

TNFA-XGBoost

seed: 793

Best Parameters: {'colsample_bytree': 0.9, 'learning_rate': 0.1, 'max_depth': 4, 'n_estimators': 1000}

R² on test set (log scale): 0.7347

R² on training set (original scale): 0.9946

R² on test set (original scale): 0.9023

Test MSE: 21294.32

Test MAE: 77.21

Test MAPE (%): 37.53

seed: 235

Best Parameters: {'colsample_bytree': 0.9, 'learning_rate': 0.1, 'max_depth': 5, 'n_estimators': 1000}

R² on test set (log scale): 0.7868

R² on training set (original scale): 0.9970

R² on test set (original scale): 0.9302

Test MSE: 28882.16

Test MAE: 108.15

Test MAPE (%): 33.05

seed: 42

Best Parameters: {'colsample_bytree': 0.8, 'learning_rate': 0.1, 'max_depth': 3, 'n_estimators': 1000}

R² on test set (log scale): 0.5003

R² on training set (original scale): 0.9919

R² on test set (original scale): 0.9540

Test MSE: 17821.68

Test MAE: 80.93

Test MAPE (%): 86.50

Average Test R² (original scale): 0.9288 ± 0.0259

Average Test R² (log scale): 0.6740 ± 0.1526

Average Test MSE: 22666.05 ± 5656.39

Average Test MAE: 88.76 ± 16.89

Average Test MAPE (%): 52.36 ± 29.65

TNFA-RF

seed: 42

Best Parameters: {'bootstrap': True, 'max_depth': 20, 'max_features': 'sqrt', 'min_samples_leaf': 10}

R² on test set (log scale) : 0.6951

R² on training set (original scale): 0.9011

R² on test set (original scale): 0.9050

Test MSE: 36821.31

Test MAE: 118.47

Test MAPE (%): 109.13

seed: 793

Best Parameters: {'bootstrap': True, 'max_depth': 10, 'max_features': 'sqrt', 'min_samples_leaf': 10, 'min_samples_split': 10, 'n_estimators': 1000, 'oob_score': False, 'random_state': 793, 'verbose': 0, 'warm_start': False}
R² on test set (log scale): 0.7739
R² on training set (original scale): 0.8832
R² on test set (original scale): 0.8091
Test MSE: 41617.48
Test MAE: 106.03
Test MAPE (%): 38.50

seed: 235

Best Parameters: {'bootstrap': True, 'max_depth': None, 'max_features': 'sqrt', 'min_samples_leaf': 10, 'min_samples_split': 10, 'n_estimators': 1000, 'oob_score': False, 'random_state': 235, 'verbose': 0, 'warm_start': False}
R² on test set (log scale): 0.7641
R² on test set (original scale): 0.8705
R² on test set (original scale): 0.8291
Test MSE: 70668.69
Test MAE: 155.35
Test MAPE (%): 44.31

Average Test R² (original scale): 0.8478 ± 0.0506

Average Test R² (log scale): 0.7443 ± 0.0429

Average Test MSE: 49702.50 ± 18314.93

Average Test MAE: 126.62 ± 25.65

Average Test MAPE (%): 63.98 ± 39.21

TNFA-MLP

seed: 42

Best Parameters: {'reg__regressor__activation': 'relu', 'reg__regressor__alpha': 0.0005, 'reg__regressor__n_estimators': 1000, 'reg__regressor__random_state': 42, 'reg__regressor__verbose': 0, 'reg__regressor__warm_start': False, 'reg__regressor__max_depth': 10, 'reg__regressor__max_features': 'sqrt', 'reg__regressor__min_samples_leaf': 10, 'reg__regressor__min_samples_split': 10, 'reg__regressor__oob_score': False, 'reg__regressor__bootstrap': True, 'reg__regressor__n_estimators': 1000, 'reg__regressor__random_state': 42, 'reg__regressor__verbose': 0, 'reg__regressor__warm_start': False}
R² on test set (log scale): 0.6606
R² on training set (original scale): 0.8254
R² on test set (original scale): 0.9162
Test MSE: 32506.24
Test MAE: 117.35
Test MAPE (%): 126.93

seed: 793

Best Parameters: {'reg__regressor__activation': 'relu', 'reg__regressor__alpha': 0.0005, 'reg__regressor__n_estimators': 1000, 'reg__regressor__random_state': 793, 'reg__regressor__verbose': 0, 'reg__regressor__warm_start': False, 'reg__regressor__max_depth': 10, 'reg__regressor__max_features': 'sqrt', 'reg__regressor__min_samples_leaf': 10, 'reg__regressor__min_samples_split': 10, 'reg__regressor__oob_score': False, 'reg__regressor__bootstrap': True, 'reg__regressor__n_estimators': 1000, 'reg__regressor__random_state': 793, 'reg__regressor__verbose': 0, 'reg__regressor__warm_start': False}
R² on test set (log scale): 0.6316
R² on training set (original scale): 0.6680
R² on test set (original scale): 0.7650
Test MSE: 51234.92
Test MAE: 126.95
Test MAPE (%): 52.98

seed: 1579

Best Parameters: {'reg__regressor__activation': 'relu', 'reg__regressor__alpha': 0.0005, 'reg__regressor__n_estimators': 1000, 'reg__regressor__random_state': 1579, 'reg__regressor__verbose': 0, 'reg__regressor__warm_start': False, 'reg__regressor__max_depth': 10, 'reg__regressor__max_features': 'sqrt', 'reg__regressor__min_samples_leaf': 10, 'reg__regressor__min_samples_split': 10, 'reg__regressor__oob_score': False, 'reg__regressor__bootstrap': True, 'reg__regressor__n_estimators': 1000, 'reg__regressor__random_state': 1579, 'reg__regressor__verbose': 0, 'reg__regressor__warm_start': False}
R² on test set (log scale): 0.6906
R² on training set (original scale): 0.7927
R² on test set (original scale): 0.6654

Test MSE: 116024.54
Test MAE: 214.31
Test MAPE (%): 68.81

===== Mean \pm Std (Test Set, Original Scale) =====

Average Test R^2 (original scale): 0.7822 ± 0.1263
Average Test R^2 (log scale): 0.6609 ± 0.0295
Average Test MSE: 66588.57 ± 43824.96
Average Test MAE: 152.87 ± 53.43
Average Test MAPE (%): 82.91 ± 38.94

IL-10 XGBoost

Running with random seed: 42
Train R^2 : 0.8862
Test R^2 : 0.7077
Test MSE: 29216.08
Test MAE: 109.46
Test MAPE (%): 37.78

Running with random seed: 173
Train R^2 : 0.8567
Test R^2 : 0.8111
Test MSE: 18360.08
Test MAE: 96.34
Test MAPE (%): 66.50

Running with random seed: 382
Train R^2 : 0.8503
Test R^2 : 0.8309
Test MSE: 20670.59
Test MAE: 94.96
Test MAPE (%): 70.26

Average Test R^2 : 0.7832 ± 0.0662
Average Test MSE: 22748.92 ± 5718.63
Average Test MAE: 100.25 ± 8.01
Average Test MAPE (%): 58.18 ± 17.76

IL-10 RF

Running with random seed: 1
Train R^2 : 0.8238
Test R^2 : 0.8075
Test MSE: 23635.01
Test MAE: 123.03
Test MAPE (%): 86.92

Running with random seed: 173
Train R^2 : 0.8101

Test R²: 0.8276
Test MSE: 16753.27
Test MAE: 116.62
Test MAPE (%): 116.28

Running with random seed: 98

Train R²: 0.8028
Test R²: 0.7368
Test MSE: 41253.77
Test MAE: 152.62
Test MAPE (%): 93.95

Average Test R²: 0.7907 ± 0.0477
Average Test MSE: 27214.02 ± 12636.29
Average Test MAE: 130.75 ± 19.20
Average Test MAPE (%): 99.05 ± 15.33

IL-10 MLP

Running with seed: 79
R² on test set (log/transformed scale): 0.3012
R² on training set (original scale): 0.9206
R² on test set (original scale): 0.7377
Test MSE: 699181.58
Test MAE: 427.93
Test MAPE (%): 188.35
Best Parameters: {'reg__regressor__activation': 'relu', 'reg__regressor__alpha': 0.0001, 'reg

Running with seed: 955

R² on test set (log/transformed scale): 0.7412
R² on training set (original scale): 0.9275
R² on test set (original scale): 0.9547
Test MSE: 120872.77
Test MAE: 233.01
Test MAPE (%): 53.68
Best Parameters: {'reg__regressor__activation': 'relu', 'reg__regressor__alpha': 0.0001, 'reg

Average Test R² (original scale): 0.8462 ± 0.1534
Average Test R² (log scale): 0.5212 ± 0.3111
Average Test MSE: 410027.18 ± 408926.08
Average Test MAE: 330.47 ± 137.83
Average Test MAPE (%): 121.01 ± 95.23