trial {trial.number}: {params} -> Mean Relative Error: {np.
↪mean(errors)}")

    return np.mean(errors) # lower is better

study = optuna.create_study(direction='minimize')
study.optimize(objective_ridge, n_trials=50, n_jobs=4)

print("Best params:", study.best_params)

```

```

[I 2025-06-18 14:28:27,682] A new study created in memory with name: no-
name-0d39f6a9-3f64-4c5c-9661-d188e505fba8
[I 2025-06-18 14:28:27,999] Trial 1 finished with value: 0.4314018275003441 and
parameters: {'alpha': 0.000103337222274179}. Best is trial 1 with value:
0.4314018275003441.
[I 2025-06-18 14:28:28,007] Trial 3 finished with value: 0.4314018185473521 and
parameters: {'alpha': 0.0022607457564932285}. Best is trial 3 with value:
0.4314018185473521.
[I 2025-06-18 14:28:28,003] Trial 2 finished with value: 0.4314018264445346 and
parameters: {'alpha': 0.00035775632920659914}. Best is trial 2 with value:
0.4314018264445346.
[I 2025-06-18 14:28:28,046] Trial 0 finished with value: 0.43140009022540765 and
parameters: {'alpha': 0.4188364297900802}. Best is trial 0 with value:
0.43140009022540765.
[I 2025-06-18 14:28:28,179] Trial 5 finished with value: 0.43140182496823154 and
parameters: {'alpha': 0.0007135020743681785}. Best is trial 0 with value:
0.43140009022540765.

Trial 1: {'alpha': 0.000103337222274179} -> Mean Relative Error:
0.4314018275003441
Trial 2: {'alpha': 0.00035775632920659914} -> Mean Relative Error:
0.4314018264445346
Trial 3: {'alpha': 0.0022607457564932285} -> Mean Relative Error:
0.4314018185473521
Trial 0: {'alpha': 0.4188364297900802} -> Mean Relative Error:
0.43140009022540765
Trial 5: {'alpha': 0.0007135020743681785} -> Mean Relative Error:
0.43140182496823154

[I 2025-06-18 14:28:28,214] Trial 4 finished with value: 0.43140182683854034 and
parameters: {'alpha': 0.00026281252751690957}. Best is trial 0 with value:
0.43140009022540765.
[I 2025-06-18 14:28:28,273] Trial 6 finished with value: 0.431401768754785 and
parameters: {'alpha': 0.014259298915322237}. Best is trial 0 with value:
0.43140009022540765.
[I 2025-06-18 14:28:28,291] Trial 7 finished with value: 0.4314018270338846 and
parameters: {'alpha': 0.00021574028595922027}. Best is trial 0 with value:
0.43140009022540765.

```

Trial 4: {'alpha': 0.00026281252751690957} -> Mean Relative Error:
 0.43140182683854034
 Trial 6: {'alpha': 0.014259298915322237} -> Mean Relative Error:
 0.431401768754785
 Trial 7: {'alpha': 0.00021574028595922027} -> Mean Relative Error:
 0.4314018270338846

 [I 2025-06-18 14:28:28,422] Trial 9 finished with value: 0.43140141491187284 and
 parameters: {'alpha': 0.09952531902707606}. Best is trial 0 with value:
 0.43140009022540765.
 [I 2025-06-18 14:28:28,473] Trial 8 finished with value: 0.4314017849597077 and
 parameters: {'alpha': 0.010354385392701528}. Best is trial 0 with value:
 0.43140009022540765.
 [I 2025-06-18 14:28:28,519] Trial 10 finished with value: 0.43139950541009886
 and parameters: {'alpha': 0.5598136304507829}. Best is trial 10 with value:
 0.43139950541009886.
 [I 2025-06-18 14:28:28,548] Trial 11 finished with value: 0.4314018021494426 and
 parameters: {'alpha': 0.0062121617645211425}. Best is trial 10 with value:
 0.43139950541009886.

 Trial 9: {'alpha': 0.09952531902707606} -> Mean Relative Error:
 0.43140141491187284
 Trial 8: {'alpha': 0.010354385392701528} -> Mean Relative Error:
 0.4314017849597077
 Trial 10: {'alpha': 0.5598136304507829} -> Mean Relative Error:
 0.43139950541009886
 Trial 11: {'alpha': 0.0062121617645211425} -> Mean Relative Error:
 0.4314018021494426

 [I 2025-06-18 14:28:28,661] Trial 12 finished with value: 0.43135640554906973
 and parameters: {'alpha': 11.04010770346246}. Best is trial 12 with value:
 0.43135640554906973.
 [I 2025-06-18 14:28:28,730] Trial 13 finished with value: 0.4313052524375989 and
 parameters: {'alpha': 23.673746111010107}. Best is trial 13 with value:
 0.4313052524375989.
 [I 2025-06-18 14:28:28,747] Trial 15 finished with value: 0.43136171647708765
 and parameters: {'alpha': 9.740430731315513}. Best is trial 13 with value:
 0.4313052524375989.
 [I 2025-06-18 14:28:28,774] Trial 14 finished with value: 0.43132109841673766
 and parameters: {'alpha': 19.724684629684823}. Best is trial 13 with value:
 0.4313052524375989.
 [I 2025-06-18 14:28:28,826] Trial 16 finished with value: 0.4312241202983594 and
 parameters: {'alpha': 44.35197794221865}. Best is trial 16 with value:
 0.4312241202983594.
 [I 2025-06-18 14:28:28,858] Trial 17 finished with value: 0.43124381124719413
 and parameters: {'alpha': 39.25369536449318}. Best is trial 16 with value:
 0.4312241202983594.

 Trial 12: {'alpha': 11.04010770346246} -> Mean Relative Error:
 0.43135640554906973

Trial 13: {'alpha': 23.673746111010107} -> Mean Relative Error:
 0.4313052524375989
 Trial 15: {'alpha': 9.740430731315513} -> Mean Relative Error:
 0.43136171647708765
 Trial 14: {'alpha': 19.724684629684823} -> Mean Relative Error:
 0.43132109841673766
 Trial 16: {'alpha': 44.35197794221865} -> Mean Relative Error:
 0.4312241202983594
 Trial 17: {'alpha': 39.25369536449318} -> Mean Relative Error:
 0.43124381124719413

 [I 2025-06-18 14:28:28,884] Trial 18 finished with value: 0.43107904222444543
 and parameters: {'alpha': 83.5104765922863}. Best is trial 18 with value:
 0.43107904222444543.
 [I 2025-06-18 14:28:28,892] Trial 19 finished with value: 0.4311505997681697 and
 parameters: {'alpha': 63.90322977566515}. Best is trial 18 with value:
 0.43107904222444543.
 [I 2025-06-18 14:28:28,992] Trial 20 finished with value: 0.43117399622751384
 and parameters: {'alpha': 57.60762507718022}. Best is trial 18 with value:
 0.43107904222444543.
 [I 2025-06-18 14:28:29,010] Trial 22 finished with value: 0.43103673686140787
 and parameters: {'alpha': 95.2759055925123}. Best is trial 22 with value:
 0.43103673686140787.
 [I 2025-06-18 14:28:29,017] Trial 21 finished with value: 0.43139209965442354
 and parameters: {'alpha': 2.3501764923385036}. Best is trial 22 with value:
 0.43103673686140787.
 [I 2025-06-18 14:28:29,065] Trial 23 finished with value: 0.43138939582676045
 and parameters: {'alpha': 3.0048682059480813}. Best is trial 22 with value:
 0.43103673686140787.

 Trial 18: {'alpha': 83.5104765922863} -> Mean Relative Error:
 0.43107904222444543
 Trial 19: {'alpha': 63.90322977566515} -> Mean Relative Error:
 0.4311505997681697
 Trial 20: {'alpha': 57.60762507718022} -> Mean Relative Error:
 0.43117399622751384
 Trial 22: {'alpha': 95.2759055925123} -> Mean Relative Error:
 0.43103673686140787
 Trial 21: {'alpha': 2.3501764923385036} -> Mean Relative Error:
 0.43139209965442354
 Trial 23: {'alpha': 3.0048682059480813} -> Mean Relative Error:
 0.43138939582676045

 [I 2025-06-18 14:28:29,200] Trial 25 finished with value: 0.4313877723795807 and
 parameters: {'alpha': 3.3980163760430773}. Best is trial 22 with value:
 0.43103673686140787.
 [I 2025-06-18 14:28:29,204] Trial 24 finished with value: 0.4313795905053427 and
 parameters: {'alpha': 5.384474655620788}. Best is trial 22 with value:
 0.43103673686140787.

[I 2025-06-18 14:28:29,223] Trial 26 finished with value: 0.43138788997413297 and parameters: {'alpha': 3.369506424842119}. Best is trial 22 with value: 0.43103673686140787.

[I 2025-06-18 14:28:29,319] Trial 27 finished with value: 0.43138916268326455 and parameters: {'alpha': 3.0613215141403374}. Best is trial 22 with value: 0.43103673686140787.

Trial 25: {'alpha': 3.3980163760430773} -> Mean Relative Error: 0.4313877723795807

Trial 24: {'alpha': 5.384474655620788} -> Mean Relative Error: 0.4313795905053427

Trial 26: {'alpha': 3.369506424842119} -> Mean Relative Error: 0.43138788997413297

Trial 27: {'alpha': 3.0613215141403374} -> Mean Relative Error: 0.43138916268326455

[I 2025-06-18 14:28:29,455] Trial 29 finished with value: 0.4310831479212449 and parameters: {'alpha': 82.37516340630408}. Best is trial 22 with value: 0.43103673686140787.

[I 2025-06-18 14:28:29,490] Trial 28 finished with value: 0.4311558170060943 and parameters: {'alpha': 62.49284719580505}. Best is trial 22 with value: 0.43103673686140787.

[I 2025-06-18 14:28:29,505] Trial 30 finished with value: 0.43120362827571 and parameters: {'alpha': 49.73459341772111}. Best is trial 22 with value: 0.43103673686140787.

[I 2025-06-18 14:28:29,576] Trial 31 finished with value: 0.43105012685579425 and parameters: {'alpha': 91.5319061429626}. Best is trial 22 with value: 0.43103673686140787.

Trial 29: {'alpha': 82.37516340630408} -> Mean Relative Error: 0.4310831479212449

Trial 28: {'alpha': 62.49284719580505} -> Mean Relative Error: 0.4311558170060943

Trial 30: {'alpha': 49.73459341772111} -> Mean Relative Error: 0.43120362827571

Trial 31: {'alpha': 91.5319061429626} -> Mean Relative Error: 0.43105012685579425

[I 2025-06-18 14:28:29,725] Trial 32 finished with value: 0.43139871451379636 and parameters: {'alpha': 0.7504830552659106}. Best is trial 22 with value: 0.43103673686140787.

[I 2025-06-18 14:28:29,791] Trial 34 finished with value: 0.431397536003868 and parameters: {'alpha': 1.0346020513081717}. Best is trial 22 with value: 0.43103673686140787.

[I 2025-06-18 14:28:29,813] Trial 33 finished with value: 0.43140013076620265 and parameters: {'alpha': 0.4090636309937964}. Best is trial 22 with value: 0.43103673686140787.

[I 2025-06-18 14:28:29,833] Trial 35 finished with value: 0.4310554096000776 and parameters: {'alpha': 90.06166650985058}. Best is trial 22 with value: 0.43103673686140787.

Trial 32: {'alpha': 0.7504830552659106} -> Mean Relative Error:
 0.43139871451379636
 Trial 34: {'alpha': 1.0346020513081717} -> Mean Relative Error:
 0.431397536003868
 Trial 33: {'alpha': 0.4090636309937964} -> Mean Relative Error:
 0.43140013076620265
 Trial 35: {'alpha': 90.06166650985058} -> Mean Relative Error:
 0.4310554096000776

 [I 2025-06-18 14:28:30,001] Trial 36 finished with value: 0.43106875090010055
 and parameters: {'alpha': 86.35917630758433}. Best is trial 22 with value:
 0.43103673686140787.
 [I 2025-06-18 14:28:30,039] Trial 37 finished with value: 0.4310287494972188 and
 parameters: {'alpha': 97.51325086254347}. Best is trial 37 with value:
 0.4310287494972188.
 [I 2025-06-18 14:28:30,130] Trial 38 finished with value: 0.4310335592378107 and
 parameters: {'alpha': 96.16546305216293}. Best is trial 37 with value:
 0.4310287494972188.
 [I 2025-06-18 14:28:30,137] Trial 39 finished with value: 0.43132666756105864
 and parameters: {'alpha': 18.34149776750626}. Best is trial 37 with value:
 0.4310287494972188.

 Trial 36: {'alpha': 86.35917630758433} -> Mean Relative Error:
 0.43106875090010055
 Trial 37: {'alpha': 97.51325086254347} -> Mean Relative Error:
 0.4310287494972188
 Trial 38: {'alpha': 96.16546305216293} -> Mean Relative Error:
 0.4310335592378107
 Trial 39: {'alpha': 18.34149776750626} -> Mean Relative Error:
 0.43132666756105864

 [I 2025-06-18 14:28:30,268] Trial 40 finished with value: 0.43132664575365276
 and parameters: {'alpha': 18.346901295661876}. Best is trial 37 with value:
 0.4310287494972188.
 [I 2025-06-18 14:28:30,377] Trial 41 finished with value: 0.4313256853498372 and
 parameters: {'alpha': 18.58495010764076}. Best is trial 37 with value:
 0.4310287494972188.
 [I 2025-06-18 14:28:30,431] Trial 42 finished with value: 0.43134564018347205
 and parameters: {'alpha': 13.676230709885424}. Best is trial 37 with value:
 0.4310287494972188.

 Trial 40: {'alpha': 18.346901295661876} -> Mean Relative Error:
 0.43132664575365276
 Trial 41: {'alpha': 18.58495010764076} -> Mean Relative Error:
 0.4313256853498372
 Trial 42: {'alpha': 13.676230709885424} -> Mean Relative Error:
 0.43134564018347205

 [I 2025-06-18 14:28:30,495] Trial 43 finished with value: 0.43136302272156923
 and parameters: {'alpha': 9.4209261023875}. Best is trial 37 with value:

0.4310287494972188.
[I 2025-06-18 14:28:30,547] Trial 44 finished with value: 0.43136716679085896 and parameters: {'alpha': 8.410220909170635}. Best is trial 37 with value: 0.4310287494972188.
[I 2025-06-18 14:28:30,661] Trial 46 finished with value: 0.4314015863225624 and parameters: {'alpha': 0.058220197498636966}. Best is trial 37 with value: 0.4310287494972188.
Trial 43: {'alpha': 9.4209261023875} -> Mean Relative Error: 0.43136302272156923
Trial 44: {'alpha': 8.410220909170635} -> Mean Relative Error: 0.43136716679085896
Trial 46: {'alpha': 0.058220197498636966} -> Mean Relative Error: 0.4314015863225624
[I 2025-06-18 14:28:30,702] Trial 45 finished with value: 0.4313623041623347 and parameters: {'alpha': 9.596630088602536}. Best is trial 37 with value: 0.4310287494972188.
[I 2025-06-18 14:28:30,791] Trial 47 finished with value: 0.43105736095477165 and parameters: {'alpha': 89.51908180271829}. Best is trial 37 with value: 0.4310287494972188.
[I 2025-06-18 14:28:30,805] Trial 48 finished with value: 0.43127369826486506 and parameters: {'alpha': 31.61805128480001}. Best is trial 37 with value: 0.4310287494972188.
[I 2025-06-18 14:28:30,823] Trial 49 finished with value: 0.4312684917338869 and parameters: {'alpha': 32.94030735990675}. Best is trial 37 with value: 0.4310287494972188.
Trial 45: {'alpha': 9.596630088602536} -> Mean Relative Error: 0.4313623041623347
Trial 47: {'alpha': 89.51908180271829} -> Mean Relative Error: 0.43105736095477165
Trial 48: {'alpha': 31.61805128480001} -> Mean Relative Error: 0.43127369826486506
Trial 49: {'alpha': 32.94030735990675} -> Mean Relative Error: 0.4312684917338869
Best params: {'alpha': 97.51325086254347}

```
[55]: model_svr = Ridge(**study.best_params)
      pipeline = Pipeline([
          ('scaler', StandardScaler()),
          ('svr', model_svr)
      ])
      pipeline.fit(X_train, y_train)
      # test the model
      y_pred = pipeline.predict(X_test)
      print("Mean Relative Error on Test Set:", mean_relative_error(y_test, y_pred))
```

Mean Relative Error on Test Set: 0.42087284869647335

We can see a high MRE then we try another better model (previous one was linear model)

```

[16]: import xgboost as xgb

def objective_xgb(trial):
    params = {
        'n_estimators': trial.suggest_int('n_estimators', 200, 1000),
        'max_depth': trial.suggest_int('max_depth', 3, 8), # Deeper trees for
        ↪non-linearity
        'learning_rate': trial.suggest_float('learning_rate', 0.01, 0.3,
        ↪log=True),
        'subsample': trial.suggest_float('subsample', 0.6, 1.0),
        'colsample_bytree': trial.suggest_float('colsample_bytree', 0.6, 1.0),
        'gamma': trial.suggest_float('gamma', 0, 5), # Regularization
        'reg_alpha': trial.suggest_float('reg_alpha', 1e-4, 1e1, log=True),
        'reg_lambda': trial.suggest_float('reg_lambda', 1e-4, 1e1, log=True)
    }

    model = xgb.XGBRegressor(
        **params,
        objective='reg:squarederror',
        tree_method='hist', # Use histogram method for speed
        n_jobs=-1
    )

    pipeline = Pipeline([('scaler', StandardScaler()), ('xgb', model)])

    # Manual cross-validation loop to use custom metric
    kf = KFold(n_splits=2, shuffle=True, random_state=42)
    errors = []

    for train_idx, val_idx in kf.split(X_train):
        X_fold_train, X_fold_val = X_train.iloc[train_idx], X_train.
        ↪iloc[val_idx]
        y_fold_train, y_fold_val = y_train.iloc[train_idx], y_train.
        ↪iloc[val_idx]

        pipeline.fit(X_fold_train, y_fold_train)
        y_pred = pipeline.predict(X_fold_val)

        error = mean_relative_error(y_fold_val, y_pred)
        errors.append(error)

    print(f"Trial {trial.number}: {params} -> Mean Relative Error: {np.
    ↪mean(errors)}")

    return np.mean(errors) # lower is better

study = optuna.create_study(direction='minimize')

```



```
study.optimize(objective_xgb, n_trials=50, n_jobs=4)

print("Best params:", study.best_params)
```

[I 2025-06-17 20:33:36,442] A new study created in memory with name: no-name-0dcc19b2-ee48-46c6-b67b-8776b5e203ba
[I 2025-06-17 20:33:45,401] Trial 2 finished with value: 0.0668499558423068 and parameters: {'n_estimators': 442, 'max_depth': 4, 'learning_rate': 0.22375051545402372, 'subsample': 0.8285433983430306, 'colsample_bytree': 0.7639915913752473, 'gamma': 1.4037784334911145, 'reg_alpha': 3.372682996967398, 'reg_lambda': 0.0001868717421224549}. Best is trial 2 with value: 0.0668499558423068.

Trial 2: {'n_estimators': 442, 'max_depth': 4, 'learning_rate': 0.22375051545402372, 'subsample': 0.8285433983430306, 'colsample_bytree': 0.7639915913752473, 'gamma': 1.4037784334911145, 'reg_alpha': 3.372682996967398, 'reg_lambda': 0.0001868717421224549} -> Mean Relative Error: 0.0668499558423068

[I 2025-06-17 20:33:48,275] Trial 3 finished with value: 0.06602194382710264 and parameters: {'n_estimators': 562, 'max_depth': 4, 'learning_rate': 0.033238770183401725, 'subsample': 0.6283000113478776, 'colsample_bytree': 0.638465682377189, 'gamma': 4.112090031228771, 'reg_alpha': 0.08101110683611396, 'reg_lambda': 0.0015196470601781195}. Best is trial 3 with value: 0.06602194382710264.

Trial 3: {'n_estimators': 562, 'max_depth': 4, 'learning_rate': 0.033238770183401725, 'subsample': 0.6283000113478776, 'colsample_bytree': 0.638465682377189, 'gamma': 4.112090031228771, 'reg_alpha': 0.08101110683611396, 'reg_lambda': 0.0015196470601781195} -> Mean Relative Error: 0.06602194382710264

[I 2025-06-17 20:33:49,238] Trial 0 finished with value: 0.05157362697951237 and parameters: {'n_estimators': 715, 'max_depth': 4, 'learning_rate': 0.04580870376215874, 'subsample': 0.6629058709537788, 'colsample_bytree': 0.9106794967229505, 'gamma': 1.4898538965472308, 'reg_alpha': 0.034310709063763774, 'reg_lambda': 4.022104127018827}. Best is trial 0 with value: 0.05157362697951237.

Trial 0: {'n_estimators': 715, 'max_depth': 4, 'learning_rate': 0.04580870376215874, 'subsample': 0.6629058709537788, 'colsample_bytree': 0.9106794967229505, 'gamma': 1.4898538965472308, 'reg_alpha': 0.034310709063763774, 'reg_lambda': 4.022104127018827} -> Mean Relative Error: 0.05157362697951237

[I 2025-06-17 20:33:53,384] Trial 4 finished with value: 0.05395141465707855 and parameters: {'n_estimators': 836, 'max_depth': 5, 'learning_rate': 0.1279524343578311, 'subsample': 0.90897547806685, 'colsample_bytree': 0.9815825225510908, 'gamma': 1.6157081229612285, 'reg_alpha': 0.0004740359952909425, 'reg_lambda': 0.0936314496380099}. Best is trial 0 with value: 0.05157362697951237.

Trial 4: {'n_estimators': 836, 'max_depth': 5, 'learning_rate':

0.1279524343578311, 'subsample': 0.90897547806685, 'colsample_bytree':
0.9815825225510908, 'gamma': 1.6157081229612285, 'reg_alpha':
0.0004740359952909425, 'reg_lambda': 0.0936314496380099} -> Mean Relative Error:
0.05395141465707855

[I 2025-06-17 20:33:54,267] Trial 6 finished with value: 0.09953390167904708 and
parameters: {'n_estimators': 290, 'max_depth': 3, 'learning_rate':
0.03398172598990776, 'subsample': 0.7752830846387383, 'colsample_bytree':
0.8691867690980777, 'gamma': 3.490175626520246, 'reg_alpha':
0.0016101557341145058, 'reg_lambda': 0.00047826441093852035}. Best is trial 0
with value: 0.05157362697951237.

Trial 6: {'n_estimators': 290, 'max_depth': 3, 'learning_rate':
0.03398172598990776, 'subsample': 0.7752830846387383, 'colsample_bytree':
0.8691867690980777, 'gamma': 3.490175626520246, 'reg_alpha':
0.0016101557341145058, 'reg_lambda': 0.00047826441093852035} -> Mean Relative
Error: 0.09953390167904708

[I 2025-06-17 20:33:58,172] Trial 5 finished with value: 0.06105907652062151 and
parameters: {'n_estimators': 966, 'max_depth': 7, 'learning_rate':
0.18173601688065288, 'subsample': 0.9831623260231417, 'colsample_bytree':
0.6020934085247042, 'gamma': 2.4129113673623053, 'reg_alpha':
0.00028808712394189263, 'reg_lambda': 0.02202999385302632}. Best is trial 0 with
value: 0.05157362697951237.

Trial 5: {'n_estimators': 966, 'max_depth': 7, 'learning_rate':
0.18173601688065288, 'subsample': 0.9831623260231417, 'colsample_bytree':
0.6020934085247042, 'gamma': 2.4129113673623053, 'reg_alpha':
0.00028808712394189263, 'reg_lambda': 0.02202999385302632} -> Mean Relative
Error: 0.06105907652062151

[I 2025-06-17 20:34:14,648] Trial 8 finished with value: 0.05462864382748703 and
parameters: {'n_estimators': 630, 'max_depth': 4, 'learning_rate':
0.05361504648026522, 'subsample': 0.9197116760486744, 'colsample_bytree':
0.9492635728320182, 'gamma': 1.8181627420441793, 'reg_alpha':
0.0019968159486539456, 'reg_lambda': 0.3599185293274995}. Best is trial 0 with
value: 0.05157362697951237.

Trial 8: {'n_estimators': 630, 'max_depth': 4, 'learning_rate':
0.05361504648026522, 'subsample': 0.9197116760486744, 'colsample_bytree':
0.9492635728320182, 'gamma': 1.8181627420441793, 'reg_alpha':
0.0019968159486539456, 'reg_lambda': 0.3599185293274995} -> Mean Relative Error:
0.05462864382748703

[I 2025-06-17 20:34:38,278] Trial 9 finished with value: 0.07234717558070307 and
parameters: {'n_estimators': 477, 'max_depth': 4, 'learning_rate':
0.12187348944172573, 'subsample': 0.9995675445568861, 'colsample_bytree':
0.6129110217787136, 'gamma': 2.9002653345627136, 'reg_alpha':
0.0005853862344028359, 'reg_lambda': 2.3230244137304488}. Best is trial 0 with
value: 0.05157362697951237.

Trial 9: {'n_estimators': 477, 'max_depth': 4, 'learning_rate': 0.12187348944172573, 'subsample': 0.9995675445568861, 'colsample_bytree': 0.6129110217787136, 'gamma': 2.9002653345627136, 'reg_alpha': 0.0005853862344028359, 'reg_lambda': 2.3230244137304488} -> Mean Relative Error: 0.07234717558070307

[I 2025-06-17 20:34:57,339] Trial 10 finished with value: 0.06676561200376946 and parameters: {'n_estimators': 634, 'max_depth': 8, 'learning_rate': 0.1075738637897836, 'subsample': 0.8891038909088929, 'colsample_bytree': 0.6799172800535783, 'gamma': 1.96738393218988, 'reg_alpha': 0.7665071982129477, 'reg_lambda': 0.0510097056266545}. Best is trial 0 with value: 0.05157362697951237.

Trial 10: {'n_estimators': 634, 'max_depth': 8, 'learning_rate': 0.1075738637897836, 'subsample': 0.8891038909088929, 'colsample_bytree': 0.6799172800535783, 'gamma': 1.96738393218988, 'reg_alpha': 0.7665071982129477, 'reg_lambda': 0.0510097056266545} -> Mean Relative Error: 0.06676561200376946

[I 2025-06-17 20:35:18,819] Trial 12 finished with value: 0.2567470777518496 and parameters: {'n_estimators': 402, 'max_depth': 4, 'learning_rate': 0.011391552815629856, 'subsample': 0.7480976707246327, 'colsample_bytree': 0.7684283522065117, 'gamma': 1.1812732748652714, 'reg_alpha': 0.0119357262139837, 'reg_lambda': 1.5001963049171905}. Best is trial 0 with value: 0.05157362697951237.

Trial 12: {'n_estimators': 402, 'max_depth': 4, 'learning_rate': 0.011391552815629856, 'subsample': 0.7480976707246327, 'colsample_bytree': 0.7684283522065117, 'gamma': 1.1812732748652714, 'reg_alpha': 0.0119357262139837, 'reg_lambda': 1.5001963049171905} -> Mean Relative Error: 0.2567470777518496

[I 2025-06-17 20:35:29,540] Trial 1 finished with value: 0.039078643551963804 and parameters: {'n_estimators': 645, 'max_depth': 6, 'learning_rate': 0.020375757151703592, 'subsample': 0.9253279767352681, 'colsample_bytree': 0.946366910193718, 'gamma': 2.426836215625655, 'reg_alpha': 0.2937419121635095, 'reg_lambda': 0.003408170610873604}. Best is trial 1 with value: 0.039078643551963804.

Trial 1: {'n_estimators': 645, 'max_depth': 6, 'learning_rate': 0.020375757151703592, 'subsample': 0.9253279767352681, 'colsample_bytree': 0.946366910193718, 'gamma': 2.426836215625655, 'reg_alpha': 0.2937419121635095, 'reg_lambda': 0.003408170610873604} -> Mean Relative Error: 0.039078643551963804

[I 2025-06-17 20:36:02,375] Trial 13 finished with value: 0.03795579392401009 and parameters: {'n_estimators': 790, 'max_depth': 6, 'learning_rate': 0.01409612923843607, 'subsample': 0.6042672640612519, 'colsample_bytree': 0.880620673062346, 'gamma': 0.11938623158875439, 'reg_alpha': 0.09660165702081018, 'reg_lambda': 9.984581276998947}. Best is trial 13 with value: 0.03795579392401009.

Trial 13: {'n_estimators': 790, 'max_depth': 6, 'learning_rate': 0.01409612923843607, 'subsample': 0.6042672640612519, 'colsample_bytree':

0.880620673062346, 'gamma': 0.11938623158875439, 'reg_alpha':
0.09660165702081018, 'reg_lambda': 9.984581276998947} -> Mean Relative Error:
0.03795579392401009

[I 2025-06-17 20:36:46,521] Trial 15 finished with value: 0.036405910972051536
and parameters: {'n_estimators': 807, 'max_depth': 6, 'learning_rate':
0.012727134509179831, 'subsample': 0.7000004194708628, 'colsample_bytree':
0.8473695438285169, 'gamma': 0.04077335887398863, 'reg_alpha':
0.39454484754030866, 'reg_lambda': 0.005340442030881511}. Best is trial 15 with
value: 0.036405910972051536.

Trial 15: {'n_estimators': 807, 'max_depth': 6, 'learning_rate':
0.012727134509179831, 'subsample': 0.7000004194708628, 'colsample_bytree':
0.8473695438285169, 'gamma': 0.04077335887398863, 'reg_alpha':
0.39454484754030866, 'reg_lambda': 0.005340442030881511} -> Mean Relative Error:
0.036405910972051536

[I 2025-06-17 20:37:23,390] Trial 16 finished with value: 0.041438522707156714
and parameters: {'n_estimators': 826, 'max_depth': 6, 'learning_rate':
0.01039954897644366, 'subsample': 0.695823104776334, 'colsample_bytree':
0.8414338344405288, 'gamma': 0.110824525766417, 'reg_alpha': 6.903946405922279,
'reg_lambda': 0.008403351476946574}. Best is trial 15 with value:
0.036405910972051536.

Trial 16: {'n_estimators': 826, 'max_depth': 6, 'learning_rate':
0.01039954897644366, 'subsample': 0.695823104776334, 'colsample_bytree':
0.8414338344405288, 'gamma': 0.110824525766417, 'reg_alpha': 6.903946405922279,
'reg_lambda': 0.008403351476946574} -> Mean Relative Error: 0.041438522707156714

[I 2025-06-17 20:37:48,678] Trial 11 finished with value: 0.03245256804117318
and parameters: {'n_estimators': 987, 'max_depth': 7, 'learning_rate':
0.013803544564778074, 'subsample': 0.8410536716287497, 'colsample_bytree':
0.8751771163444744, 'gamma': 0.04779743277798898, 'reg_alpha':
0.8308629956135741, 'reg_lambda': 0.0025650414891188163}. Best is trial 11 with
value: 0.03245256804117318.

Trial 11: {'n_estimators': 987, 'max_depth': 7, 'learning_rate':
0.013803544564778074, 'subsample': 0.8410536716287497, 'colsample_bytree':
0.8751771163444744, 'gamma': 0.04779743277798898, 'reg_alpha':
0.8308629956135741, 'reg_lambda': 0.0025650414891188163} -> Mean Relative Error:
0.03245256804117318

[I 2025-06-17 20:37:57,328] Trial 7 finished with value: 0.05192118964288041 and
parameters: {'n_estimators': 502, 'max_depth': 6, 'learning_rate':
0.01323045408574911, 'subsample': 0.804210232699929, 'colsample_bytree':
0.9096118239376929, 'gamma': 3.7471450352878755, 'reg_alpha':
0.0005371364677706422, 'reg_lambda': 1.8225286314420295}. Best is trial 11 with
value: 0.03245256804117318.

Trial 7: {'n_estimators': 502, 'max_depth': 6, 'learning_rate':
0.01323045408574911, 'subsample': 0.804210232699929, 'colsample_bytree':
0.9096118239376929, 'gamma': 3.7471450352878755, 'reg_alpha':

0.0005371364677706422, 'reg_lambda': 1.8225286314420295} -> Mean Relative Error: 0.05192118964288041

[I 2025-06-17 20:40:18,016] Trial 17 finished with value: 0.02894788128217178 and parameters: {'n_estimators': 975, 'max_depth': 7, 'learning_rate': 0.018179676001914204, 'subsample': 0.6016473791529032, 'colsample_bytree': 0.8226817475114728, 'gamma': 0.047039573896635045, 'reg_alpha': 0.33259653853976745, 'reg_lambda': 0.2789298159677029}. Best is trial 17 with value: 0.02894788128217178.

Trial 17: {'n_estimators': 975, 'max_depth': 7, 'learning_rate': 0.018179676001914204, 'subsample': 0.6016473791529032, 'colsample_bytree': 0.8226817475114728, 'gamma': 0.047039573896635045, 'reg_alpha': 0.33259653853976745, 'reg_lambda': 0.2789298159677029} -> Mean Relative Error: 0.02894788128217178

[I 2025-06-17 20:40:18,690] Trial 18 finished with value: 0.036615392625897976 and parameters: {'n_estimators': 953, 'max_depth': 8, 'learning_rate': 0.019942622823333953, 'subsample': 0.8409542206906679, 'colsample_bytree': 0.812423984238314, 'gamma': 0.6775223891097802, 'reg_alpha': 0.9703377017280687, 'reg_lambda': 0.001269705787539411}. Best is trial 17 with value: 0.02894788128217178.

Trial 18: {'n_estimators': 953, 'max_depth': 8, 'learning_rate': 0.019942622823333953, 'subsample': 0.8409542206906679, 'colsample_bytree': 0.812423984238314, 'gamma': 0.6775223891097802, 'reg_alpha': 0.9703377017280687, 'reg_lambda': 0.001269705787539411} -> Mean Relative Error: 0.036615392625897976

[I 2025-06-17 20:42:01,664] Trial 21 finished with value: 0.05265185880810783 and parameters: {'n_estimators': 998, 'max_depth': 7, 'learning_rate': 0.021002615700553437, 'subsample': 0.738293741307648, 'colsample_bytree': 0.7402420029993847, 'gamma': 4.755004541335958, 'reg_alpha': 2.0012433130574316, 'reg_lambda': 0.21889588163433643}. Best is trial 17 with value: 0.02894788128217178.

Trial 21: {'n_estimators': 998, 'max_depth': 7, 'learning_rate': 0.021002615700553437, 'subsample': 0.738293741307648, 'colsample_bytree': 0.7402420029993847, 'gamma': 4.755004541335958, 'reg_alpha': 2.0012433130574316, 'reg_lambda': 0.21889588163433643} -> Mean Relative Error: 0.05265185880810783

[I 2025-06-17 20:42:28,056] Trial 22 finished with value: 0.051531836580253884 and parameters: {'n_estimators': 869, 'max_depth': 7, 'learning_rate': 0.08038680414149142, 'subsample': 0.8700020481913786, 'colsample_bytree': 0.7157620168061406, 'gamma': 0.7905238309828844, 'reg_alpha': 0.009153246017686849, 'reg_lambda': 0.019360955332947558}. Best is trial 17 with value: 0.02894788128217178.

Trial 22: {'n_estimators': 869, 'max_depth': 7, 'learning_rate': 0.08038680414149142, 'subsample': 0.8700020481913786, 'colsample_bytree': 0.7157620168061406, 'gamma': 0.7905238309828844, 'reg_alpha': 0.009153246017686849, 'reg_lambda': 0.019360955332947558} -> Mean Relative Error: 0.051531836580253884

[I 2025-06-17 20:43:00,095] Trial 20 finished with value: 0.03696975363687307 and parameters: {'n_estimators': 994, 'max_depth': 8, 'learning_rate': 0.021516977156508778, 'subsample': 0.832788615560942, 'colsample_bytree': 0.8002854688584278, 'gamma': 0.720654998411239, 'reg_alpha': 1.6193234043883715, 'reg_lambda': 0.2418490858558121}. Best is trial 17 with value: 0.02894788128217178.

Trial 20: {'n_estimators': 994, 'max_depth': 8, 'learning_rate': 0.021516977156508778, 'subsample': 0.832788615560942, 'colsample_bytree': 0.8002854688584278, 'gamma': 0.720654998411239, 'reg_alpha': 1.6193234043883715, 'reg_lambda': 0.2418490858558121} -> Mean Relative Error: 0.03696975363687307

[I 2025-06-17 20:43:32,165] Trial 23 finished with value: 0.05689207022712274 and parameters: {'n_estimators': 907, 'max_depth': 8, 'learning_rate': 0.030537155874313677, 'subsample': 0.7704267586448063, 'colsample_bytree': 0.7960477298670806, 'gamma': 0.6631326258448541, 'reg_alpha': 0.2010674821099855, 'reg_lambda': 0.498607597707375}. Best is trial 17 with value: 0.02894788128217178.

Trial 23: {'n_estimators': 907, 'max_depth': 8, 'learning_rate': 0.030537155874313677, 'subsample': 0.7704267586448063, 'colsample_bytree': 0.7960477298670806, 'gamma': 0.6631326258448541, 'reg_alpha': 0.2010674821099855, 'reg_lambda': 0.498607597707375} -> Mean Relative Error: 0.05689207022712274

[I 2025-06-17 20:43:47,336] Trial 19 finished with value: 0.036150281565912545 and parameters: {'n_estimators': 1000, 'max_depth': 8, 'learning_rate': 0.02186218397938367, 'subsample': 0.7227787114467378, 'colsample_bytree': 0.8093785856241931, 'gamma': 0.7772310417441121, 'reg_alpha': 1.0924506095765574, 'reg_lambda': 0.0010621423408808245}. Best is trial 17 with value: 0.02894788128217178.

Trial 19: {'n_estimators': 1000, 'max_depth': 8, 'learning_rate': 0.02186218397938367, 'subsample': 0.7227787114467378, 'colsample_bytree': 0.8093785856241931, 'gamma': 0.7772310417441121, 'reg_alpha': 1.0924506095765574, 'reg_lambda': 0.0010621423408808245} -> Mean Relative Error: 0.036150281565912545

[I 2025-06-17 20:46:39,800] Trial 25 finished with value: 0.03174593347380686 and parameters: {'n_estimators': 754, 'max_depth': 7, 'learning_rate': 0.015996623228430727, 'subsample': 0.6683622168940248, 'colsample_bytree': 0.8383179442567628, 'gamma': 0.14985745569873302, 'reg_alpha': 0.4012734474939306, 'reg_lambda': 0.009005022157623645}. Best is trial 17 with value: 0.02894788128217178.

Trial 25: {'n_estimators': 754, 'max_depth': 7, 'learning_rate': 0.015996623228430727, 'subsample': 0.6683622168940248, 'colsample_bytree': 0.8383179442567628, 'gamma': 0.14985745569873302, 'reg_alpha': 0.4012734474939306, 'reg_lambda': 0.009005022157623645} -> Mean Relative Error: 0.03174593347380686

[I 2025-06-17 20:46:44,631] Trial 24 finished with value: 0.028894207310136897 and parameters: {'n_estimators': 891, 'max_depth': 7, 'learning_rate': 0.030267408829608676, 'subsample': 0.6894441319406317, 'colsample_bytree': 0.8327795495741424, 'gamma': 0.08453454791221958, 'reg_alpha': 0.40645360107966444, 'reg_lambda': 0.006445618774930366}. Best is trial 24 with value: 0.028894207310136897.

Trial 24: {'n_estimators': 891, 'max_depth': 7, 'learning_rate': 0.030267408829608676, 'subsample': 0.6894441319406317, 'colsample_bytree': 0.8327795495741424, 'gamma': 0.08453454791221958, 'reg_alpha': 0.40645360107966444, 'reg_lambda': 0.006445618774930366} -> Mean Relative Error: 0.028894207310136897

[I 2025-06-17 20:46:45,263] Trial 14 finished with value: 0.03520918543148403 and parameters: {'n_estimators': 780, 'max_depth': 6, 'learning_rate': 0.014657492254086163, 'subsample': 0.6363822183104114, 'colsample_bytree': 0.8963613620231876, 'gamma': 0.029263042926952476, 'reg_alpha': 0.12336765465938912, 'reg_lambda': 0.005586139911683476}. Best is trial 24 with value: 0.028894207310136897.

Trial 14: {'n_estimators': 780, 'max_depth': 6, 'learning_rate': 0.014657492254086163, 'subsample': 0.6363822183104114, 'colsample_bytree': 0.8963613620231876, 'gamma': 0.029263042926952476, 'reg_alpha': 0.12336765465938912, 'reg_lambda': 0.005586139911683476} -> Mean Relative Error: 0.03520918543148403

[I 2025-06-17 20:47:33,368] Trial 26 finished with value: 0.033644476327414616 and parameters: {'n_estimators': 904, 'max_depth': 7, 'learning_rate': 0.01638979416258188, 'subsample': 0.6505120516392093, 'colsample_bytree': 0.8309495124442763, 'gamma': 0.4099577055751428, 'reg_alpha': 5.6388582296891485, 'reg_lambda': 0.00018208483500290666}. Best is trial 24 with value: 0.028894207310136897.

Trial 26: {'n_estimators': 904, 'max_depth': 7, 'learning_rate': 0.01638979416258188, 'subsample': 0.6505120516392093, 'colsample_bytree': 0.8309495124442763, 'gamma': 0.4099577055751428, 'reg_alpha': 5.6388582296891485, 'reg_lambda': 0.00018208483500290666} -> Mean Relative Error: 0.033644476327414616

[I 2025-06-17 20:47:43,414] Trial 28 finished with value: 0.03251141137121542 and parameters: {'n_estimators': 772, 'max_depth': 7, 'learning_rate': 0.02849047284690616, 'subsample': 0.6572986072895411, 'colsample_bytree': 0.8346532119354421, 'gamma': 0.4114691915001626, 'reg_alpha': 0.12678967718547393, 'reg_lambda': 0.008530447842751608}. Best is trial 24 with value: 0.028894207310136897.

Trial 28: {'n_estimators': 772, 'max_depth': 7, 'learning_rate': 0.02849047284690616, 'subsample': 0.6572986072895411, 'colsample_bytree': 0.8346532119354421, 'gamma': 0.4114691915001626, 'reg_alpha': 0.12678967718547393, 'reg_lambda': 0.008530447842751608} -> Mean Relative Error: 0.03251141137121542

[I 2025-06-17 20:47:58,487] Trial 29 finished with value: 0.03477847674644423 and parameters: {'n_estimators': 717, 'max_depth': 7, 'learning_rate': 0.028366781419028826, 'subsample': 0.6775616257482052, 'colsample_bytree': 0.8384908142151846, 'gamma': 1.0004213553583163, 'reg_alpha': 0.037009234268981825, 'reg_lambda': 0.07181827510340692}. Best is trial 24 with value: 0.028894207310136897.

Trial 29: {'n_estimators': 717, 'max_depth': 7, 'learning_rate': 0.028366781419028826, 'subsample': 0.6775616257482052, 'colsample_bytree': 0.8384908142151846, 'gamma': 1.0004213553583163, 'reg_alpha': 0.037009234268981825, 'reg_lambda': 0.07181827510340692} -> Mean Relative Error: 0.03477847674644423

[I 2025-06-17 20:48:00,995] Trial 30 finished with value: 0.05036593530152381 and parameters: {'n_estimators': 687, 'max_depth': 5, 'learning_rate': 0.03052828797558941, 'subsample': 0.6717131874149399, 'colsample_bytree': 0.7710555008885818, 'gamma': 1.078454576387763, 'reg_alpha': 0.033944432437185194, 'reg_lambda': 0.0745092415375304}. Best is trial 24 with value: 0.028894207310136897.

Trial 30: {'n_estimators': 687, 'max_depth': 5, 'learning_rate': 0.03052828797558941, 'subsample': 0.6717131874149399, 'colsample_bytree': 0.7710555008885818, 'gamma': 1.078454576387763, 'reg_alpha': 0.033944432437185194, 'reg_lambda': 0.0745092415375304} -> Mean Relative Error: 0.05036593530152381

[I 2025-06-17 20:48:05,252] Trial 27 finished with value: 0.036367495764635056 and parameters: {'n_estimators': 727, 'max_depth': 7, 'learning_rate': 0.014113611079231798, 'subsample': 0.6521036950303681, 'colsample_bytree': 0.8475281357760825, 'gamma': 0.3411314694203824, 'reg_alpha': 7.6170764648828495, 'reg_lambda': 0.011308353895543083}. Best is trial 24 with value: 0.028894207310136897.

Trial 27: {'n_estimators': 727, 'max_depth': 7, 'learning_rate': 0.014113611079231798, 'subsample': 0.6521036950303681, 'colsample_bytree': 0.8475281357760825, 'gamma': 0.3411314694203824, 'reg_alpha': 7.6170764648828495, 'reg_lambda': 0.011308353895543083} -> Mean Relative Error: 0.036367495764635056

[I 2025-06-17 20:48:17,238] Trial 31 finished with value: 0.04763446766718665 and parameters: {'n_estimators': 711, 'max_depth': 7, 'learning_rate': 0.04075393924977276, 'subsample': 0.602870073209577, 'colsample_bytree': 0.7611661485888103, 'gamma': 0.9048903405404078, 'reg_alpha': 0.03073284822466699, 'reg_lambda': 0.08408525464286892}. Best is trial 24 with value: 0.028894207310136897.

Trial 31: {'n_estimators': 711, 'max_depth': 7, 'learning_rate': 0.04075393924977276, 'subsample': 0.602870073209577, 'colsample_bytree': 0.7611661485888103, 'gamma': 0.9048903405404078, 'reg_alpha': 0.03073284822466699, 'reg_lambda': 0.08408525464286892} -> Mean Relative Error: 0.04763446766718665

[I 2025-06-17 20:48:24,288] Trial 32 finished with value: 0.049079570488751494 and parameters: {'n_estimators': 725, 'max_depth': 5, 'learning_rate': 0.04428168262651604, 'subsample': 0.6097339633267214, 'colsample_bytree': 0.7701678781950255, 'gamma': 1.2032934607894121, 'reg_alpha': 0.03490463912374381, 'reg_lambda': 0.01437671433199672}. Best is trial 24 with value: 0.028894207310136897.

Trial 32: {'n_estimators': 725, 'max_depth': 5, 'learning_rate': 0.04428168262651604, 'subsample': 0.6097339633267214, 'colsample_bytree': 0.7701678781950255, 'gamma': 1.2032934607894121, 'reg_alpha': 0.03490463912374381, 'reg_lambda': 0.01437671433199672} -> Mean Relative Error: 0.049079570488751494

[I 2025-06-17 20:48:25,289] Trial 33 finished with value: 0.03647768994230247 and parameters: {'n_estimators': 909, 'max_depth': 5, 'learning_rate': 0.04336986393241837, 'subsample': 0.6013806459934754, 'colsample_bytree': 0.9368853944365061, 'gamma': 0.4426204269839049, 'reg_alpha': 0.4313548310482636, 'reg_lambda': 0.01595157877519704}. Best is trial 24 with value: 0.028894207310136897.

Trial 33: {'n_estimators': 909, 'max_depth': 5, 'learning_rate': 0.04336986393241837, 'subsample': 0.6013806459934754, 'colsample_bytree': 0.9368853944365061, 'gamma': 0.4426204269839049, 'reg_alpha': 0.4313548310482636, 'reg_lambda': 0.01595157877519704} -> Mean Relative Error: 0.03647768994230247

[I 2025-06-17 20:48:30,253] Trial 34 finished with value: 0.033438054273743106 and parameters: {'n_estimators': 912, 'max_depth': 7, 'learning_rate': 0.038454694506997886, 'subsample': 0.7038333691424103, 'colsample_bytree': 0.8772948330057196, 'gamma': 0.4091884294803542, 'reg_alpha': 0.4195832628332674, 'reg_lambda': 0.0030431688137139853}. Best is trial 24 with value: 0.028894207310136897.

Trial 34: {'n_estimators': 912, 'max_depth': 7, 'learning_rate': 0.038454694506997886, 'subsample': 0.7038333691424103, 'colsample_bytree': 0.8772948330057196, 'gamma': 0.4091884294803542, 'reg_alpha': 0.4195832628332674, 'reg_lambda': 0.0030431688137139853} -> Mean Relative Error: 0.033438054273743106

[I 2025-06-17 20:48:37,734] Trial 35 finished with value: 0.040705173942816975 and parameters: {'n_estimators': 903, 'max_depth': 5, 'learning_rate': 0.01767118259794993, 'subsample': 0.7043103383111096, 'colsample_bytree': 0.9328884187700109, 'gamma': 0.4158618131263926, 'reg_alpha': 0.35814230731162866, 'reg_lambda': 0.002604550342059443}. Best is trial 24 with value: 0.028894207310136897.

Trial 35: {'n_estimators': 903, 'max_depth': 5, 'learning_rate': 0.01767118259794993, 'subsample': 0.7043103383111096, 'colsample_bytree': 0.9328884187700109, 'gamma': 0.4158618131263926, 'reg_alpha': 0.35814230731162866, 'reg_lambda': 0.002604550342059443} -> Mean Relative Error: 0.040705173942816975

[I 2025-06-17 20:48:49,103] Trial 37 finished with value: 0.03350626373624697 and parameters: {'n_estimators': 881, 'max_depth': 8, 'learning_rate': 0.018072669694372948, 'subsample': 0.7009249357057185, 'colsample_bytree': 0.8858369851178846, 'gamma': 0.3311133954772897, 'reg_alpha': 0.34853963833160023, 'reg_lambda': 0.00247131661465838}. Best is trial 24 with value: 0.028894207310136897.

Trial 37: {'n_estimators': 881, 'max_depth': 8, 'learning_rate': 0.018072669694372948, 'subsample': 0.7009249357057185, 'colsample_bytree': 0.8858369851178846, 'gamma': 0.3311133954772897, 'reg_alpha': 0.34853963833160023, 'reg_lambda': 0.00247131661465838} -> Mean Relative Error: 0.03350626373624697

[I 2025-06-17 20:48:51,494] Trial 36 finished with value: 0.03402879995383346 and parameters: {'n_estimators': 900, 'max_depth': 8, 'learning_rate': 0.016914193019201575, 'subsample': 0.711730144277161, 'colsample_bytree': 0.9247243672380948, 'gamma': 0.391001126973189, 'reg_alpha': 0.4032043589210155, 'reg_lambda': 0.0025647775747857753}. Best is trial 24 with value: 0.028894207310136897.

Trial 36: {'n_estimators': 900, 'max_depth': 8, 'learning_rate': 0.016914193019201575, 'subsample': 0.711730144277161, 'colsample_bytree': 0.9247243672380948, 'gamma': 0.391001126973189, 'reg_alpha': 0.4032043589210155, 'reg_lambda': 0.0025647775747857753} -> Mean Relative Error: 0.03402879995383346

[I 2025-06-17 20:48:54,071] Trial 39 finished with value: 0.03774928858811705 and parameters: {'n_estimators': 856, 'max_depth': 8, 'learning_rate': 0.026033157729344173, 'subsample': 0.6327430963338654, 'colsample_bytree': 0.8603349716093712, 'gamma': 1.3786895323271247, 'reg_alpha': 2.594439473398416, 'reg_lambda': 0.0005003442139523252}. Best is trial 24 with value: 0.028894207310136897.

Trial 39: {'n_estimators': 856, 'max_depth': 8, 'learning_rate': 0.026033157729344173, 'subsample': 0.6327430963338654, 'colsample_bytree': 0.8603349716093712, 'gamma': 1.3786895323271247, 'reg_alpha': 2.594439473398416, 'reg_lambda': 0.0005003442139523252} -> Mean Relative Error: 0.03774928858811705

[I 2025-06-17 20:48:55,069] Trial 38 finished with value: 0.03873105474112622 and parameters: {'n_estimators': 870, 'max_depth': 8, 'learning_rate': 0.01757024582547906, 'subsample': 0.7990402992525553, 'colsample_bytree': 0.9313472590418262, 'gamma': 1.4721821545414924, 'reg_alpha': 2.9595853279089606, 'reg_lambda': 0.0028244132112461807}. Best is trial 24 with value: 0.028894207310136897.

Trial 38: {'n_estimators': 870, 'max_depth': 8, 'learning_rate': 0.01757024582547906, 'subsample': 0.7990402992525553, 'colsample_bytree': 0.9313472590418262, 'gamma': 1.4721821545414924, 'reg_alpha': 2.9595853279089606, 'reg_lambda': 0.0028244132112461807} -> Mean Relative Error: 0.03873105474112622

[I 2025-06-17 20:49:02,625] Trial 42 finished with value: 0.0659686413710957 and parameters: {'n_estimators': 949, 'max_depth': 6, 'learning_rate':

0.29595001641593743, 'subsample': 0.7959779682724811, 'colsample_bytree':
0.9650787304967774, 'gamma': 2.7916431899836494, 'reg_alpha': 4.136814236949746,
'reg_lambda': 0.031187890771754788}. Best is trial 24 with value:
0.028894207310136897.

Trial 42: {'n_estimators': 949, 'max_depth': 6, 'learning_rate':
0.29595001641593743, 'subsample': 0.7959779682724811, 'colsample_bytree':
0.9650787304967774, 'gamma': 2.7916431899836494, 'reg_alpha': 4.136814236949746,
'reg_lambda': 0.031187890771754788} -> Mean Relative Error: 0.0659686413710957

[I 2025-06-17 20:49:10,841] Trial 43 finished with value: 0.04287121944031087
and parameters: {'n_estimators': 959, 'max_depth': 6, 'learning_rate':
0.06272708085545774, 'subsample': 0.8519469954006723, 'colsample_bytree':
0.9751148175965635, 'gamma': 2.8198001886947055, 'reg_alpha':
0.7255786341185306, 'reg_lambda': 0.03571053637363958}. Best is trial 24 with
value: 0.028894207310136897.

Trial 43: {'n_estimators': 959, 'max_depth': 6, 'learning_rate':
0.06272708085545774, 'subsample': 0.8519469954006723, 'colsample_bytree':
0.9751148175965635, 'gamma': 2.8198001886947055, 'reg_alpha':
0.7255786341185306, 'reg_lambda': 0.03571053637363958} -> Mean Relative Error:
0.04287121944031087

[I 2025-06-17 20:49:14,291] Trial 40 finished with value: 0.039316720680641064
and parameters: {'n_estimators': 954, 'max_depth': 6, 'learning_rate':
0.024677770964706237, 'subsample': 0.9494462868867829, 'colsample_bytree':
0.865906668250285, 'gamma': 1.340210637182031, 'reg_alpha': 2.9520906866109207,
'reg_lambda': 0.0006995049662156739}. Best is trial 24 with value:
0.028894207310136897.

Trial 40: {'n_estimators': 954, 'max_depth': 6, 'learning_rate':
0.024677770964706237, 'subsample': 0.9494462868867829, 'colsample_bytree':
0.865906668250285, 'gamma': 1.340210637182031, 'reg_alpha': 2.9520906866109207,
'reg_lambda': 0.0006995049662156739} -> Mean Relative Error:
0.039316720680641064

[I 2025-06-17 20:49:19,557] Trial 41 finished with value: 0.039292164963107515
and parameters: {'n_estimators': 944, 'max_depth': 6, 'learning_rate':
0.023898954609096194, 'subsample': 0.9573450880306446, 'colsample_bytree':
0.8684094977488639, 'gamma': 1.4728323752180346, 'reg_alpha':
2.9305913735805316, 'reg_lambda': 0.0393609747344126}. Best is trial 24 with
value: 0.028894207310136897.

Trial 41: {'n_estimators': 944, 'max_depth': 6, 'learning_rate':
0.023898954609096194, 'subsample': 0.9573450880306446, 'colsample_bytree':
0.8684094977488639, 'gamma': 1.4728323752180346, 'reg_alpha':
2.9305913735805316, 'reg_lambda': 0.0393609747344126} -> Mean Relative Error:
0.039292164963107515

[I 2025-06-17 20:49:23,132] Trial 44 finished with value: 0.03188389958616887
and parameters: {'n_estimators': 560, 'max_depth': 7, 'learning_rate':
0.022490246715099436, 'subsample': 0.6685333457539886, 'colsample_bytree':

0.8261308984074519, 'gamma': 0.014243932824648642, 'reg_alpha':
0.18279794935767057, 'reg_lambda': 0.00629789825014194}. Best is trial 24 with
value: 0.028894207310136897.

Trial 44: {'n_estimators': 560, 'max_depth': 7, 'learning_rate':
0.022490246715099436, 'subsample': 0.6685333457539886, 'colsample_bytree':
0.8261308984074519, 'gamma': 0.014243932824648642, 'reg_alpha':
0.18279794935767057, 'reg_lambda': 0.00629789825014194} -> Mean Relative Error:
0.03188389958616887

[I 2025-06-17 20:49:28,630] Trial 45 finished with value: 0.03419487065318903
and parameters: {'n_estimators': 556, 'max_depth': 7, 'learning_rate':
0.025093901908510904, 'subsample': 0.9458281299323591, 'colsample_bytree':
0.8166570622255613, 'gamma': 0.18748005503636953, 'reg_alpha':
0.17238783272785774, 'reg_lambda': 0.0005556766252143734}. Best is trial 24 with
value: 0.028894207310136897.

Trial 45: {'n_estimators': 556, 'max_depth': 7, 'learning_rate':
0.025093901908510904, 'subsample': 0.9458281299323591, 'colsample_bytree':
0.8166570622255613, 'gamma': 0.18748005503636953, 'reg_alpha':
0.17238783272785774, 'reg_lambda': 0.0005556766252143734} -> Mean Relative
Error: 0.03419487065318903

[I 2025-06-17 20:49:30,438] Trial 46 finished with value: 0.04756286053636612
and parameters: {'n_estimators': 568, 'max_depth': 7, 'learning_rate':
0.02399174700357855, 'subsample': 0.66721973934408, 'colsample_bytree':
0.7897145678768954, 'gamma': 0.04434642902239505, 'reg_alpha':
0.15912593031803748, 'reg_lambda': 0.008280387758285176}. Best is trial 24 with
value: 0.028894207310136897.

Trial 46: {'n_estimators': 568, 'max_depth': 7, 'learning_rate':
0.02399174700357855, 'subsample': 0.66721973934408, 'colsample_bytree':
0.7897145678768954, 'gamma': 0.04434642902239505, 'reg_alpha':
0.15912593031803748, 'reg_lambda': 0.008280387758285176} -> Mean Relative Error:
0.04756286053636612

[I 2025-06-17 20:49:31,828] Trial 48 finished with value: 0.15522934541316197
and parameters: {'n_estimators': 329, 'max_depth': 7, 'learning_rate':
0.011223277382286461, 'subsample': 0.6261325886713965, 'colsample_bytree':
0.8216063822093747, 'gamma': 0.21095217761561635, 'reg_alpha':
0.20196688796037837, 'reg_lambda': 0.005109106747625429}. Best is trial 24 with
value: 0.028894207310136897.

Trial 48: {'n_estimators': 329, 'max_depth': 7, 'learning_rate':
0.011223277382286461, 'subsample': 0.6261325886713965, 'colsample_bytree':
0.8216063822093747, 'gamma': 0.21095217761561635, 'reg_alpha':
0.20196688796037837, 'reg_lambda': 0.005109106747625429} -> Mean Relative Error:
0.15522934541316197

[I 2025-06-17 20:49:33,311] Trial 49 finished with value: 0.1650987269338608 and
parameters: {'n_estimators': 582, 'max_depth': 3, 'learning_rate':
0.011315242510438119, 'subsample': 0.6784984787490749, 'colsample_bytree':

0.9115640242148659, 'gamma': 2.090609874772633, 'reg_alpha':
0.07721690290952775, 'reg_lambda': 0.00521318162468791}. Best is trial 24 with
value: 0.028894207310136897.

Trial 49: {'n_estimators': 582, 'max_depth': 3, 'learning_rate':
0.011315242510438119, 'subsample': 0.6784984787490749, 'colsample_bytree':
0.9115640242148659, 'gamma': 2.090609874772633, 'reg_alpha':
0.07721690290952775, 'reg_lambda': 0.00521318162468791} -> Mean Relative Error:
0.1650987269338608

[I 2025-06-17 20:49:34,622] Trial 47 finished with value: 0.040448733958988514
and parameters: {'n_estimators': 596, 'max_depth': 7, 'learning_rate':
0.01173539483042204, 'subsample': 0.6660817301927366, 'colsample_bytree':
0.8185998979586605, 'gamma': 0.18838079783075323, 'reg_alpha':
0.17037418277589864, 'reg_lambda': 0.008055952646781443}. Best is trial 24 with
value: 0.028894207310136897.

Trial 47: {'n_estimators': 596, 'max_depth': 7, 'learning_rate':
0.01173539483042204, 'subsample': 0.6660817301927366, 'colsample_bytree':
0.8185998979586605, 'gamma': 0.18838079783075323, 'reg_alpha':
0.17037418277589864, 'reg_lambda': 0.008055952646781443} -> Mean Relative Error:
0.040448733958988514

Best params: {'n_estimators': 891, 'max_depth': 7, 'learning_rate':
0.030267408829608676, 'subsample': 0.6894441319406317, 'colsample_bytree':
0.8327795495741424, 'gamma': 0.08453454791221958, 'reg_alpha':
0.40645360107966444, 'reg_lambda': 0.006445618774930366}

We can see that using xgb better is already having a better results

```
[17]: # test the model
model_xgb = xgb.XGBRegressor(**study.best_params, objective='reg:squarederror',
    ↪tree_method='hist', n_jobs=-1)
pipeline = Pipeline([
    ('scaler', StandardScaler()),
    ('xgb', model_xgb)
])
pipeline.fit(X_train, y_train)
y_pred = pipeline.predict(X_test)
print("Mean Relative Error on Test Set:", mean_relative_error(y_test, y_pred))
```

Mean Relative Error on Test Set: 0.0246801910707378

```
[19]: #save the model
import joblib
joblib.dump(pipeline, 'xgb_model.pkl')
```

```
[19]: ['xgb_model.pkl']
```

```
[20]: # Load the model
pipeline_loaded = joblib.load('xgb_model.pkl')
# Test the loaded model
y_pred_loaded = pipeline_loaded.predict(X_test)
print("Mean Relative Error on Test Set (Loaded Model):",
      ↪mean_relative_error(y_test, y_pred_loaded))
```

Mean Relative Error on Test Set (Loaded Model): 0.0246801910707378

```
[ ]: # try neural network
from torch.optim.lr_scheduler import LinearLR, ReduceLROnPlateau

class SimpleNN(torch.nn.Module):
    def __init__(self, input_dim):
        super(SimpleNN, self).__init__()
        self.net = torch.nn.Sequential(
            torch.nn.Linear(input_dim, 128),
            torch.nn.BatchNorm1d(128),
            torch.nn.ReLU(),
            torch.nn.Linear(128, 256),
            torch.nn.BatchNorm1d(256),
            torch.nn.ReLU(),
            torch.nn.Linear(256, 128),
            torch.nn.BatchNorm1d(128),
            torch.nn.ReLU(),
            torch.nn.Dropout(0.2),
            torch.nn.Linear(128, 64),
            torch.nn.BatchNorm1d(64),
            torch.nn.ReLU(),
            torch.nn.Linear(64, 1)
        )
    def forward(self, x):
        x = self.net(x)
        return x

import torch
import numpy as np
from sklearn.preprocessing import StandardScaler
import copy

def train_nn(model, X_train, y_train, X_val, y_val, epochs=100, batch_size=32,
             ↪device='cpu'):
    model.to(device)

    criterion = torch.nn.MSELoss()
    optimizer = torch.optim.RMSprop(model.parameters(), lr=0.001)
```

```

    # Warmup for first 10 epochs
    warmup_scheduler = LinearLR(optimizer, start_factor=0.1, end_factor=1.0,
    ↪total_iters=10)
    plateau_scheduler = ReduceLROnPlateau(optimizer, mode='min', factor=0.5,
    ↪patience=10, verbose=True)

    X_scaler = StandardScaler().fit(X_train)
    y_scaler = StandardScaler().fit(y_train.values.reshape(-1, 1))

    X_train_scaled = X_scaler.transform(X_train)
    X_val_scaled = X_scaler.transform(X_val)
    y_train_scaled = y_scaler.transform(y_train.values.reshape(-1, 1)).flatten()
    y_val_scaled = y_scaler.transform(y_val.values.reshape(-1, 1)).flatten()

    train_dataset = torch.utils.data.TensorDataset(torch.tensor(X_train_scaled,
    ↪dtype=torch.float32), torch.tensor(y_train_scaled, dtype=torch.float32))
    val_dataset = torch.utils.data.TensorDataset(torch.tensor(X_val_scaled,
    ↪dtype=torch.float32), torch.tensor(y_val_scaled, dtype=torch.float32))

    train_loader = torch.utils.data.DataLoader(train_dataset,
    ↪batch_size=batch_size, shuffle=True)
    val_loader = torch.utils.data.DataLoader(val_dataset,
    ↪batch_size=batch_size, shuffle=False)

    best_model_wts = copy.deepcopy(model.state_dict())
    best_loss = float('inf')

    for epoch in range(epochs):
        model.train()
        for X_batch, y_batch in train_loader:
            X_batch, y_batch = X_batch.to(device), y_batch.to(device)
            optimizer.zero_grad()
            outputs = model(X_batch).squeeze()
            loss = criterion(outputs, y_batch)
            loss.backward()
            optimizer.step()

        model.eval()
        val_loss = 0.0
        relative_error = 0.0
        with torch.no_grad():
            for X_batch, y_batch in val_loader:
                X_batch, y_batch = X_batch.to(device), y_batch.to(device)
                outputs = model(X_batch).squeeze()

```

```

        loss = criterion(outputs, y_batch)
        val_loss += loss.item()
        relative_error += mean_relative_error(y_batch.cpu().numpy(),
↪outputs.cpu().numpy())

    avg_val_loss = val_loss / len(val_loader)
    avg_mre = relative_error / len(val_loader)

    # Update learning rate
    if epoch < 10:
        warmup_scheduler.step()
    else:
        plateau_scheduler.step(avg_val_loss)

    # Save best model
    if avg_val_loss < best_loss:
        best_loss = avg_val_loss
        best_model_wts = copy.deepcopy(model.state_dict())

    print(f"Epoch {epoch+1}/{epochs}, Val Loss: {avg_val_loss:.4f}, MRE:
↪{avg_mre:.4f}")

    # Load best model weights
    model.load_state_dict(best_model_wts)
    return model, X_scaler, y_scaler

```

```

[44]: model, x_scaler, y_scaler = train_nn(SimpleNN(input_dim=X_train.shape[1]),
↪X_train, y_train, X_test, y_test, epochs=50, batch_size=128, device='cuda')

```

```

/home/mohamed/miniconda3/lib/python3.12/site-
packages/torch/optim/lr_scheduler.py:28: UserWarning: The verbose parameter is
deprecated. Please use get_last_lr() to access the learning rate.
  warnings.warn("The verbose parameter is deprecated. Please use get_last_lr() "

```

```

Epoch 1/50, Val Loss: 0.0038, MRE: 0.3714
Epoch 2/50, Val Loss: 0.0031, MRE: 0.2917
Epoch 3/50, Val Loss: 0.0058, MRE: 0.2550
Epoch 4/50, Val Loss: 0.0039, MRE: 0.2337
Epoch 5/50, Val Loss: 0.0054, MRE: 0.2482
Epoch 6/50, Val Loss: 0.0046, MRE: 0.3591
Epoch 7/50, Val Loss: 0.0044, MRE: 0.2536
Epoch 8/50, Val Loss: 0.0025, MRE: 0.2881
Epoch 9/50, Val Loss: 0.0047, MRE: 0.3155
Epoch 10/50, Val Loss: 0.0066, MRE: 0.2282
Epoch 11/50, Val Loss: 0.0093, MRE: 0.2286
Epoch 12/50, Val Loss: 0.0132, MRE: 0.2499
Epoch 13/50, Val Loss: 0.0017, MRE: 0.2250
Epoch 14/50, Val Loss: 0.0063, MRE: 0.2347

```



```

Epoch 15/50, Val Loss: 0.0028, MRE: 0.1752
Epoch 16/50, Val Loss: 0.0022, MRE: 0.1576
Epoch 17/50, Val Loss: 0.0016, MRE: 0.2336
Epoch 18/50, Val Loss: 0.0012, MRE: 0.1363
Epoch 19/50, Val Loss: 0.0033, MRE: 0.2132
Epoch 20/50, Val Loss: 0.0015, MRE: 0.2403
Epoch 21/50, Val Loss: 0.0032, MRE: 0.1977
Epoch 22/50, Val Loss: 0.0025, MRE: 0.1607
Epoch 23/50, Val Loss: 0.0023, MRE: 0.1622
Epoch 24/50, Val Loss: 0.0029, MRE: 0.2048
Epoch 25/50, Val Loss: 0.0017, MRE: 0.1450
Epoch 26/50, Val Loss: 0.0023, MRE: 0.1705
Epoch 27/50, Val Loss: 0.0026, MRE: 0.2125
Epoch 28/50, Val Loss: 0.0029, MRE: 0.2945
Epoch 29/50, Val Loss: 0.0035, MRE: 0.1825
Epoch 30/50, Val Loss: 0.0011, MRE: 0.1645
Epoch 31/50, Val Loss: 0.0012, MRE: 0.2517
Epoch 32/50, Val Loss: 0.0011, MRE: 0.1506
Epoch 33/50, Val Loss: 0.0016, MRE: 0.1183
Epoch 34/50, Val Loss: 0.0010, MRE: 0.2139
Epoch 35/50, Val Loss: 0.0010, MRE: 0.1630
Epoch 36/50, Val Loss: 0.0006, MRE: 0.1512
Epoch 37/50, Val Loss: 0.0009, MRE: 0.1380
Epoch 38/50, Val Loss: 0.0009, MRE: 0.1520
Epoch 39/50, Val Loss: 0.0009, MRE: 0.1546
Epoch 40/50, Val Loss: 0.0008, MRE: 0.1643
Epoch 41/50, Val Loss: 0.0024, MRE: 0.1849
Epoch 42/50, Val Loss: 0.0007, MRE: 0.1759
Epoch 43/50, Val Loss: 0.0015, MRE: 0.1897
Epoch 44/50, Val Loss: 0.0014, MRE: 0.2753
Epoch 45/50, Val Loss: 0.0009, MRE: 0.1844
Epoch 46/50, Val Loss: 0.0021, MRE: 0.1581
Epoch 47/50, Val Loss: 0.0017, MRE: 0.2346
Epoch 48/50, Val Loss: 0.0015, MRE: 0.1926
Epoch 49/50, Val Loss: 0.0009, MRE: 0.1327
Epoch 50/50, Val Loss: 0.0019, MRE: 0.2342

```

```

[45]: # Get predictions
X_test_scaled = x_scaler.transform(X_test)
with torch.no_grad():
    y_pred_scaled = model(torch.tensor(X_test_scaled, dtype=torch.float32).
        ↪to('cuda')).cpu().numpy()

# Inverse transform both predictions and true labels
y_pred = y_scaler.inverse_transform(y_pred_scaled)
y_true = y_test.values.reshape(-1, 1)

```

```

# Now compute MRE
mre_test = mean_relative_error(y_true, y_pred)
print("Mean Relative Error on Test Set (Neural Network):", mre_test)

```

Mean Relative Error on Test Set (Neural Network): 0.02423414100864286

```

[46]: import numpy as np
import pandas as pd
from pytorch_tabnet.tab_model import TabNetRegressor
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import mean_absolute_error
from sklearn.model_selection import train_test_split
import torch

# Move TabNet to GPU
device = 'cuda' if torch.cuda.is_available() else 'cpu'

# Example: X_train, X_val, y_train, y_val, X_test, y_test must be numpy arrays
# If you already have them as pandas DataFrames, use .values to convert

# Step 1: Scale features and target
x_scaler = StandardScaler()
y_scaler = StandardScaler()

X_train_scaled = x_scaler.fit_transform(X_train)
X_val_scaled = x_scaler.transform(X_validation)
X_test_scaled = x_scaler.transform(X_test)

y_train_scaled = y_scaler.fit_transform(y_train.values.reshape(-1, 1)).flatten()
y_val_scaled = y_scaler.transform(y_validation.values.reshape(-1, 1)).flatten()
y_test_scaled = y_scaler.transform(y_test.values.reshape(-1, 1)).flatten()

# Step 2: Initialize and train TabNet
model = TabNetRegressor(
    device_name=device,
    optimizer_fn=torch.optim.AdamW,
    optimizer_params=dict(lr=2e-3, weight_decay=1e-4),
    scheduler_params={"step_size": 20, "gamma": 0.9},
    scheduler_fn=torch.optim.lr_scheduler.StepLR,
    mask_type='entmax' # "sparsemax" is also an option
)

model.fit(
    X_train=X_train_scaled, y_train=y_train_scaled.reshape(-1, 1),
    eval_set=[(X_val_scaled, y_val_scaled.reshape(-1, 1))],
    eval_metric=['mae'],
    max_epochs=200,

```

```

    patience=20,
    batch_size=1024,
    virtual_batch_size=128,
    num_workers=0,
    drop_last=False,
    loss_fn=torch.nn.MSELoss()
)

# Step 3: Predict on test set
y_pred_scaled = model.predict(X_test_scaled)
y_pred = y_scaler.inverse_transform(y_pred_scaled)

# Step 4: Evaluate
mre = np.mean(np.abs((y_test.values - y_pred.flatten()) / y_test.values))
print("Test MRE (TabNet):", mre)

```

```

/home/mohamed/miniconda3/lib/python3.12/site-
packages/pytorch_tabnet/abstract_model.py:82: UserWarning: Device used : cuda
  warnings.warn(f"Device used : {self.device}")

```

```

epoch 0 | loss: 0.4549 | val_0_mae: 0.21145 | 0:00:05s
epoch 1 | loss: 0.0873 | val_0_mae: 0.1345 | 0:00:10s
epoch 2 | loss: 0.05717 | val_0_mae: 0.11385 | 0:00:16s
epoch 3 | loss: 0.04546 | val_0_mae: 0.09873 | 0:00:21s
epoch 4 | loss: 0.03858 | val_0_mae: 0.08947 | 0:00:26s
epoch 5 | loss: 0.0334 | val_0_mae: 0.08083 | 0:00:31s
epoch 6 | loss: 0.02896 | val_0_mae: 0.07388 | 0:00:37s
epoch 7 | loss: 0.02534 | val_0_mae: 0.07017 | 0:00:42s
epoch 8 | loss: 0.024 | val_0_mae: 0.06337 | 0:00:47s
epoch 9 | loss: 0.02204 | val_0_mae: 0.06256 | 0:00:52s
epoch 10 | loss: 0.02066 | val_0_mae: 0.06089 | 0:00:58s
epoch 11 | loss: 0.01892 | val_0_mae: 0.05569 | 0:01:02s
epoch 12 | loss: 0.01708 | val_0_mae: 0.05154 | 0:01:08s
epoch 13 | loss: 0.01684 | val_0_mae: 0.05201 | 0:01:13s
epoch 14 | loss: 0.01672 | val_0_mae: 0.0506 | 0:01:19s
epoch 15 | loss: 0.01529 | val_0_mae: 0.04885 | 0:01:24s
epoch 16 | loss: 0.01532 | val_0_mae: 0.0477 | 0:01:29s
epoch 17 | loss: 0.01406 | val_0_mae: 0.04654 | 0:01:34s
epoch 18 | loss: 0.01418 | val_0_mae: 0.04925 | 0:01:39s
epoch 19 | loss: 0.01333 | val_0_mae: 0.04893 | 0:01:44s
epoch 20 | loss: 0.0125 | val_0_mae: 0.04529 | 0:01:50s
epoch 21 | loss: 0.01282 | val_0_mae: 0.04064 | 0:01:55s
epoch 22 | loss: 0.01217 | val_0_mae: 0.04158 | 0:02:00s
epoch 23 | loss: 0.01184 | val_0_mae: 0.04248 | 0:02:05s
epoch 24 | loss: 0.01124 | val_0_mae: 0.03732 | 0:02:11s
epoch 25 | loss: 0.01164 | val_0_mae: 0.04582 | 0:02:16s
epoch 26 | loss: 0.01141 | val_0_mae: 0.04219 | 0:02:21s
epoch 27 | loss: 0.0111 | val_0_mae: 0.04285 | 0:02:27s

```

epoch 28		loss: 0.01077		val_0_mae: 0.04673		0:02:32s
epoch 29		loss: 0.01083		val_0_mae: 0.0359		0:02:36s
epoch 30		loss: 0.01018		val_0_mae: 0.05052		0:02:41s
epoch 31		loss: 0.01104		val_0_mae: 0.03698		0:02:46s
epoch 32		loss: 0.00977		val_0_mae: 0.03713		0:02:51s
epoch 33		loss: 0.01003		val_0_mae: 0.03604		0:02:56s
epoch 34		loss: 0.00936		val_0_mae: 0.03941		0:03:01s
epoch 35		loss: 0.00971		val_0_mae: 0.03091		0:03:07s
epoch 36		loss: 0.00912		val_0_mae: 0.03211		0:03:11s
epoch 37		loss: 0.00945		val_0_mae: 0.03982		0:03:16s
epoch 38		loss: 0.00901		val_0_mae: 0.03513		0:03:21s
epoch 39		loss: 0.00875		val_0_mae: 0.03136		0:03:26s
epoch 40		loss: 0.00833		val_0_mae: 0.02967		0:03:31s
epoch 41		loss: 0.00901		val_0_mae: 0.04454		0:03:36s
epoch 42		loss: 0.00888		val_0_mae: 0.03161		0:03:41s
epoch 43		loss: 0.00886		val_0_mae: 0.03306		0:03:46s
epoch 44		loss: 0.00876		val_0_mae: 0.03421		0:03:51s
epoch 45		loss: 0.0077		val_0_mae: 0.0313		0:03:56s
epoch 46		loss: 0.00821		val_0_mae: 0.03177		0:04:01s
epoch 47		loss: 0.00828		val_0_mae: 0.03827		0:04:06s
epoch 48		loss: 0.00897		val_0_mae: 0.033		0:04:11s
epoch 49		loss: 0.00787		val_0_mae: 0.02652		0:04:16s
epoch 50		loss: 0.00797		val_0_mae: 0.02739		0:04:21s
epoch 51		loss: 0.00807		val_0_mae: 0.03146		0:04:26s
epoch 52		loss: 0.00757		val_0_mae: 0.03767		0:04:32s
epoch 53		loss: 0.00737		val_0_mae: 0.03128		0:04:37s
epoch 54		loss: 0.00778		val_0_mae: 0.03645		0:04:42s
epoch 55		loss: 0.00744		val_0_mae: 0.0289		0:04:46s
epoch 56		loss: 0.00739		val_0_mae: 0.02806		0:04:51s
epoch 57		loss: 0.00735		val_0_mae: 0.03313		0:04:57s
epoch 58		loss: 0.00683		val_0_mae: 0.02536		0:05:02s
epoch 59		loss: 0.0075		val_0_mae: 0.02635		0:05:07s
epoch 60		loss: 0.00709		val_0_mae: 0.02767		0:05:12s
epoch 61		loss: 0.00708		val_0_mae: 0.02935		0:05:17s
epoch 62		loss: 0.00655		val_0_mae: 0.02792		0:05:22s
epoch 63		loss: 0.00649		val_0_mae: 0.03357		0:05:27s
epoch 64		loss: 0.00696		val_0_mae: 0.02781		0:05:32s
epoch 65		loss: 0.00664		val_0_mae: 0.03007		0:05:37s
epoch 66		loss: 0.00652		val_0_mae: 0.0287		0:05:42s
epoch 67		loss: 0.00703		val_0_mae: 0.02709		0:05:46s
epoch 68		loss: 0.0065		val_0_mae: 0.0343		0:05:51s
epoch 69		loss: 0.00664		val_0_mae: 0.03043		0:05:56s
epoch 70		loss: 0.00694		val_0_mae: 0.02393		0:06:01s
epoch 71		loss: 0.00641		val_0_mae: 0.02708		0:06:06s
epoch 72		loss: 0.00694		val_0_mae: 0.02525		0:06:11s
epoch 73		loss: 0.00623		val_0_mae: 0.02871		0:06:16s
epoch 74		loss: 0.00614		val_0_mae: 0.0283		0:06:21s
epoch 75		loss: 0.00626		val_0_mae: 0.03192		0:06:26s

epoch 76		loss: 0.00717		val_0_mae: 0.02343		0:06:31s
epoch 77		loss: 0.00605		val_0_mae: 0.02514		0:06:36s
epoch 78		loss: 0.00663		val_0_mae: 0.02625		0:06:41s
epoch 79		loss: 0.00617		val_0_mae: 0.0296		0:06:46s
epoch 80		loss: 0.00576		val_0_mae: 0.03094		0:06:51s
epoch 81		loss: 0.00621		val_0_mae: 0.03583		0:06:56s
epoch 82		loss: 0.00619		val_0_mae: 0.02423		0:07:01s
epoch 83		loss: 0.00627		val_0_mae: 0.02764		0:07:06s
epoch 84		loss: 0.00614		val_0_mae: 0.02584		0:07:11s
epoch 85		loss: 0.00633		val_0_mae: 0.02465		0:07:16s
epoch 86		loss: 0.00696		val_0_mae: 0.02628		0:07:21s
epoch 87		loss: 0.00573		val_0_mae: 0.02279		0:07:26s
epoch 88		loss: 0.00589		val_0_mae: 0.02697		0:07:30s
epoch 89		loss: 0.00624		val_0_mae: 0.02271		0:07:35s
epoch 90		loss: 0.00559		val_0_mae: 0.02762		0:07:40s
epoch 91		loss: 0.00626		val_0_mae: 0.02628		0:07:45s
epoch 92		loss: 0.00582		val_0_mae: 0.02301		0:07:50s
epoch 93		loss: 0.00588		val_0_mae: 0.02872		0:07:55s
epoch 94		loss: 0.00606		val_0_mae: 0.03305		0:08:00s
epoch 95		loss: 0.00605		val_0_mae: 0.02171		0:08:05s
epoch 96		loss: 0.00563		val_0_mae: 0.03232		0:08:10s
epoch 97		loss: 0.00538		val_0_mae: 0.02523		0:08:15s
epoch 98		loss: 0.00616		val_0_mae: 0.02851		0:08:20s
epoch 99		loss: 0.00568		val_0_mae: 0.02665		0:08:25s
epoch 100		loss: 0.00574		val_0_mae: 0.02064		0:08:30s
epoch 101		loss: 0.00535		val_0_mae: 0.02304		0:08:35s
epoch 102		loss: 0.00524		val_0_mae: 0.02462		0:08:41s
epoch 103		loss: 0.00557		val_0_mae: 0.02061		0:08:46s
epoch 104		loss: 0.00571		val_0_mae: 0.02486		0:08:51s
epoch 105		loss: 0.00566		val_0_mae: 0.02063		0:08:56s
epoch 106		loss: 0.00576		val_0_mae: 0.02747		0:09:01s
epoch 107		loss: 0.00531		val_0_mae: 0.02538		0:09:06s
epoch 108		loss: 0.0056		val_0_mae: 0.02527		0:09:11s
epoch 109		loss: 0.00547		val_0_mae: 0.01934		0:09:16s
epoch 110		loss: 0.0052		val_0_mae: 0.02584		0:09:21s
epoch 111		loss: 0.00548		val_0_mae: 0.02289		0:09:26s
epoch 112		loss: 0.00527		val_0_mae: 0.02663		0:09:30s
epoch 113		loss: 0.00523		val_0_mae: 0.0252		0:09:36s
epoch 114		loss: 0.00501		val_0_mae: 0.02178		0:09:41s
epoch 115		loss: 0.00546		val_0_mae: 0.02077		0:09:46s
epoch 116		loss: 0.00515		val_0_mae: 0.02557		0:09:51s
epoch 117		loss: 0.00496		val_0_mae: 0.03028		0:09:56s
epoch 118		loss: 0.00553		val_0_mae: 0.03653		0:10:00s
epoch 119		loss: 0.00586		val_0_mae: 0.0385		0:10:05s
epoch 120		loss: 0.00549		val_0_mae: 0.02223		0:10:10s
epoch 121		loss: 0.00495		val_0_mae: 0.01855		0:10:15s
epoch 122		loss: 0.00525		val_0_mae: 0.02235		0:10:20s
epoch 123		loss: 0.00497		val_0_mae: 0.02491		0:10:25s

```

epoch 124| loss: 0.00559 | val_0_mae: 0.02836 | 0:10:30s
epoch 125| loss: 0.00506 | val_0_mae: 0.02987 | 0:10:35s
epoch 126| loss: 0.00496 | val_0_mae: 0.02053 | 0:10:40s
epoch 127| loss: 0.00512 | val_0_mae: 0.02503 | 0:10:45s
epoch 128| loss: 0.00521 | val_0_mae: 0.02163 | 0:10:50s
epoch 129| loss: 0.00488 | val_0_mae: 0.02444 | 0:10:54s
epoch 130| loss: 0.00516 | val_0_mae: 0.02358 | 0:10:59s
epoch 131| loss: 0.00476 | val_0_mae: 0.02197 | 0:11:04s
epoch 132| loss: 0.0049 | val_0_mae: 0.02788 | 0:11:09s
epoch 133| loss: 0.00475 | val_0_mae: 0.02111 | 0:11:14s
epoch 134| loss: 0.00482 | val_0_mae: 0.03122 | 0:11:19s
epoch 135| loss: 0.00491 | val_0_mae: 0.02321 | 0:11:24s
epoch 136| loss: 0.00489 | val_0_mae: 0.02703 | 0:11:29s
epoch 137| loss: 0.00488 | val_0_mae: 0.02401 | 0:11:34s
epoch 138| loss: 0.0051 | val_0_mae: 0.02957 | 0:11:38s
epoch 139| loss: 0.00489 | val_0_mae: 0.0288 | 0:11:43s
epoch 140| loss: 0.00487 | val_0_mae: 0.03097 | 0:11:48s
epoch 141| loss: 0.00463 | val_0_mae: 0.02742 | 0:11:53s

```

Early stopping occurred at epoch 141 with best_epoch = 121 and best_val_0_mae = 0.01855

```

/home/mohamed/miniconda3/lib/python3.12/site-
packages/pytorch_tabnet/callbacks.py:172: UserWarning: Best weights from best
epoch are automatically used!
  warnings.warn(wrn_msg)

```

Test MRE (TabNet): 0.03354027375340802

```

[53]: #save the model
import joblib
joblib.dump(model, 'tabnet_model.pkl')
# Load the model
model_loaded = joblib.load('tabnet_model.pkl')
y_pred_scaled = model.predict(X_test_scaled)
y_pred = y_scaler.inverse_transform(y_pred_scaled)
# Evaluate the loaded model
print("Mean Relative Error on Test Set (Loaded TabNet Model):",
      ↪mean_relative_error(y_test.values, y_pred.flatten()))

```

Mean Relative Error on Test Set (Loaded TabNet Model): 0.03354027375340802

```

[ ]: print("Summary of the models:")
print(f"Ridge Model: ~0.42 training time: < 1s")
print(f"XGBoost Model: ~0.024 training time: < 1s")
print(f"Simple Neural Network Model: ~0.024 training time: < 2m 27s (50
      ↪epochs)")
print(f"TabNet Model: ~0.033 training time: 11m 56s (200 epochs)")

```

Summary of the models:

Ridge Model: ~0.42 training time: < 1s

XGBoost Model: ~0.024 training time: < 1s

Simple Neural Network Model: ~0.024 training time: < 2m 27s (50 epochs)

TabNet Model: ~0.033 training time 11m 56s

[]: