

Supporting Information to “TropMol: A Cloud-based web tool to predict acetylcholinesterase inhibitors by machine learning”

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1 Tuning Parameters

Here are shown the tuning values used in the Random Forest, Gradient Boosting, XGBoost, and LightGBM models.

1.1 Random Forest

Testing different parameter combinations for RANDOM FOREST on the normalized dataset (with 15% test set)

```
param_grid_normalized = {  
    'n_estimators': [10, 50, 100, 110, 150, 200, 500, 1000, 2000],  
    'max_depth': [10, 15, 20, 25, 30, 35, 40],  
    'min_samples_leaf': [1, 2, 4],  
    'max_features': ['sqrt', 'log2']  
}
```

Testing different parameter combinations on the normalized dataset:

R²

R² with n_estimators=10, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.5583
R² with n_estimators=10, max_depth=10, min_samples_leaf=1, max_features=log2: 0.5413
R² with n_estimators=10, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.5385
R² with n_estimators=10, max_depth=10, min_samples_leaf=2, max_features=log2: 0.5276
R² with n_estimators=10, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.5371
R² with n_estimators=10, max_depth=10, min_samples_leaf=4, max_features=log2: 0.5282
R² with n_estimators=10, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.6897
R² with n_estimators=10, max_depth=15, min_samples_leaf=1, max_features=log2: 0.6809
R² with n_estimators=10, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.6715
R² with n_estimators=10, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6635
R² with n_estimators=10, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6404
R² with n_estimators=10, max_depth=15, min_samples_leaf=4, max_features=log2: 0.6371
R² with n_estimators=10, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.7276
R² with n_estimators=10, max_depth=20, min_samples_leaf=1, max_features=log2: 0.7249
R² with n_estimators=10, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.7072

R² with n_estimators=10, max_depth=20, min_samples_leaf=2, max_features=log2: 0.6985
R² with n_estimators=10, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.6843
R² with n_estimators=10, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6747
R² with n_estimators=10, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.7243
R² with n_estimators=10, max_depth=25, min_samples_leaf=1, max_features=log2: 0.7257
R² with n_estimators=10, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.7173
R² with n_estimators=10, max_depth=25, min_samples_leaf=2, max_features=log2: 0.7052
R² with n_estimators=10, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.6872
R² with n_estimators=10, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6723
R² with n_estimators=10, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.7146
R² with n_estimators=10, max_depth=30, min_samples_leaf=1, max_features=log2: 0.7170
R² with n_estimators=10, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.7053
R² with n_estimators=10, max_depth=30, min_samples_leaf=2, max_features=log2: 0.7103
R² with n_estimators=10, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.6848
R² with n_estimators=10, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6626
R² with n_estimators=10, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.7316
R² with n_estimators=10, max_depth=35, min_samples_leaf=1, max_features=log2: 0.7233
R² with n_estimators=10, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.7123
R² with n_estimators=10, max_depth=35, min_samples_leaf=2, max_features=log2: 0.7169
R² with n_estimators=10, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.6863
R² with n_estimators=10, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6593
R² with n_estimators=10, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.7276
R² with n_estimators=10, max_depth=40, min_samples_leaf=1, max_features=log2: 0.7197
R² with n_estimators=10, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.7123
R² with n_estimators=10, max_depth=40, min_samples_leaf=2, max_features=log2: 0.7184
R² with n_estimators=10, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.6863
R² with n_estimators=10, max_depth=40, min_samples_leaf=4, max_features=log2: 0.6593
R² with n_estimators=50, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.5773
R² with n_estimators=50, max_depth=10, min_samples_leaf=1, max_features=log2: 0.5475
R² with n_estimators=50, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.5669
R² with n_estimators=50, max_depth=10, min_samples_leaf=2, max_features=log2: 0.5350
R² with n_estimators=50, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.5636

R² with n_estimators=50, max_depth=10, min_samples_leaf=4, max_features=log2: 0.5336
R² with n_estimators=50, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.7107
R² with n_estimators=50, max_depth=15, min_samples_leaf=1, max_features=log2: 0.7009
R² with n_estimators=50, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.6994
R² with n_estimators=50, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6899
R² with n_estimators=50, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6762
R² with n_estimators=50, max_depth=15, min_samples_leaf=4, max_features=log2: 0.6571
R² with n_estimators=50, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.7551
R² with n_estimators=50, max_depth=20, min_samples_leaf=1, max_features=log2: 0.7505
R² with n_estimators=50, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.7354
R² with n_estimators=50, max_depth=20, min_samples_leaf=2, max_features=log2: 0.7237
R² with n_estimators=50, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.7093
R² with n_estimators=50, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6903
R² with n_estimators=50, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.7577
R² with n_estimators=50, max_depth=25, min_samples_leaf=1, max_features=log2: 0.7561
R² with n_estimators=50, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.7440
R² with n_estimators=50, max_depth=25, min_samples_leaf=2, max_features=log2: 0.7310
R² with n_estimators=50, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.7109
R² with n_estimators=50, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6947
R² with n_estimators=50, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.7564
R² with n_estimators=50, max_depth=30, min_samples_leaf=1, max_features=log2: 0.7578
R² with n_estimators=50, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.7422
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R² with n_estimators=50, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6950
R² with n_estimators=50, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.7582
R² with n_estimators=50, max_depth=35, min_samples_leaf=1, max_features=log2: 0.7582
R² with n_estimators=50, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.7446
R² with n_estimators=50, max_depth=35, min_samples_leaf=2, max_features=log2: 0.7366
R² with n_estimators=50, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.7106
R² with n_estimators=50, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6945
R² with n_estimators=50, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.7590

R² with n_estimators=50, max_depth=40, min_samples_leaf=1, max_features=log2: 0.7564
R² with n_estimators=50, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.7446
R² with n_estimators=50, max_depth=40, min_samples_leaf=2, max_features=log2: 0.7372
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R² with n_estimators=100, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.5641
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R² with n_estimators=100, max_depth=20, min_samples_leaf=1, max_features=log2: 0.7535
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R² with n_estimators=100, max_depth=25, min_samples_leaf=2, max_features=log2: 0.7372
R² with n_estimators=100, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.7133
R² with n_estimators=100, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6981
R² with n_estimators=100, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.7650
R² with n_estimators=100, max_depth=30, min_samples_leaf=1, max_features=log2: 0.7628
R² with n_estimators=100, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.7465

R² with n_estimators=100, max_depth=30, min_samples_leaf=2, max_features=log2: 0.7408
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R² with n_estimators=100, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.7627
R² with n_estimators=100, max_depth=35, min_samples_leaf=1, max_features=log2: 0.7635
R² with n_estimators=100, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.7479
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R² with n_estimators=100, max_depth=40, min_samples_leaf=1, max_features=log2: 0.7613
R² with n_estimators=100, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.7480
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R² with n_estimators=110, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.5799
R² with n_estimators=110, max_depth=10, min_samples_leaf=1, max_features=log2: 0.5480
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R² with n_estimators=110, max_depth=10, min_samples_leaf=2, max_features=log2: 0.5399
R² with n_estimators=110, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.5657
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R² with n_estimators=110, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6946
R² with n_estimators=110, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6824
R² with n_estimators=110, max_depth=15, min_samples_leaf=4, max_features=log2: 0.6604
R² with n_estimators=110, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.7589
R² with n_estimators=110, max_depth=20, min_samples_leaf=1, max_features=log2: 0.7536
R² with n_estimators=110, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.7413
R² with n_estimators=110, max_depth=20, min_samples_leaf=2, max_features=log2: 0.7317
R² with n_estimators=110, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.7111

R² with n_estimators=110, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6924
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R² with n_estimators=110, max_depth=25, min_samples_leaf=1, max_features=log2: 0.7603
R² with n_estimators=110, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.7485
R² with n_estimators=110, max_depth=25, min_samples_leaf=2, max_features=log2: 0.7377
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R² with n_estimators=110, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.7652
R² with n_estimators=110, max_depth=30, min_samples_leaf=1, max_features=log2: 0.7629
R² with n_estimators=110, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.7465
R² with n_estimators=110, max_depth=30, min_samples_leaf=2, max_features=log2: 0.7410
R² with n_estimators=110, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.7141
R² with n_estimators=110, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6970
R² with n_estimators=110, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.7631
R² with n_estimators=110, max_depth=35, min_samples_leaf=1, max_features=log2: 0.7630
R² with n_estimators=110, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.7486
R² with n_estimators=110, max_depth=35, min_samples_leaf=2, max_features=log2: 0.7404
R² with n_estimators=110, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.7142
R² with n_estimators=110, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6976
R² with n_estimators=110, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.7637
R² with n_estimators=110, max_depth=40, min_samples_leaf=1, max_features=log2: 0.7616
R² with n_estimators=110, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.7483
R² with n_estimators=110, max_depth=40, min_samples_leaf=2, max_features=log2: 0.7407
R² with n_estimators=110, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.7141
R² with n_estimators=110, max_depth=40, min_samples_leaf=4, max_features=log2: 0.6981
R² with n_estimators=150, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.5827
R² with n_estimators=150, max_depth=10, min_samples_leaf=1, max_features=log2: 0.5503
R² with n_estimators=150, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.5741
R² with n_estimators=150, max_depth=10, min_samples_leaf=2, max_features=log2: 0.5440
R² with n_estimators=150, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.5695
R² with n_estimators=150, max_depth=10, min_samples_leaf=4, max_features=log2: 0.5377
R² with n_estimators=150, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.7230

R² with n_estimators=150, max_depth=15, min_samples_leaf=1, max_features=log2: 0.7093
R² with n_estimators=150, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.7095
R² with n_estimators=150, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6959
R² with n_estimators=150, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6859
R² with n_estimators=150, max_depth=15, min_samples_leaf=4, max_features=log2: 0.6614
R² with n_estimators=150, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.7605
R² with n_estimators=150, max_depth=20, min_samples_leaf=1, max_features=log2: 0.7543
R² with n_estimators=150, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.7433
R² with n_estimators=150, max_depth=20, min_samples_leaf=2, max_features=log2: 0.7340
R² with n_estimators=150, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.7128
R² with n_estimators=150, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6949
R² with n_estimators=150, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.7648
R² with n_estimators=150, max_depth=25, min_samples_leaf=1, max_features=log2: 0.7619
R² with n_estimators=150, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.7516
R² with n_estimators=150, max_depth=25, min_samples_leaf=2, max_features=log2: 0.7407
R² with n_estimators=150, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.7146
R² with n_estimators=150, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6997
R² with n_estimators=150, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.7667
R² with n_estimators=150, max_depth=30, min_samples_leaf=1, max_features=log2: 0.7652
R² with n_estimators=150, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.7495
R² with n_estimators=150, max_depth=30, min_samples_leaf=2, max_features=log2: 0.7425
R² with n_estimators=150, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.7161
R² with n_estimators=150, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6999
R² with n_estimators=150, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.7658
R² with n_estimators=150, max_depth=35, min_samples_leaf=1, max_features=log2: 0.7655
R² with n_estimators=150, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.7504
R² with n_estimators=150, max_depth=35, min_samples_leaf=2, max_features=log2: 0.7417
R² with n_estimators=150, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.7159
R² with n_estimators=150, max_depth=35, min_samples_leaf=4, max_features=log2: 0.7002
R² with n_estimators=150, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.7658
R² with n_estimators=150, max_depth=40, min_samples_leaf=1, max_features=log2: 0.7636
R² with n_estimators=150, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.7503

R² with n_estimators=150, max_depth=40, min_samples_leaf=2, max_features=log2: 0.7419
R² with n_estimators=150, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.7159
R² with n_estimators=150, max_depth=40, min_samples_leaf=4, max_features=log2: 0.7004
R² with n_estimators=200, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.5820
R² with n_estimators=200, max_depth=10, min_samples_leaf=1, max_features=log2: 0.5517
R² with n_estimators=200, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.5757
R² with n_estimators=200, max_depth=10, min_samples_leaf=2, max_features=log2: 0.5429
R² with n_estimators=200, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.5692
R² with n_estimators=200, max_depth=10, min_samples_leaf=4, max_features=log2: 0.5368
R² with n_estimators=200, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.7238
R² with n_estimators=200, max_depth=15, min_samples_leaf=1, max_features=log2: 0.7092
R² with n_estimators=200, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.7111
R² with n_estimators=200, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6968
R² with n_estimators=200, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6859
R² with n_estimators=200, max_depth=15, min_samples_leaf=4, max_features=log2: 0.6614
R² with n_estimators=200, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.7601
R² with n_estimators=200, max_depth=20, min_samples_leaf=1, max_features=log2: 0.7552
R² with n_estimators=200, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.7444
R² with n_estimators=200, max_depth=20, min_samples_leaf=2, max_features=log2: 0.7341
R² with n_estimators=200, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.7140
R² with n_estimators=200, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6961
R² with n_estimators=200, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.7653
R² with n_estimators=200, max_depth=25, min_samples_leaf=1, max_features=log2: 0.7630
R² with n_estimators=200, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.7521
R² with n_estimators=200, max_depth=25, min_samples_leaf=2, max_features=log2: 0.7417
R² with n_estimators=200, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.7160
R² with n_estimators=200, max_depth=25, min_samples_leaf=4, max_features=log2: 0.7001
R² with n_estimators=200, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.7664
R² with n_estimators=200, max_depth=30, min_samples_leaf=1, max_features=log2: 0.7658
R² with n_estimators=200, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.7493
R² with n_estimators=200, max_depth=30, min_samples_leaf=2, max_features=log2: 0.7438
R² with n_estimators=200, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.7169

R² with n_estimators=200, max_depth=30, min_samples_leaf=4, max_features=log2: 0.7005
R² with n_estimators=200, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.7661
R² with n_estimators=200, max_depth=35, min_samples_leaf=1, max_features=log2: 0.7657
R² with n_estimators=200, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.7496
R² with n_estimators=200, max_depth=35, min_samples_leaf=2, max_features=log2: 0.7428
R² with n_estimators=200, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.7168
R² with n_estimators=200, max_depth=35, min_samples_leaf=4, max_features=log2: 0.7006
R² with n_estimators=200, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.7653
R² with n_estimators=200, max_depth=40, min_samples_leaf=1, max_features=log2: 0.7649
R² with n_estimators=200, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.7496
R² with n_estimators=200, max_depth=40, min_samples_leaf=2, max_features=log2: 0.7427
R² with n_estimators=200, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.7169
R² with n_estimators=200, max_depth=40, min_samples_leaf=4, max_features=log2: 0.7008
R² with n_estimators=500, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.5836
R² with n_estimators=500, max_depth=10, min_samples_leaf=1, max_features=log2: 0.5521
R² with n_estimators=500, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.5768
R² with n_estimators=500, max_depth=10, min_samples_leaf=2, max_features=log2: 0.5452
R² with n_estimators=500, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.5691
R² with n_estimators=500, max_depth=10, min_samples_leaf=4, max_features=log2: 0.5346
R² with n_estimators=500, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.7244
R² with n_estimators=500, max_depth=15, min_samples_leaf=1, max_features=log2: 0.7109
R² with n_estimators=500, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.7131
R² with n_estimators=500, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6977
R² with n_estimators=500, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6872
R² with n_estimators=500, max_depth=15, min_samples_leaf=4, max_features=log2: 0.6638
R² with n_estimators=500, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.7612
R² with n_estimators=500, max_depth=20, min_samples_leaf=1, max_features=log2: 0.7557
R² with n_estimators=500, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.7463
R² with n_estimators=500, max_depth=20, min_samples_leaf=2, max_features=log2: 0.7349
R² with n_estimators=500, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.7142
R² with n_estimators=500, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6954
R² with n_estimators=500, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.7668

R² with n_estimators=500, max_depth=25, min_samples_leaf=1, max_features=log2: 0.7639
R² with n_estimators=500, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.7524
R² with n_estimators=500, max_depth=25, min_samples_leaf=2, max_features=log2: 0.7428
R² with n_estimators=500, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.7181
R² with n_estimators=500, max_depth=25, min_samples_leaf=4, max_features=log2: 0.7004
R² with n_estimators=500, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.7680
R² with n_estimators=500, max_depth=30, min_samples_leaf=1, max_features=log2: 0.7662
R² with n_estimators=500, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.7511
R² with n_estimators=500, max_depth=30, min_samples_leaf=2, max_features=log2: 0.7437
R² with n_estimators=500, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.7181
R² with n_estimators=500, max_depth=30, min_samples_leaf=4, max_features=log2: 0.7001
R² with n_estimators=500, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.7672
R² with n_estimators=500, max_depth=35, min_samples_leaf=1, max_features=log2: 0.7656
R² with n_estimators=500, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.7516
R² with n_estimators=500, max_depth=35, min_samples_leaf=2, max_features=log2: 0.7425
R² with n_estimators=500, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.7181
R² with n_estimators=500, max_depth=35, min_samples_leaf=4, max_features=log2: 0.7000
R² with n_estimators=500, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.7677
R² with n_estimators=500, max_depth=40, min_samples_leaf=1, max_features=log2: 0.7651
R² with n_estimators=500, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.7513
R² with n_estimators=500, max_depth=40, min_samples_leaf=2, max_features=log2: 0.7428
R² with n_estimators=500, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.7182
R² with n_estimators=500, max_depth=40, min_samples_leaf=4, max_features=log2: 0.7001
R² with n_estimators=1000, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.5817
R² with n_estimators=1000, max_depth=10, min_samples_leaf=1, max_features=log2: 0.5527
R² with n_estimators=1000, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.5772
R² with n_estimators=1000, max_depth=10, min_samples_leaf=2, max_features=log2: 0.5449
R² with n_estimators=1000, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.5679
R² with n_estimators=1000, max_depth=10, min_samples_leaf=4, max_features=log2: 0.5359
R² with n_estimators=1000, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.7246
R² with n_estimators=1000, max_depth=15, min_samples_leaf=1, max_features=log2: 0.7123
R² with n_estimators=1000, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.7129

R² with n_estimators=1000, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6967
R² with n_estimators=1000, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6874
R² with n_estimators=1000, max_depth=15, min_samples_leaf=4, max_features=log2: 0.6651
R² with n_estimators=1000, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.7611
R² with n_estimators=1000, max_depth=20, min_samples_leaf=1, max_features=log2: 0.7559
R² with n_estimators=1000, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.7461
R² with n_estimators=1000, max_depth=20, min_samples_leaf=2, max_features=log2: 0.7350
R² with n_estimators=1000, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.7141
R² with n_estimators=1000, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6962
R² with n_estimators=1000, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.7669
R² with n_estimators=1000, max_depth=25, min_samples_leaf=1, max_features=log2: 0.7641
R² with n_estimators=1000, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.7527
R² with n_estimators=1000, max_depth=25, min_samples_leaf=2, max_features=log2: 0.7429
R² with n_estimators=1000, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.7180
R² with n_estimators=1000, max_depth=25, min_samples_leaf=4, max_features=log2: 0.7007
R² with n_estimators=1000, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.7677
R² with n_estimators=1000, max_depth=30, min_samples_leaf=1, max_features=log2: 0.7653
R² with n_estimators=1000, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.7513
R² with n_estimators=1000, max_depth=30, min_samples_leaf=2, max_features=log2: 0.7433
R² with n_estimators=1000, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.7176
R² with n_estimators=1000, max_depth=30, min_samples_leaf=4, max_features=log2: 0.7006
R² with n_estimators=1000, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.7674
R² with n_estimators=1000, max_depth=35, min_samples_leaf=1, max_features=log2: 0.7658
R² with n_estimators=1000, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.7517
R² with n_estimators=1000, max_depth=35, min_samples_leaf=2, max_features=log2: 0.7428
R² with n_estimators=1000, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.7176
R² with n_estimators=1000, max_depth=35, min_samples_leaf=4, max_features=log2: 0.7002
R² with n_estimators=1000, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.7682
R² with n_estimators=1000, max_depth=40, min_samples_leaf=1, max_features=log2: 0.7651
R² with n_estimators=1000, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.7516
R² with n_estimators=1000, max_depth=40, min_samples_leaf=2, max_features=log2: 0.7430
R² with n_estimators=1000, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.7177

R² with n_estimators=1000, max_depth=40, min_samples_leaf=4, max_features=log2: 0.7003
R² with n_estimators=2000, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.5819
R² with n_estimators=2000, max_depth=10, min_samples_leaf=1, max_features=log2: 0.5534
R² with n_estimators=2000, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.5776
R² with n_estimators=2000, max_depth=10, min_samples_leaf=2, max_features=log2: 0.5472
R² with n_estimators=2000, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.5684
R² with n_estimators=2000, max_depth=10, min_samples_leaf=4, max_features=log2: 0.5367
R² with n_estimators=2000, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.7256
R² with n_estimators=2000, max_depth=15, min_samples_leaf=1, max_features=log2: 0.7125
R² with n_estimators=2000, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.7137
R² with n_estimators=2000, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6957
R² with n_estimators=2000, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6881
R² with n_estimators=2000, max_depth=15, min_samples_leaf=4, max_features=log2: 0.6653
R² with n_estimators=2000, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.7615
R² with n_estimators=2000, max_depth=20, min_samples_leaf=1, max_features=log2: 0.7564
R² with n_estimators=2000, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.7466
R² with n_estimators=2000, max_depth=20, min_samples_leaf=2, max_features=log2: 0.7352
R² with n_estimators=2000, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.7142
R² with n_estimators=2000, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6968
R² with n_estimators=2000, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.7676
R² with n_estimators=2000, max_depth=25, min_samples_leaf=1, max_features=log2: 0.7643
R² with n_estimators=2000, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.7523
R² with n_estimators=2000, max_depth=25, min_samples_leaf=2, max_features=log2: 0.7430
R² with n_estimators=2000, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.7179
R² with n_estimators=2000, max_depth=25, min_samples_leaf=4, max_features=log2: 0.7009
R² with n_estimators=2000, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.7679
R² with n_estimators=2000, max_depth=30, min_samples_leaf=1, max_features=log2: 0.7651
R² with n_estimators=2000, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.7515
R² with n_estimators=2000, max_depth=30, min_samples_leaf=2, max_features=log2: 0.7436
R² with n_estimators=2000, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.7183
R² with n_estimators=2000, max_depth=30, min_samples_leaf=4, max_features=log2: 0.7011
R² with n_estimators=2000, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.7679

R² with n_estimators=2000, max_depth=35, min_samples_leaf=1, max_features=log2: 0.7654
R² with n_estimators=2000, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.7519
R² with n_estimators=2000, max_depth=35, min_samples_leaf=2, max_features=log2: 0.7431
R² with n_estimators=2000, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.7182
R² with n_estimators=2000, max_depth=35, min_samples_leaf=4, max_features=log2: 0.7010
R² with n_estimators=2000, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.7683
R² with n_estimators=2000, max_depth=40, min_samples_leaf=1, max_features=log2: 0.7652
R² with n_estimators=2000, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.7520
R² with n_estimators=2000, max_depth=40, min_samples_leaf=2, max_features=log2: 0.7431
R² with n_estimators=2000, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.7182
R² with n_estimators=2000, max_depth=40, min_samples_leaf=4, max_features=log2: 0.7010

Best parameters found on the normalized dataset:

{'n_estimators': 2000, 'max_depth': 40, 'min_samples_leaf': 1, 'max_features': 'sqrt'} 0.7683

Testing different parameter combinations for Random Forest with PCA (test set 15%)

```
param_grid_normalized = {  
    'n_estimators': [10, 50, 100, 110, 150, 200, 500, 1000],  
    'max_depth': [10, 15, 20, 25, 30, 35, 40],  
    'min_samples_leaf': [1, 2, 4],  
    'max_features': ['sqrt', 'log2']  
}
```

Testing different parameter combinations with PCA:

R²

R² with n_estimators=10, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.4346
R² with n_estimators=10, max_depth=10, min_samples_leaf=1, max_features=log2: 0.3907
R² with n_estimators=10, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.4227
R² with n_estimators=10, max_depth=10, min_samples_leaf=2, max_features=log2: 0.4089
R² with n_estimators=10, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.4288
R² with n_estimators=10, max_depth=10, min_samples_leaf=4, max_features=log2: 0.3823
R² with n_estimators=10, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.5787
R² with n_estimators=10, max_depth=15, min_samples_leaf=1, max_features=log2: 0.5759
R² with n_estimators=10, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.5690
R² with n_estimators=10, max_depth=15, min_samples_leaf=2, max_features=log2: 0.5606
R² with n_estimators=10, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.5751
R² with n_estimators=10, max_depth=15, min_samples_leaf=4, max_features=log2: 0.5424
R² with n_estimators=10, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.6397
R² with n_estimators=10, max_depth=20, min_samples_leaf=1, max_features=log2: 0.6231
R² with n_estimators=10, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.6426
R² with n_estimators=10, max_depth=20, min_samples_leaf=2, max_features=log2: 0.6200
R² with n_estimators=10, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.6095
R² with n_estimators=10, max_depth=20, min_samples_leaf=4, max_features=log2: 0.5972
R² with n_estimators=10, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.6463
R² with n_estimators=10, max_depth=25, min_samples_leaf=1, max_features=log2: 0.6423
R² with n_estimators=10, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.6376

R² with n_estimators=10, max_depth=25, min_samples_leaf=2, max_features=log2: 0.6345
R² with n_estimators=10, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.6105
R² with n_estimators=10, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6016
R² with n_estimators=10, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.6446
R² with n_estimators=10, max_depth=30, min_samples_leaf=1, max_features=log2: 0.6367
R² with n_estimators=10, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.6366
R² with n_estimators=10, max_depth=30, min_samples_leaf=2, max_features=log2: 0.6469
R² with n_estimators=10, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.6086
R² with n_estimators=10, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6042
R² with n_estimators=10, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.6477
R² with n_estimators=10, max_depth=35, min_samples_leaf=1, max_features=log2: 0.6257
R² with n_estimators=10, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.6488
R² with n_estimators=10, max_depth=35, min_samples_leaf=2, max_features=log2: 0.6458
R² with n_estimators=10, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.6125
R² with n_estimators=10, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6034
R² with n_estimators=10, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.6485
R² with n_estimators=10, max_depth=40, min_samples_leaf=1, max_features=log2: 0.6225
R² with n_estimators=10, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.6492
R² with n_estimators=10, max_depth=40, min_samples_leaf=2, max_features=log2: 0.6442
R² with n_estimators=10, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.6145
R² with n_estimators=10, max_depth=40, min_samples_leaf=4, max_features=log2: 0.6034
R² with n_estimators=50, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.4470
R² with n_estimators=50, max_depth=10, min_samples_leaf=1, max_features=log2: 0.4334
R² with n_estimators=50, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.4395
R² with n_estimators=50, max_depth=10, min_samples_leaf=2, max_features=log2: 0.4354
R² with n_estimators=50, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.4356
R² with n_estimators=50, max_depth=10, min_samples_leaf=4, max_features=log2: 0.4158
R² with n_estimators=50, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.6164
R² with n_estimators=50, max_depth=15, min_samples_leaf=1, max_features=log2: 0.6074
R² with n_estimators=50, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.6120
R² with n_estimators=50, max_depth=15, min_samples_leaf=2, max_features=log2: 0.5935
R² with n_estimators=50, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.5984

R² with n_estimators=50, max_depth=15, min_samples_leaf=4, max_features=log2: 0.5720
R² with n_estimators=50, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.6789
R² with n_estimators=50, max_depth=20, min_samples_leaf=1, max_features=log2: 0.6663
R² with n_estimators=50, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.6671
R² with n_estimators=50, max_depth=20, min_samples_leaf=2, max_features=log2: 0.6617
R² with n_estimators=50, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.6422
R² with n_estimators=50, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6356
R² with n_estimators=50, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.6878
R² with n_estimators=50, max_depth=25, min_samples_leaf=1, max_features=log2: 0.6824
R² with n_estimators=50, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.6802
R² with n_estimators=50, max_depth=25, min_samples_leaf=2, max_features=log2: 0.6739
R² with n_estimators=50, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.6444
R² with n_estimators=50, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6414
R² with n_estimators=50, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.6863
R² with n_estimators=50, max_depth=30, min_samples_leaf=1, max_features=log2: 0.6851
R² with n_estimators=50, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.6756
R² with n_estimators=50, max_depth=30, min_samples_leaf=2, max_features=log2: 0.6748
R² with n_estimators=50, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.6489
R² with n_estimators=50, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6426
R² with n_estimators=50, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.6853
R² with n_estimators=50, max_depth=35, min_samples_leaf=1, max_features=log2: 0.6813
R² with n_estimators=50, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.6784
R² with n_estimators=50, max_depth=35, min_samples_leaf=2, max_features=log2: 0.6718
R² with n_estimators=50, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.6510
R² with n_estimators=50, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6411
R² with n_estimators=50, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.6863
R² with n_estimators=50, max_depth=40, min_samples_leaf=1, max_features=log2: 0.6806
R² with n_estimators=50, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.6790
R² with n_estimators=50, max_depth=40, min_samples_leaf=2, max_features=log2: 0.6714
R² with n_estimators=50, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.6513
R² with n_estimators=50, max_depth=40, min_samples_leaf=4, max_features=log2: 0.6421
R² with n_estimators=100, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.4527

R² with n_estimators=100, max_depth=10, min_samples_leaf=1, max_features=log2: 0.4312
R² with n_estimators=100, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.4489
R² with n_estimators=100, max_depth=10, min_samples_leaf=2, max_features=log2: 0.4353
R² with n_estimators=100, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.4411
R² with n_estimators=100, max_depth=10, min_samples_leaf=4, max_features=log2: 0.4191
R² with n_estimators=100, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.6222
R² with n_estimators=100, max_depth=15, min_samples_leaf=1, max_features=log2: 0.6081
R² with n_estimators=100, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.6193
R² with n_estimators=100, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6010
R² with n_estimators=100, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6008
R² with n_estimators=100, max_depth=15, min_samples_leaf=4, max_features=log2: 0.5767
R² with n_estimators=100, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.6829
R² with n_estimators=100, max_depth=20, min_samples_leaf=1, max_features=log2: 0.6714
R² with n_estimators=100, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.6716
R² with n_estimators=100, max_depth=20, min_samples_leaf=2, max_features=log2: 0.6653
R² with n_estimators=100, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.6458
R² with n_estimators=100, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6395
R² with n_estimators=100, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.6928
R² with n_estimators=100, max_depth=25, min_samples_leaf=1, max_features=log2: 0.6869
R² with n_estimators=100, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.6830
R² with n_estimators=100, max_depth=25, min_samples_leaf=2, max_features=log2: 0.6779
R² with n_estimators=100, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.6504
R² with n_estimators=100, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6450
R² with n_estimators=100, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.6946
R² with n_estimators=100, max_depth=30, min_samples_leaf=1, max_features=log2: 0.6899
R² with n_estimators=100, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.6813
R² with n_estimators=100, max_depth=30, min_samples_leaf=2, max_features=log2: 0.6808
R² with n_estimators=100, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.6544
R² with n_estimators=100, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6462
R² with n_estimators=100, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.6928
R² with n_estimators=100, max_depth=35, min_samples_leaf=1, max_features=log2: 0.6897
R² with n_estimators=100, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.6833

R² with n_estimators=100, max_depth=35, min_samples_leaf=2, max_features=log2: 0.6790
R² with n_estimators=100, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.6544
R² with n_estimators=100, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6450
R² with n_estimators=100, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.6930
R² with n_estimators=100, max_depth=40, min_samples_leaf=1, max_features=log2: 0.6902
R² with n_estimators=100, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.6839
R² with n_estimators=100, max_depth=40, min_samples_leaf=2, max_features=log2: 0.6789
R² with n_estimators=100, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.6546
R² with n_estimators=100, max_depth=40, min_samples_leaf=4, max_features=log2: 0.6454
R² with n_estimators=110, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.4547
R² with n_estimators=110, max_depth=10, min_samples_leaf=1, max_features=log2: 0.4332
R² with n_estimators=110, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.4512
R² with n_estimators=110, max_depth=10, min_samples_leaf=2, max_features=log2: 0.4359
R² with n_estimators=110, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.4439
R² with n_estimators=110, max_depth=10, min_samples_leaf=4, max_features=log2: 0.4180
R² with n_estimators=110, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.6236
R² with n_estimators=110, max_depth=15, min_samples_leaf=1, max_features=log2: 0.6084
R² with n_estimators=110, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.6207
R² with n_estimators=110, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6008
R² with n_estimators=110, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6008
R² with n_estimators=110, max_depth=15, min_samples_leaf=4, max_features=log2: 0.5775
R² with n_estimators=110, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.6840
R² with n_estimators=110, max_depth=20, min_samples_leaf=1, max_features=log2: 0.6716
R² with n_estimators=110, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.6728
R² with n_estimators=110, max_depth=20, min_samples_leaf=2, max_features=log2: 0.6655
R² with n_estimators=110, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.6457
R² with n_estimators=110, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6391
R² with n_estimators=110, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.6929
R² with n_estimators=110, max_depth=25, min_samples_leaf=1, max_features=log2: 0.6866
R² with n_estimators=110, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.6835
R² with n_estimators=110, max_depth=25, min_samples_leaf=2, max_features=log2: 0.6782
R² with n_estimators=110, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.6508

R² with n_estimators=110, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6450
R² with n_estimators=110, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.6945
R² with n_estimators=110, max_depth=30, min_samples_leaf=1, max_features=log2: 0.6901
R² with n_estimators=110, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.6817
R² with n_estimators=110, max_depth=30, min_samples_leaf=2, max_features=log2: 0.6799
R² with n_estimators=110, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.6534
R² with n_estimators=110, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6463
R² with n_estimators=110, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.6931
R² with n_estimators=110, max_depth=35, min_samples_leaf=1, max_features=log2: 0.6896
R² with n_estimators=110, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.6837
R² with n_estimators=110, max_depth=35, min_samples_leaf=2, max_features=log2: 0.6779
R² with n_estimators=110, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.6535
R² with n_estimators=110, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6451
R² with n_estimators=110, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.6935
R² with n_estimators=110, max_depth=40, min_samples_leaf=1, max_features=log2: 0.6905
R² with n_estimators=110, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.6841
R² with n_estimators=110, max_depth=40, min_samples_leaf=2, max_features=log2: 0.6780
R² with n_estimators=110, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.6536
R² with n_estimators=110, max_depth=40, min_samples_leaf=4, max_features=log2: 0.6455
R² with n_estimators=150, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.4561
R² with n_estimators=150, max_depth=10, min_samples_leaf=1, max_features=log2: 0.4327
R² with n_estimators=150, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.4537
R² with n_estimators=150, max_depth=10, min_samples_leaf=2, max_features=log2: 0.4373
R² with n_estimators=150, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.4472
R² with n_estimators=150, max_depth=10, min_samples_leaf=4, max_features=log2: 0.4213
R² with n_estimators=150, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.6250
R² with n_estimators=150, max_depth=15, min_samples_leaf=1, max_features=log2: 0.6114
R² with n_estimators=150, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.6228
R² with n_estimators=150, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6022
R² with n_estimators=150, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6018
R² with n_estimators=150, max_depth=15, min_samples_leaf=4, max_features=log2: 0.5820
R² with n_estimators=150, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.6850

R² with n_estimators=150, max_depth=20, min_samples_leaf=1, max_features=log2: 0.6748
R² with n_estimators=150, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.6742
R² with n_estimators=150, max_depth=20, min_samples_leaf=2, max_features=log2: 0.6672
R² with n_estimators=150, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.6466
R² with n_estimators=150, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6412
R² with n_estimators=150, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.6952
R² with n_estimators=150, max_depth=25, min_samples_leaf=1, max_features=log2: 0.6871
R² with n_estimators=150, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.6851
R² with n_estimators=150, max_depth=25, min_samples_leaf=2, max_features=log2: 0.6794
R² with n_estimators=150, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.6528
R² with n_estimators=150, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6460
R² with n_estimators=150, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.6954
R² with n_estimators=150, max_depth=30, min_samples_leaf=1, max_features=log2: 0.6910
R² with n_estimators=150, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.6835
R² with n_estimators=150, max_depth=30, min_samples_leaf=2, max_features=log2: 0.6805
R² with n_estimators=150, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.6550
R² with n_estimators=150, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6466
R² with n_estimators=150, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.6953
R² with n_estimators=150, max_depth=35, min_samples_leaf=1, max_features=log2: 0.6902
R² with n_estimators=150, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.6857
R² with n_estimators=150, max_depth=35, min_samples_leaf=2, max_features=log2: 0.6784
R² with n_estimators=150, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.6550
R² with n_estimators=150, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6452
R² with n_estimators=150, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.6958
R² with n_estimators=150, max_depth=40, min_samples_leaf=1, max_features=log2: 0.6918
R² with n_estimators=150, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.6858
R² with n_estimators=150, max_depth=40, min_samples_leaf=2, max_features=log2: 0.6787
R² with n_estimators=150, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.6551
R² with n_estimators=150, max_depth=40, min_samples_leaf=4, max_features=log2: 0.6455
R² with n_estimators=200, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.4543
R² with n_estimators=200, max_depth=10, min_samples_leaf=1, max_features=log2: 0.4341
R² with n_estimators=200, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.4523

R² with n_estimators=200, max_depth=10, min_samples_leaf=2, max_features=log2: 0.4374
R² with n_estimators=200, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.4453
R² with n_estimators=200, max_depth=10, min_samples_leaf=4, max_features=log2: 0.4264
R² with n_estimators=200, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.6259
R² with n_estimators=200, max_depth=15, min_samples_leaf=1, max_features=log2: 0.6137
R² with n_estimators=200, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.6220
R² with n_estimators=200, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6036
R² with n_estimators=200, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6022
R² with n_estimators=200, max_depth=15, min_samples_leaf=4, max_features=log2: 0.5844
R² with n_estimators=200, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.6860
R² with n_estimators=200, max_depth=20, min_samples_leaf=1, max_features=log2: 0.6765
R² with n_estimators=200, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.6744
R² with n_estimators=200, max_depth=20, min_samples_leaf=2, max_features=log2: 0.6686
R² with n_estimators=200, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.6471
R² with n_estimators=200, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6415
R² with n_estimators=200, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.6953
R² with n_estimators=200, max_depth=25, min_samples_leaf=1, max_features=log2: 0.6903
R² with n_estimators=200, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.6866
R² with n_estimators=200, max_depth=25, min_samples_leaf=2, max_features=log2: 0.6796
R² with n_estimators=200, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.6563
R² with n_estimators=200, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6474
R² with n_estimators=200, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.6962
R² with n_estimators=200, max_depth=30, min_samples_leaf=1, max_features=log2: 0.6933
R² with n_estimators=200, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.6852
R² with n_estimators=200, max_depth=30, min_samples_leaf=2, max_features=log2: 0.6804
R² with n_estimators=200, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.6565
R² with n_estimators=200, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6499
R² with n_estimators=200, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.6967
R² with n_estimators=200, max_depth=35, min_samples_leaf=1, max_features=log2: 0.6914
R² with n_estimators=200, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.6864
R² with n_estimators=200, max_depth=35, min_samples_leaf=2, max_features=log2: 0.6801
R² with n_estimators=200, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.6571

R² with n_estimators=200, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6487
R² with n_estimators=200, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.6966
R² with n_estimators=200, max_depth=40, min_samples_leaf=1, max_features=log2: 0.6925
R² with n_estimators=200, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.6873
R² with n_estimators=200, max_depth=40, min_samples_leaf=2, max_features=log2: 0.6801
R² with n_estimators=200, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.6572
R² with n_estimators=200, max_depth=40, min_samples_leaf=4, max_features=log2: 0.6487
R² with n_estimators=500, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.4578
R² with n_estimators=500, max_depth=10, min_samples_leaf=1, max_features=log2: 0.4360
R² with n_estimators=500, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.4552
R² with n_estimators=500, max_depth=10, min_samples_leaf=2, max_features=log2: 0.4372
R² with n_estimators=500, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.4502
R² with n_estimators=500, max_depth=10, min_samples_leaf=4, max_features=log2: 0.4286
R² with n_estimators=500, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.6277
R² with n_estimators=500, max_depth=15, min_samples_leaf=1, max_features=log2: 0.6140
R² with n_estimators=500, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.6229
R² with n_estimators=500, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6056
R² with n_estimators=500, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6048
R² with n_estimators=500, max_depth=15, min_samples_leaf=4, max_features=log2: 0.5862
R² with n_estimators=500, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.6873
R² with n_estimators=500, max_depth=20, min_samples_leaf=1, max_features=log2: 0.6782
R² with n_estimators=500, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.6757
R² with n_estimators=500, max_depth=20, min_samples_leaf=2, max_features=log2: 0.6685
R² with n_estimators=500, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.6496
R² with n_estimators=500, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6402
R² with n_estimators=500, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.6973
R² with n_estimators=500, max_depth=25, min_samples_leaf=1, max_features=log2: 0.6921
R² with n_estimators=500, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.6868
R² with n_estimators=500, max_depth=25, min_samples_leaf=2, max_features=log2: 0.6806
R² with n_estimators=500, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.6568
R² with n_estimators=500, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6489
R² with n_estimators=500, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.6987

R² with n_estimators=500, max_depth=30, min_samples_leaf=1, max_features=log2: 0.6945
R² with n_estimators=500, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.6876
R² with n_estimators=500, max_depth=30, min_samples_leaf=2, max_features=log2: 0.6816
R² with n_estimators=500, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.6569
R² with n_estimators=500, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6501
R² with n_estimators=500, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.6980
R² with n_estimators=500, max_depth=35, min_samples_leaf=1, max_features=log2: 0.6943
R² with n_estimators=500, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.6874
R² with n_estimators=500, max_depth=35, min_samples_leaf=2, max_features=log2: 0.6806
R² with n_estimators=500, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.6576
R² with n_estimators=500, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6496
R² with n_estimators=500, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.6971
R² with n_estimators=500, max_depth=40, min_samples_leaf=1, max_features=log2: 0.6950
R² with n_estimators=500, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.6877
R² with n_estimators=500, max_depth=40, min_samples_leaf=2, max_features=log2: 0.6808
R² with n_estimators=500, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.6578
R² with n_estimators=500, max_depth=40, min_samples_leaf=4, max_features=log2: 0.6496
R² with n_estimators=1000, max_depth=10, min_samples_leaf=1, max_features=sqrt: 0.4593
R² with n_estimators=1000, max_depth=10, min_samples_leaf=1, max_features=log2: 0.4364
R² with n_estimators=1000, max_depth=10, min_samples_leaf=2, max_features=sqrt: 0.4562
R² with n_estimators=1000, max_depth=10, min_samples_leaf=2, max_features=log2: 0.4348
R² with n_estimators=1000, max_depth=10, min_samples_leaf=4, max_features=sqrt: 0.4508
R² with n_estimators=1000, max_depth=10, min_samples_leaf=4, max_features=log2: 0.4284
R² with n_estimators=1000, max_depth=15, min_samples_leaf=1, max_features=sqrt: 0.6282
R² with n_estimators=1000, max_depth=15, min_samples_leaf=1, max_features=log2: 0.6139
R² with n_estimators=1000, max_depth=15, min_samples_leaf=2, max_features=sqrt: 0.6232
R² with n_estimators=1000, max_depth=15, min_samples_leaf=2, max_features=log2: 0.6063
R² with n_estimators=1000, max_depth=15, min_samples_leaf=4, max_features=sqrt: 0.6055
R² with n_estimators=1000, max_depth=15, min_samples_leaf=4, max_features=log2: 0.5871
R² with n_estimators=1000, max_depth=20, min_samples_leaf=1, max_features=sqrt: 0.6874
R² with n_estimators=1000, max_depth=20, min_samples_leaf=1, max_features=log2: 0.6771
R² with n_estimators=1000, max_depth=20, min_samples_leaf=2, max_features=sqrt: 0.6762

R² with n_estimators=1000, max_depth=20, min_samples_leaf=2, max_features=log2: 0.6693
R² with n_estimators=1000, max_depth=20, min_samples_leaf=4, max_features=sqrt: 0.6511
R² with n_estimators=1000, max_depth=20, min_samples_leaf=4, max_features=log2: 0.6408
R² with n_estimators=1000, max_depth=25, min_samples_leaf=1, max_features=sqrt: 0.6977
R² with n_estimators=1000, max_depth=25, min_samples_leaf=1, max_features=log2: 0.6927
R² with n_estimators=1000, max_depth=25, min_samples_leaf=2, max_features=sqrt: 0.6862
R² with n_estimators=1000, max_depth=25, min_samples_leaf=2, max_features=log2: 0.6808
R² with n_estimators=1000, max_depth=25, min_samples_leaf=4, max_features=sqrt: 0.6578
R² with n_estimators=1000, max_depth=25, min_samples_leaf=4, max_features=log2: 0.6495
R² with n_estimators=1000, max_depth=30, min_samples_leaf=1, max_features=sqrt: 0.6992
R² with n_estimators=1000, max_depth=30, min_samples_leaf=1, max_features=log2: 0.6947
R² with n_estimators=1000, max_depth=30, min_samples_leaf=2, max_features=sqrt: 0.6875
R² with n_estimators=1000, max_depth=30, min_samples_leaf=2, max_features=log2: 0.6833
R² with n_estimators=1000, max_depth=30, min_samples_leaf=4, max_features=sqrt: 0.6582
R² with n_estimators=1000, max_depth=30, min_samples_leaf=4, max_features=log2: 0.6510
R² with n_estimators=1000, max_depth=35, min_samples_leaf=1, max_features=sqrt: 0.6994
R² with n_estimators=1000, max_depth=35, min_samples_leaf=1, max_features=log2: 0.6942
R² with n_estimators=1000, max_depth=35, min_samples_leaf=2, max_features=sqrt: 0.6869
R² with n_estimators=1000, max_depth=35, min_samples_leaf=2, max_features=log2: 0.6824
R² with n_estimators=1000, max_depth=35, min_samples_leaf=4, max_features=sqrt: 0.6587
R² with n_estimators=1000, max_depth=35, min_samples_leaf=4, max_features=log2: 0.6508
R² with n_estimators=1000, max_depth=40, min_samples_leaf=1, max_features=sqrt: 0.6988
R² with n_estimators=1000, max_depth=40, min_samples_leaf=1, max_features=log2: 0.6954
R² with n_estimators=1000, max_depth=40, min_samples_leaf=2, max_features=sqrt: 0.6872
R² with n_estimators=1000, max_depth=40, min_samples_leaf=2, max_features=log2: 0.6826
R² with n_estimators=1000, max_depth=40, min_samples_leaf=4, max_features=sqrt: 0.6587
R² with n_estimators=1000, max_depth=40, min_samples_leaf=4, max_features=log2: 0.6509

Best parameters found with PCA:

{'n_estimators': 1000, 'max_depth': 35, 'min_samples_leaf': 1, 'max_features': 'sqrt'} 0.6994

1.2 RF-PCA Descriptors Loading Summary

| Principal Component | Explained Variance (%) | Cumulative Variance (%) |
|---------------------|------------------------|-------------------------|
| 0 | 6.256397034 | 6.256397034 |
| 1 | 6.156985254 | 12.41338229 |
| 2 | 4.590169043 | 17.00355133 |
| 3 | 3.903430199 | 20.90698153 |
| 4 | 3.420704615 | 24.32768614 |
| 5 | 3.225403876 | 27.55309002 |
| 6 | 2.945288712 | 30.49837873 |
| 7 | 2.561933642 | 33.06031238 |
| 8 | 2.313643773 | 35.37395615 |
| 9 | 2.190826473 | 37.56478262 |
| 10 | 2.148873282 | 39.7136559 |
| 11 | 1.919967902 | 41.63362381 |
| 12 | 1.672947571 | 43.30657138 |
| 13 | 1.616981541 | 44.92355292 |
| 14 | 1.484596313 | 46.40814923 |
| 15 | 1.46465973 | 47.87280896 |
| 16 | 1.385700944 | 49.25850991 |
| 17 | 1.344809208 | 50.60331911 |
| 18 | 1.292001199 | 51.89532031 |
| 19 | 1.236434985 | 53.1317553 |
| 20 | 1.197485075 | 54.32924037 |

| | | |
|----|-------------|-------------|
| 21 | 1.167944065 | 55.49718444 |
| 22 | 1.108375841 | 56.60556028 |
| 23 | 1.085933459 | 57.69149374 |
| 24 | 1.075143007 | 58.76663675 |
| 25 | 1.036431451 | 59.8030682 |
| 26 | 1.00000472 | 60.80307292 |
| 27 | 0.977428226 | 61.78050114 |
| 28 | 0.958662157 | 62.7391633 |
| 29 | 0.944612094 | 63.68377539 |
| 30 | 0.917614671 | 64.60139006 |
| 31 | 0.908969154 | 65.51035922 |
| 32 | 0.897524151 | 66.40788337 |
| 33 | 0.881116715 | 67.28900008 |
| 34 | 0.862501484 | 68.15150157 |
| 35 | 0.85800234 | 69.00950391 |
| 36 | 0.848589563 | 69.85809347 |
| 37 | 0.842541385 | 70.70063486 |
| 38 | 0.827230657 | 71.52786551 |
| 39 | 0.821309879 | 72.34917539 |
| 40 | 0.81036412 | 73.15953951 |
| 41 | 0.801740028 | 73.96127954 |
| 42 | 0.797612028 | 74.75889157 |
| 43 | 0.788553671 | 75.54744524 |
| 44 | 0.782004453 | 76.32944969 |

| | | |
|----|-------------|-------------|
| 45 | 0.762329632 | 77.09177932 |
| 46 | 0.752904778 | 77.8446841 |
| 47 | 0.740186873 | 78.58487097 |
| 48 | 0.721847832 | 79.30671881 |
| 49 | 0.718747291 | 80.0254661 |
| 50 | 0.713929958 | 80.73939605 |
| 51 | 0.689073609 | 81.42846966 |
| 52 | 0.671398781 | 82.09986844 |
| 53 | 0.659041754 | 82.7589102 |
| 54 | 0.657193436 | 83.41610363 |
| 55 | 0.650879666 | 84.0669833 |
| 56 | 0.644906299 | 84.7118896 |
| 57 | 0.617546889 | 85.32943649 |
| 58 | 0.611293178 | 85.94072967 |
| 59 | 0.599544702 | 86.54027437 |
| 60 | 0.589469091 | 87.12974346 |
| 61 | 0.558743301 | 87.68848676 |
| 62 | 0.544447761 | 88.23293452 |
| 63 | 0.536892808 | 88.76982733 |
| 64 | 0.518558848 | 89.28838618 |
| 65 | 0.512876437 | 89.80126261 |
| 66 | 0.490010709 | 90.29127332 |
| 67 | 0.470812338 | 90.76208566 |
| 68 | 0.453065467 | 91.21515113 |

| | | |
|----|-------------|-------------|
| 69 | 0.446100229 | 91.66125136 |
| 70 | 0.42408913 | 92.08534049 |
| 71 | 0.418875626 | 92.50421611 |
| 72 | 0.403017082 | 92.90723319 |
| 73 | 0.368531302 | 93.2757645 |
| 74 | 0.355475842 | 93.63124034 |
| 75 | 0.346742445 | 93.97798278 |
| 76 | 0.316932146 | 94.29491493 |
| 77 | 0.310909887 | 94.60582482 |
| 78 | 0.300431221 | 94.90625604 |
| 79 | 0.293552858 | 95.19980889 |

1.3 Gradient Boosting

Testing different parameter combinations for Gradient Boosting on the normalized dataset (test set 15%)

```
param_grid_normalized = {
    'n_estimators': [10, 50, 100, 110, 150, 300, 500, 1000],
    'max_depth': [3, 5, 7, 10, 15],
    'learning_rate': [0.01, 0.05, 0.1],
    'min_samples_leaf': [1, 2, 4]
}
```

R²

Testing different parameter combinations on the normalized dataset:

R² with n_estimators=10, max_depth=3, learning_rate=0.01, min_samples_leaf=1: 0.0375

R² with n_estimators=10, max_depth=3, learning_rate=0.01, min_samples_leaf=2: 0.0375

R² with n_estimators=10, max_depth=3, learning_rate=0.01, min_samples_leaf=4: 0.0375

R² with n_estimators=10, max_depth=3, learning_rate=0.05, min_samples_leaf=1: 0.1410

R² with n_estimators=10, max_depth=3, learning_rate=0.05, min_samples_leaf=2: 0.1410
R² with n_estimators=10, max_depth=3, learning_rate=0.05, min_samples_leaf=4: 0.1410
R² with n_estimators=10, max_depth=3, learning_rate=0.1, min_samples_leaf=1: 0.2132
R² with n_estimators=10, max_depth=3, learning_rate=0.1, min_samples_leaf=2: 0.2132
R² with n_estimators=10, max_depth=3, learning_rate=0.1, min_samples_leaf=4: 0.2132
R² with n_estimators=10, max_depth=5, learning_rate=0.01, min_samples_leaf=1: 0.0571
R² with n_estimators=10, max_depth=5, learning_rate=0.01, min_samples_leaf=2: 0.0571
R² with n_estimators=10, max_depth=5, learning_rate=0.01, min_samples_leaf=4: 0.0571
R² with n_estimators=10, max_depth=5, learning_rate=0.05, min_samples_leaf=1: 0.2057
R² with n_estimators=10, max_depth=5, learning_rate=0.05, min_samples_leaf=2: 0.2057
R² with n_estimators=10, max_depth=5, learning_rate=0.05, min_samples_leaf=4: 0.2057
R² with n_estimators=10, max_depth=5, learning_rate=0.1, min_samples_leaf=1: 0.3196
R² with n_estimators=10, max_depth=5, learning_rate=0.1, min_samples_leaf=2: 0.3196
R² with n_estimators=10, max_depth=5, learning_rate=0.1, min_samples_leaf=4: 0.3192
R² with n_estimators=10, max_depth=7, learning_rate=0.01, min_samples_leaf=1: 0.0796
R² with n_estimators=10, max_depth=7, learning_rate=0.01, min_samples_leaf=2: 0.0797
R² with n_estimators=10, max_depth=7, learning_rate=0.01, min_samples_leaf=4: 0.0791
R² with n_estimators=10, max_depth=7, learning_rate=0.05, min_samples_leaf=1: 0.2881
R² with n_estimators=10, max_depth=7, learning_rate=0.05, min_samples_leaf=2: 0.2898
R² with n_estimators=10, max_depth=7, learning_rate=0.05, min_samples_leaf=4: 0.2874
R² with n_estimators=10, max_depth=7, learning_rate=0.1, min_samples_leaf=1: 0.4313
R² with n_estimators=10, max_depth=7, learning_rate=0.1, min_samples_leaf=2: 0.4332
R² with n_estimators=10, max_depth=7, learning_rate=0.1, min_samples_leaf=4: 0.4370
R² with n_estimators=10, max_depth=10, learning_rate=0.01, min_samples_leaf=1: 0.1025
R² with n_estimators=10, max_depth=10, learning_rate=0.01, min_samples_leaf=2: 0.1022
R² with n_estimators=10, max_depth=10, learning_rate=0.01, min_samples_leaf=4: 0.1008
R² with n_estimators=10, max_depth=10, learning_rate=0.05, min_samples_leaf=1: 0.3879
R² with n_estimators=10, max_depth=10, learning_rate=0.05, min_samples_leaf=2: 0.3875
R² with n_estimators=10, max_depth=10, learning_rate=0.05, min_samples_leaf=4: 0.3825
R² with n_estimators=10, max_depth=10, learning_rate=0.1, min_samples_leaf=1: 0.5437
R² with n_estimators=10, max_depth=10, learning_rate=0.1, min_samples_leaf=2: 0.5536
R² with n_estimators=10, max_depth=10, learning_rate=0.1, min_samples_leaf=4: 0.5458

R² with n_estimators=10, max_depth=15, learning_rate=0.01, min_samples_leaf=1: 0.1306
R² with n_estimators=10, max_depth=15, learning_rate=0.01, min_samples_leaf=2: 0.1303
R² with n_estimators=10, max_depth=15, learning_rate=0.01, min_samples_leaf=4: 0.1258
R² with n_estimators=10, max_depth=15, learning_rate=0.05, min_samples_leaf=1: 0.4653
R² with n_estimators=10, max_depth=15, learning_rate=0.05, min_samples_leaf=2: 0.4619
R² with n_estimators=10, max_depth=15, learning_rate=0.05, min_samples_leaf=4: 0.4561
R² with n_estimators=10, max_depth=15, learning_rate=0.1, min_samples_leaf=1: 0.6382
R² with n_estimators=10, max_depth=15, learning_rate=0.1, min_samples_leaf=2: 0.6405
R² with n_estimators=10, max_depth=15, learning_rate=0.1, min_samples_leaf=4: 0.6399
R² with n_estimators=50, max_depth=3, learning_rate=0.01, min_samples_leaf=1: 0.1389
R² with n_estimators=50, max_depth=3, learning_rate=0.01, min_samples_leaf=2: 0.1389
R² with n_estimators=50, max_depth=3, learning_rate=0.01, min_samples_leaf=4: 0.1389
R² with n_estimators=50, max_depth=3, learning_rate=0.05, min_samples_leaf=1: 0.3163
R² with n_estimators=50, max_depth=3, learning_rate=0.05, min_samples_leaf=2: 0.3163
R² with n_estimators=50, max_depth=3, learning_rate=0.05, min_samples_leaf=4: 0.3163
R² with n_estimators=50, max_depth=3, learning_rate=0.1, min_samples_leaf=1: 0.3882
R² with n_estimators=50, max_depth=3, learning_rate=0.1, min_samples_leaf=2: 0.3879
R² with n_estimators=50, max_depth=3, learning_rate=0.1, min_samples_leaf=4: 0.3871
R² with n_estimators=50, max_depth=5, learning_rate=0.01, min_samples_leaf=1: 0.2061
R² with n_estimators=50, max_depth=5, learning_rate=0.01, min_samples_leaf=2: 0.2061
R² with n_estimators=50, max_depth=5, learning_rate=0.01, min_samples_leaf=4: 0.2062
R² with n_estimators=50, max_depth=5, learning_rate=0.05, min_samples_leaf=1: 0.4650
R² with n_estimators=50, max_depth=5, learning_rate=0.05, min_samples_leaf=2: 0.4697
R² with n_estimators=50, max_depth=5, learning_rate=0.05, min_samples_leaf=4: 0.4714
R² with n_estimators=50, max_depth=5, learning_rate=0.1, min_samples_leaf=1: 0.5546
R² with n_estimators=50, max_depth=5, learning_rate=0.1, min_samples_leaf=2: 0.5584
R² with n_estimators=50, max_depth=5, learning_rate=0.1, min_samples_leaf=4: 0.5518
R² with n_estimators=50, max_depth=7, learning_rate=0.01, min_samples_leaf=1: 0.2838
R² with n_estimators=50, max_depth=7, learning_rate=0.01, min_samples_leaf=2: 0.2839
R² with n_estimators=50, max_depth=7, learning_rate=0.01, min_samples_leaf=4: 0.2824
R² with n_estimators=50, max_depth=7, learning_rate=0.05, min_samples_leaf=1: 0.5978
R² with n_estimators=50, max_depth=7, learning_rate=0.05, min_samples_leaf=2: 0.5998

R² with n_estimators=50, max_depth=7, learning_rate=0.05, min_samples_leaf=4: 0.5969
R² with n_estimators=50, max_depth=7, learning_rate=0.1, min_samples_leaf=1: 0.6695
R² with n_estimators=50, max_depth=7, learning_rate=0.1, min_samples_leaf=2: 0.6671
R² with n_estimators=50, max_depth=7, learning_rate=0.1, min_samples_leaf=4: 0.6663
R² with n_estimators=50, max_depth=10, learning_rate=0.01, min_samples_leaf=1: 0.3792
R² with n_estimators=50, max_depth=10, learning_rate=0.01, min_samples_leaf=2: 0.3781
R² with n_estimators=50, max_depth=10, learning_rate=0.01, min_samples_leaf=4: 0.3750
R² with n_estimators=50, max_depth=10, learning_rate=0.05, min_samples_leaf=1: 0.7054
R² with n_estimators=50, max_depth=10, learning_rate=0.05, min_samples_leaf=2: 0.7049
R² with n_estimators=50, max_depth=10, learning_rate=0.05, min_samples_leaf=4: 0.7078
R² with n_estimators=50, max_depth=10, learning_rate=0.1, min_samples_leaf=1: 0.7571
R² with n_estimators=50, max_depth=10, learning_rate=0.1, min_samples_leaf=2: 0.7517
R² with n_estimators=50, max_depth=10, learning_rate=0.1, min_samples_leaf=4: 0.7475
R² with n_estimators=50, max_depth=15, learning_rate=0.01, min_samples_leaf=1: 0.4618
R² with n_estimators=50, max_depth=15, learning_rate=0.01, min_samples_leaf=2: 0.4572
R² with n_estimators=50, max_depth=15, learning_rate=0.01, min_samples_leaf=4: 0.4492
R² with n_estimators=50, max_depth=15, learning_rate=0.05, min_samples_leaf=1: 0.7381
R² with n_estimators=50, max_depth=15, learning_rate=0.05, min_samples_leaf=2: 0.7447
R² with n_estimators=50, max_depth=15, learning_rate=0.05, min_samples_leaf=4: 0.7526
R² with n_estimators=50, max_depth=15, learning_rate=0.1, min_samples_leaf=1: 0.7420
R² with n_estimators=50, max_depth=15, learning_rate=0.1, min_samples_leaf=2: 0.7546
R² with n_estimators=50, max_depth=15, learning_rate=0.1, min_samples_leaf=4: 0.7614
R² with n_estimators=100, max_depth=3, learning_rate=0.01, min_samples_leaf=1: 0.2090
R² with n_estimators=100, max_depth=3, learning_rate=0.01, min_samples_leaf=2: 0.2090
R² with n_estimators=100, max_depth=3, learning_rate=0.01, min_samples_leaf=4: 0.2090
R² with n_estimators=100, max_depth=3, learning_rate=0.05, min_samples_leaf=1: 0.3880
R² with n_estimators=100, max_depth=3, learning_rate=0.05, min_samples_leaf=2: 0.3876
R² with n_estimators=100, max_depth=3, learning_rate=0.05, min_samples_leaf=4: 0.3899
R² with n_estimators=100, max_depth=3, learning_rate=0.1, min_samples_leaf=1: 0.4705
R² with n_estimators=100, max_depth=3, learning_rate=0.1, min_samples_leaf=2: 0.4749
R² with n_estimators=100, max_depth=3, learning_rate=0.1, min_samples_leaf=4: 0.4690
R² with n_estimators=100, max_depth=5, learning_rate=0.01, min_samples_leaf=1: 0.3139

R² with n_estimators=100, max_depth=5, learning_rate=0.01, min_samples_leaf=2: 0.3137
R² with n_estimators=100, max_depth=5, learning_rate=0.01, min_samples_leaf=4: 0.3131
R² with n_estimators=100, max_depth=5, learning_rate=0.05, min_samples_leaf=1: 0.5532
R² with n_estimators=100, max_depth=5, learning_rate=0.05, min_samples_leaf=2: 0.5519
R² with n_estimators=100, max_depth=5, learning_rate=0.05, min_samples_leaf=4: 0.5555
R² with n_estimators=100, max_depth=5, learning_rate=0.1, min_samples_leaf=1: 0.6218
R² with n_estimators=100, max_depth=5, learning_rate=0.1, min_samples_leaf=2: 0.6198
R² with n_estimators=100, max_depth=5, learning_rate=0.1, min_samples_leaf=4: 0.6247
R² with n_estimators=100, max_depth=7, learning_rate=0.01, min_samples_leaf=1: 0.4244
R² with n_estimators=100, max_depth=7, learning_rate=0.01, min_samples_leaf=2: 0.4245
R² with n_estimators=100, max_depth=7, learning_rate=0.01, min_samples_leaf=4: 0.4233
R² with n_estimators=100, max_depth=7, learning_rate=0.05, min_samples_leaf=1: 0.6732
R² with n_estimators=100, max_depth=7, learning_rate=0.05, min_samples_leaf=2: 0.6703
R² with n_estimators=100, max_depth=7, learning_rate=0.05, min_samples_leaf=4: 0.6707
R² with n_estimators=100, max_depth=7, learning_rate=0.1, min_samples_leaf=1: 0.7172
R² with n_estimators=100, max_depth=7, learning_rate=0.1, min_samples_leaf=2: 0.7147
R² with n_estimators=100, max_depth=7, learning_rate=0.1, min_samples_leaf=4: 0.7164
R² with n_estimators=100, max_depth=10, learning_rate=0.01, min_samples_leaf=1: 0.5437
R² with n_estimators=100, max_depth=10, learning_rate=0.01, min_samples_leaf=2: 0.5468
R² with n_estimators=100, max_depth=10, learning_rate=0.01, min_samples_leaf=4: 0.5437
R² with n_estimators=100, max_depth=10, learning_rate=0.05, min_samples_leaf=1: 0.7531
R² with n_estimators=100, max_depth=10, learning_rate=0.05, min_samples_leaf=2: 0.7543
R² with n_estimators=100, max_depth=10, learning_rate=0.05, min_samples_leaf=4: 0.7575
R² with n_estimators=100, max_depth=10, learning_rate=0.1, min_samples_leaf=1: 0.7710
R² with n_estimators=100, max_depth=10, learning_rate=0.1, min_samples_leaf=2: 0.7686
R² with n_estimators=100, max_depth=10, learning_rate=0.1, min_samples_leaf=4: 0.7655
R² with n_estimators=100, max_depth=15, learning_rate=0.01, min_samples_leaf=1: 0.6357
R² with n_estimators=100, max_depth=15, learning_rate=0.01, min_samples_leaf=2: 0.6340
R² with n_estimators=100, max_depth=15, learning_rate=0.01, min_samples_leaf=4: 0.6331
R² with n_estimators=100, max_depth=15, learning_rate=0.05, min_samples_leaf=1: 0.7444
R² with n_estimators=100, max_depth=15, learning_rate=0.05, min_samples_leaf=2: 0.7544
R² with n_estimators=100, max_depth=15, learning_rate=0.05, min_samples_leaf=4: 0.7647

R² with n_estimators=100, max_depth=15, learning_rate=0.1, min_samples_leaf=1: 0.7403
R² with n_estimators=100, max_depth=15, learning_rate=0.1, min_samples_leaf=2: 0.7535
R² with n_estimators=100, max_depth=15, learning_rate=0.1, min_samples_leaf=4: 0.7612
R² with n_estimators=110, max_depth=3, learning_rate=0.01, min_samples_leaf=1: 0.2201
R² with n_estimators=110, max_depth=3, learning_rate=0.01, min_samples_leaf=2: 0.2201
R² with n_estimators=110, max_depth=3, learning_rate=0.01, min_samples_leaf=4: 0.2201
R² with n_estimators=110, max_depth=3, learning_rate=0.05, min_samples_leaf=1: 0.3989
R² with n_estimators=110, max_depth=3, learning_rate=0.05, min_samples_leaf=2: 0.3983
R² with n_estimators=110, max_depth=3, learning_rate=0.05, min_samples_leaf=4: 0.4016
R² with n_estimators=110, max_depth=3, learning_rate=0.1, min_samples_leaf=1: 0.4846
R² with n_estimators=110, max_depth=3, learning_rate=0.1, min_samples_leaf=2: 0.4844
R² with n_estimators=110, max_depth=3, learning_rate=0.1, min_samples_leaf=4: 0.4802
R² with n_estimators=110, max_depth=5, learning_rate=0.01, min_samples_leaf=1: 0.3293
R² with n_estimators=110, max_depth=5, learning_rate=0.01, min_samples_leaf=2: 0.3290
R² with n_estimators=110, max_depth=5, learning_rate=0.01, min_samples_leaf=4: 0.3288
R² with n_estimators=110, max_depth=5, learning_rate=0.05, min_samples_leaf=1: 0.5645
R² with n_estimators=110, max_depth=5, learning_rate=0.05, min_samples_leaf=2: 0.5622
R² with n_estimators=110, max_depth=5, learning_rate=0.05, min_samples_leaf=4: 0.5653
R² with n_estimators=110, max_depth=5, learning_rate=0.1, min_samples_leaf=1: 0.6284
R² with n_estimators=110, max_depth=5, learning_rate=0.1, min_samples_leaf=2: 0.6302
R² with n_estimators=110, max_depth=5, learning_rate=0.1, min_samples_leaf=4: 0.6333
R² with n_estimators=110, max_depth=7, learning_rate=0.01, min_samples_leaf=1: 0.4453
R² with n_estimators=110, max_depth=7, learning_rate=0.01, min_samples_leaf=2: 0.4457
R² with n_estimators=110, max_depth=7, learning_rate=0.01, min_samples_leaf=4: 0.4436
R² with n_estimators=110, max_depth=7, learning_rate=0.05, min_samples_leaf=1: 0.6809
R² with n_estimators=110, max_depth=7, learning_rate=0.05, min_samples_leaf=2: 0.6774
R² with n_estimators=110, max_depth=7, learning_rate=0.05, min_samples_leaf=4: 0.6789
R² with n_estimators=110, max_depth=7, learning_rate=0.1, min_samples_leaf=1: 0.7214
R² with n_estimators=110, max_depth=7, learning_rate=0.1, min_samples_leaf=2: 0.7220
R² with n_estimators=110, max_depth=7, learning_rate=0.1, min_samples_leaf=4: 0.7203
R² with n_estimators=110, max_depth=10, learning_rate=0.01, min_samples_leaf=1: 0.5653
R² with n_estimators=110, max_depth=10, learning_rate=0.01, min_samples_leaf=2: 0.5688

R² with n_estimators=110, max_depth=10, learning_rate=0.01, min_samples_leaf=4: 0.5641
R² with n_estimators=110, max_depth=10, learning_rate=0.05, min_samples_leaf=1: 0.7571
R² with n_estimators=110, max_depth=10, learning_rate=0.05, min_samples_leaf=2: 0.7570
R² with n_estimators=110, max_depth=10, learning_rate=0.05, min_samples_leaf=4: 0.7607
R² with n_estimators=110, max_depth=10, learning_rate=0.1, min_samples_leaf=1: 0.7722
R² with n_estimators=110, max_depth=10, learning_rate=0.1, min_samples_leaf=2: 0.7701
R² with n_estimators=110, max_depth=10, learning_rate=0.1, min_samples_leaf=4: 0.7667
R² with n_estimators=110, max_depth=15, learning_rate=0.01, min_samples_leaf=1: 0.6546
R² with n_estimators=110, max_depth=15, learning_rate=0.01, min_samples_leaf=2: 0.6533
R² with n_estimators=110, max_depth=15, learning_rate=0.01, min_samples_leaf=4: 0.6532
R² with n_estimators=110, max_depth=15, learning_rate=0.05, min_samples_leaf=1: 0.7439
R² with n_estimators=110, max_depth=15, learning_rate=0.05, min_samples_leaf=2: 0.7541
R² with n_estimators=110, max_depth=15, learning_rate=0.05, min_samples_leaf=4: 0.7651
R² with n_estimators=110, max_depth=15, learning_rate=0.1, min_samples_leaf=1: 0.7402
R² with n_estimators=110, max_depth=15, learning_rate=0.1, min_samples_leaf=2: 0.7533
R² with n_estimators=110, max_depth=15, learning_rate=0.1, min_samples_leaf=4: 0.7609
R² with n_estimators=150, max_depth=3, learning_rate=0.01, min_samples_leaf=1: 0.2572
R² with n_estimators=150, max_depth=3, learning_rate=0.01, min_samples_leaf=2: 0.2572
R² with n_estimators=150, max_depth=3, learning_rate=0.01, min_samples_leaf=4: 0.2572
R² with n_estimators=150, max_depth=3, learning_rate=0.05, min_samples_leaf=1: 0.4346
R² with n_estimators=150, max_depth=3, learning_rate=0.05, min_samples_leaf=2: 0.4344
R² with n_estimators=150, max_depth=3, learning_rate=0.05, min_samples_leaf=4: 0.4388
R² with n_estimators=150, max_depth=3, learning_rate=0.1, min_samples_leaf=1: 0.5175
R² with n_estimators=150, max_depth=3, learning_rate=0.1, min_samples_leaf=2: 0.5179
R² with n_estimators=150, max_depth=3, learning_rate=0.1, min_samples_leaf=4: 0.5123
R² with n_estimators=150, max_depth=5, learning_rate=0.01, min_samples_leaf=1: 0.3821
R² with n_estimators=150, max_depth=5, learning_rate=0.01, min_samples_leaf=2: 0.3827
R² with n_estimators=150, max_depth=5, learning_rate=0.01, min_samples_leaf=4: 0.3816
R² with n_estimators=150, max_depth=5, learning_rate=0.05, min_samples_leaf=1: 0.5943
R² with n_estimators=150, max_depth=5, learning_rate=0.05, min_samples_leaf=2: 0.5914
R² with n_estimators=150, max_depth=5, learning_rate=0.05, min_samples_leaf=4: 0.5941
R² with n_estimators=150, max_depth=5, learning_rate=0.1, min_samples_leaf=1: 0.6539

R² with n_estimators=150, max_depth=5, learning_rate=0.1, min_samples_leaf=2: 0.6619
R² with n_estimators=150, max_depth=5, learning_rate=0.1, min_samples_leaf=4: 0.6616
R² with n_estimators=150, max_depth=7, learning_rate=0.01, min_samples_leaf=1: 0.5041
R² with n_estimators=150, max_depth=7, learning_rate=0.01, min_samples_leaf=2: 0.5045
R² with n_estimators=150, max_depth=7, learning_rate=0.01, min_samples_leaf=4: 0.5020
R² with n_estimators=150, max_depth=7, learning_rate=0.05, min_samples_leaf=1: 0.7053
R² with n_estimators=150, max_depth=7, learning_rate=0.05, min_samples_leaf=2: 0.6993
R² with n_estimators=150, max_depth=7, learning_rate=0.05, min_samples_leaf=4: 0.7005
R² with n_estimators=150, max_depth=7, learning_rate=0.1, min_samples_leaf=1: 0.7376
R² with n_estimators=150, max_depth=7, learning_rate=0.1, min_samples_leaf=2: 0.7397
R² with n_estimators=150, max_depth=7, learning_rate=0.1, min_samples_leaf=4: 0.7400
R² with n_estimators=150, max_depth=10, learning_rate=0.01, min_samples_leaf=1: 0.6314
R² with n_estimators=150, max_depth=10, learning_rate=0.01, min_samples_leaf=2: 0.6335
R² with n_estimators=150, max_depth=10, learning_rate=0.01, min_samples_leaf=4: 0.6263
R² with n_estimators=150, max_depth=10, learning_rate=0.05, min_samples_leaf=1: 0.7637
R² with n_estimators=150, max_depth=10, learning_rate=0.05, min_samples_leaf=2: 0.7642
R² with n_estimators=150, max_depth=10, learning_rate=0.05, min_samples_leaf=4: 0.7692
R² with n_estimators=150, max_depth=10, learning_rate=0.1, min_samples_leaf=1: 0.7742
R² with n_estimators=150, max_depth=10, learning_rate=0.1, min_samples_leaf=2: 0.7724
R² with n_estimators=150, max_depth=10, learning_rate=0.1, min_samples_leaf=4: 0.7711
R² with n_estimators=150, max_depth=15, learning_rate=0.01, min_samples_leaf=1: 0.7033
R² with n_estimators=150, max_depth=15, learning_rate=0.01, min_samples_leaf=2: 0.7039
R² with n_estimators=150, max_depth=15, learning_rate=0.01, min_samples_leaf=4: 0.7063
R² with n_estimators=150, max_depth=15, learning_rate=0.05, min_samples_leaf=1: 0.7427
R² with n_estimators=150, max_depth=15, learning_rate=0.05, min_samples_leaf=2: 0.7535
R² with n_estimators=150, max_depth=15, learning_rate=0.05, min_samples_leaf=4: 0.7651
R² with n_estimators=150, max_depth=15, learning_rate=0.1, min_samples_leaf=1: 0.7400
R² with n_estimators=150, max_depth=15, learning_rate=0.1, min_samples_leaf=2: 0.7527
R² with n_estimators=150, max_depth=15, learning_rate=0.1, min_samples_leaf=4: 0.7603
R² with n_estimators=300, max_depth=3, learning_rate=0.01, min_samples_leaf=1: 0.3359
R² with n_estimators=300, max_depth=3, learning_rate=0.01, min_samples_leaf=2: 0.3359
R² with n_estimators=300, max_depth=3, learning_rate=0.01, min_samples_leaf=4: 0.3359

R² with n_estimators=300, max_depth=3, learning_rate=0.05, min_samples_leaf=1: 0.5160
R² with n_estimators=300, max_depth=3, learning_rate=0.05, min_samples_leaf=2: 0.5149
R² with n_estimators=300, max_depth=3, learning_rate=0.05, min_samples_leaf=4: 0.5175
R² with n_estimators=300, max_depth=3, learning_rate=0.1, min_samples_leaf=1: 0.5897
R² with n_estimators=300, max_depth=3, learning_rate=0.1, min_samples_leaf=2: 0.5894
R² with n_estimators=300, max_depth=3, learning_rate=0.1, min_samples_leaf=4: 0.5863
R² with n_estimators=300, max_depth=5, learning_rate=0.01, min_samples_leaf=1: 0.4918
R² with n_estimators=300, max_depth=5, learning_rate=0.01, min_samples_leaf=2: 0.4931
R² with n_estimators=300, max_depth=5, learning_rate=0.01, min_samples_leaf=4: 0.4915
R² with n_estimators=300, max_depth=5, learning_rate=0.05, min_samples_leaf=1: 0.6612
R² with n_estimators=300, max_depth=5, learning_rate=0.05, min_samples_leaf=2: 0.6622
R² with n_estimators=300, max_depth=5, learning_rate=0.05, min_samples_leaf=4: 0.6614
R² with n_estimators=300, max_depth=5, learning_rate=0.1, min_samples_leaf=1: 0.7157
R² with n_estimators=300, max_depth=5, learning_rate=0.1, min_samples_leaf=2: 0.7146
R² with n_estimators=300, max_depth=5, learning_rate=0.1, min_samples_leaf=4: 0.7149
R² with n_estimators=300, max_depth=7, learning_rate=0.01, min_samples_leaf=1: 0.6209
R² with n_estimators=300, max_depth=7, learning_rate=0.01, min_samples_leaf=2: 0.6184
R² with n_estimators=300, max_depth=7, learning_rate=0.01, min_samples_leaf=4: 0.6204
R² with n_estimators=300, max_depth=7, learning_rate=0.05, min_samples_leaf=1: 0.7428
R² with n_estimators=300, max_depth=7, learning_rate=0.05, min_samples_leaf=2: 0.7433
R² with n_estimators=300, max_depth=7, learning_rate=0.05, min_samples_leaf=4: 0.7419
R² with n_estimators=300, max_depth=7, learning_rate=0.1, min_samples_leaf=1: 0.7619
R² with n_estimators=300, max_depth=7, learning_rate=0.1, min_samples_leaf=2: 0.7667
R² with n_estimators=300, max_depth=7, learning_rate=0.1, min_samples_leaf=4: 0.7677
R² with n_estimators=300, max_depth=10, learning_rate=0.01, min_samples_leaf=1: 0.7241
R² with n_estimators=300, max_depth=10, learning_rate=0.01, min_samples_leaf=2: 0.7247
R² with n_estimators=300, max_depth=10, learning_rate=0.01, min_samples_leaf=4: 0.7210
R² with n_estimators=300, max_depth=10, learning_rate=0.05, min_samples_leaf=1: 0.7709
R² with n_estimators=300, max_depth=10, learning_rate=0.05, min_samples_leaf=2: 0.7733
R² with n_estimators=300, max_depth=10, learning_rate=0.05, min_samples_leaf=4: 0.7782
R² with n_estimators=300, max_depth=10, learning_rate=0.1, min_samples_leaf=1: 0.7764
R² with n_estimators=300, max_depth=10, learning_rate=0.1, min_samples_leaf=2: 0.7749

R² with n_estimators=300, max_depth=10, learning_rate=0.1, min_samples_leaf=4: 0.7735
R² with n_estimators=300, max_depth=15, learning_rate=0.01, min_samples_leaf=1: 0.7450
R² with n_estimators=300, max_depth=15, learning_rate=0.01, min_samples_leaf=2: 0.7524
R² with n_estimators=300, max_depth=15, learning_rate=0.01, min_samples_leaf=4: 0.7599
R² with n_estimators=300, max_depth=15, learning_rate=0.05, min_samples_leaf=1: 0.7419
R² with n_estimators=300, max_depth=15, learning_rate=0.05, min_samples_leaf=2: 0.7521
R² with n_estimators=300, max_depth=15, learning_rate=0.05, min_samples_leaf=4: 0.7645
R² with n_estimators=300, max_depth=15, learning_rate=0.1, min_samples_leaf=1: 0.7398
R² with n_estimators=300, max_depth=15, learning_rate=0.1, min_samples_leaf=2: 0.7519
R² with n_estimators=300, max_depth=15, learning_rate=0.1, min_samples_leaf=4: 0.7581
R² with n_estimators=500, max_depth=3, learning_rate=0.01, min_samples_leaf=1: 0.3887
R² with n_estimators=500, max_depth=3, learning_rate=0.01, min_samples_leaf=2: 0.3893
R² with n_estimators=500, max_depth=3, learning_rate=0.01, min_samples_leaf=4: 0.3891
R² with n_estimators=500, max_depth=3, learning_rate=0.05, min_samples_leaf=1: 0.5712
R² with n_estimators=500, max_depth=3, learning_rate=0.05, min_samples_leaf=2: 0.5741
R² with n_estimators=500, max_depth=3, learning_rate=0.05, min_samples_leaf=4: 0.5740
R² with n_estimators=500, max_depth=3, learning_rate=0.1, min_samples_leaf=1: 0.6362
R² with n_estimators=500, max_depth=3, learning_rate=0.1, min_samples_leaf=2: 0.6336
R² with n_estimators=500, max_depth=3, learning_rate=0.1, min_samples_leaf=4: 0.6340
R² with n_estimators=500, max_depth=5, learning_rate=0.01, min_samples_leaf=1: 0.5507
R² with n_estimators=500, max_depth=5, learning_rate=0.01, min_samples_leaf=2: 0.5519
R² with n_estimators=500, max_depth=5, learning_rate=0.01, min_samples_leaf=4: 0.5521
R² with n_estimators=500, max_depth=5, learning_rate=0.05, min_samples_leaf=1: 0.7023
R² with n_estimators=500, max_depth=5, learning_rate=0.05, min_samples_leaf=2: 0.7061
R² with n_estimators=500, max_depth=5, learning_rate=0.05, min_samples_leaf=4: 0.7029
R² with n_estimators=500, max_depth=5, learning_rate=0.1, min_samples_leaf=1: 0.7459
R² with n_estimators=500, max_depth=5, learning_rate=0.1, min_samples_leaf=2: 0.7456
R² with n_estimators=500, max_depth=5, learning_rate=0.1, min_samples_leaf=4: 0.7420
R² with n_estimators=500, max_depth=7, learning_rate=0.01, min_samples_leaf=1: 0.6718
R² with n_estimators=500, max_depth=7, learning_rate=0.01, min_samples_leaf=2: 0.6707
R² with n_estimators=500, max_depth=7, learning_rate=0.01, min_samples_leaf=4: 0.6715
R² with n_estimators=500, max_depth=7, learning_rate=0.05, min_samples_leaf=1: 0.7611

R² with n_estimators=500, max_depth=7, learning_rate=0.05, min_samples_leaf=2: 0.7635
R² with n_estimators=500, max_depth=7, learning_rate=0.05, min_samples_leaf=4: 0.7618
R² with n_estimators=500, max_depth=7, learning_rate=0.1, min_samples_leaf=1: 0.7707
R² with n_estimators=500, max_depth=7, learning_rate=0.1, min_samples_leaf=2: 0.7756
R² with n_estimators=500, max_depth=7, learning_rate=0.1, min_samples_leaf=4: 0.7775
R² with n_estimators=500, max_depth=10, learning_rate=0.01, min_samples_leaf=1: 0.7548
R² with n_estimators=500, max_depth=10, learning_rate=0.01, min_samples_leaf=2: 0.7559
R² with n_estimators=500, max_depth=10, learning_rate=0.01, min_samples_leaf=4: 0.7500
R² with n_estimators=500, max_depth=10, learning_rate=0.05, min_samples_leaf=1: 0.7725
R² with n_estimators=500, max_depth=10, learning_rate=0.05, min_samples_leaf=2: 0.7745
R² with n_estimators=500, max_depth=10, learning_rate=0.05, min_samples_leaf=4: 0.7798
R² with n_estimators=500, max_depth=10, learning_rate=0.1, min_samples_leaf=1: 0.7748
R² with n_estimators=500, max_depth=10, learning_rate=0.1, min_samples_leaf=2: 0.7732
R² with n_estimators=500, max_depth=10, learning_rate=0.1, min_samples_leaf=4: 0.7729
R² with n_estimators=500, max_depth=15, learning_rate=0.01, min_samples_leaf=1: 0.7478
R² with n_estimators=500, max_depth=15, learning_rate=0.01, min_samples_leaf=2: 0.7562
R² with n_estimators=500, max_depth=15, learning_rate=0.01, min_samples_leaf=4: 0.7662
R² with n_estimators=500, max_depth=15, learning_rate=0.05, min_samples_leaf=1: 0.7417
R² with n_estimators=500, max_depth=15, learning_rate=0.05, min_samples_leaf=2: 0.7513
R² with n_estimators=500, max_depth=15, learning_rate=0.05, min_samples_leaf=4: 0.7631
R² with n_estimators=500, max_depth=15, learning_rate=0.1, min_samples_leaf=1: 0.7398
R² with n_estimators=500, max_depth=15, learning_rate=0.1, min_samples_leaf=2: 0.7517
R² with n_estimators=500, max_depth=15, learning_rate=0.1, min_samples_leaf=4: 0.7572
R² with n_estimators=1000, max_depth=3, learning_rate=0.01, min_samples_leaf=1: 0.4709
R² with n_estimators=1000, max_depth=3, learning_rate=0.01, min_samples_leaf=2: 0.4725
R² with n_estimators=1000, max_depth=3, learning_rate=0.01, min_samples_leaf=4: 0.4722
R² with n_estimators=1000, max_depth=3, learning_rate=0.05, min_samples_leaf=1: 0.6378
R² with n_estimators=1000, max_depth=3, learning_rate=0.05, min_samples_leaf=2: 0.6384
R² with n_estimators=1000, max_depth=3, learning_rate=0.05, min_samples_leaf=4: 0.6386
R² with n_estimators=1000, max_depth=3, learning_rate=0.1, min_samples_leaf=1: 0.6910
R² with n_estimators=1000, max_depth=3, learning_rate=0.1, min_samples_leaf=2: 0.6893
R² with n_estimators=1000, max_depth=3, learning_rate=0.1, min_samples_leaf=4: 0.6904

R² with n_estimators=1000, max_depth=5, learning_rate=0.01, min_samples_leaf=1: 0.6190
R² with n_estimators=1000, max_depth=5, learning_rate=0.01, min_samples_leaf=2: 0.6189
R² with n_estimators=1000, max_depth=5, learning_rate=0.01, min_samples_leaf=4: 0.6181
R² with n_estimators=1000, max_depth=5, learning_rate=0.05, min_samples_leaf=1: 0.7447
R² with n_estimators=1000, max_depth=5, learning_rate=0.05, min_samples_leaf=2: 0.7488
R² with n_estimators=1000, max_depth=5, learning_rate=0.05, min_samples_leaf=4: 0.7454
R² with n_estimators=1000, max_depth=5, learning_rate=0.1, min_samples_leaf=1: 0.7665
R² with n_estimators=1000, max_depth=5, learning_rate=0.1, min_samples_leaf=2: 0.7685
R² with n_estimators=1000, max_depth=5, learning_rate=0.1, min_samples_leaf=4: 0.7677
R² with n_estimators=1000, max_depth=7, learning_rate=0.01, min_samples_leaf=1: 0.7216
R² with n_estimators=1000, max_depth=7, learning_rate=0.01, min_samples_leaf=2: 0.7220
R² with n_estimators=1000, max_depth=7, learning_rate=0.01, min_samples_leaf=4: 0.7219
R² with n_estimators=1000, max_depth=7, learning_rate=0.05, min_samples_leaf=1: 0.7767
R² with n_estimators=1000, max_depth=7, learning_rate=0.05, min_samples_leaf=2: 0.7780
R² with n_estimators=1000, max_depth=7, learning_rate=0.05, min_samples_leaf=4: 0.7761
R² with n_estimators=1000, max_depth=7, learning_rate=0.1, min_samples_leaf=1: 0.7729
R² with n_estimators=1000, max_depth=7, learning_rate=0.1, min_samples_leaf=2: 0.7773
R² with n_estimators=1000, max_depth=7, learning_rate=0.1, min_samples_leaf=4: 0.7808
R² with n_estimators=1000, max_depth=10, learning_rate=0.01, min_samples_leaf=1: 0.7693
R² with n_estimators=1000, max_depth=10, learning_rate=0.01, min_samples_leaf=2: 0.7713
R² with n_estimators=1000, max_depth=10, learning_rate=0.01, min_samples_leaf=4: 0.7669
R² with n_estimators=1000, max_depth=10, learning_rate=0.05, min_samples_leaf=1: 0.7715
R² with n_estimators=1000, max_depth=10, learning_rate=0.05, min_samples_leaf=2: 0.7731
R² with n_estimators=1000, max_depth=10, learning_rate=0.05, min_samples_leaf=4: 0.7796
R² with n_estimators=1000, max_depth=10, learning_rate=0.1, min_samples_leaf=1: 0.7737
R² with n_estimators=1000, max_depth=10, learning_rate=0.1, min_samples_leaf=2: 0.7718
R² with n_estimators=1000, max_depth=10, learning_rate=0.1, min_samples_leaf=4: 0.7709
R² with n_estimators=1000, max_depth=15, learning_rate=0.01, min_samples_leaf=1: 0.7465
R² with n_estimators=1000, max_depth=15, learning_rate=0.01, min_samples_leaf=2: 0.7548
R² with n_estimators=1000, max_depth=15, learning_rate=0.01, min_samples_leaf=4: 0.7664
R² with n_estimators=1000, max_depth=15, learning_rate=0.05, min_samples_leaf=1: 0.7416
R² with n_estimators=1000, max_depth=15, learning_rate=0.05, min_samples_leaf=2: 0.7510

R² with n_estimators=1000, max_depth=15, learning_rate=0.05, min_samples_leaf=4: 0.7615

R² with n_estimators=1000, max_depth=15, learning_rate=0.1, min_samples_leaf=1: 0.7398

R² with n_estimators=1000, max_depth=15, learning_rate=0.1, min_samples_leaf=2: 0.7517

R² with n_estimators=1000, max_depth=15, learning_rate=0.1, min_samples_leaf=4: 0.7569

Best parameters found on the normalized dataset:

{'n_estimators': 1000, 'max_depth': 7, 'learning_rate': 0.1, 'min_samples_leaf': 4} 0.7808

1.4 XGBoost

Testing different parameter combinations for XGBoost on the normalized dataset (15% test set)

```
param_grid_normalized = {  
    'n_estimators': [10, 50, 100, 110, 150, 300, 500, 1000],  
    'max_depth': [3, 5, 7, 10, 15],  
    'learning_rate': [0.01, 0.05, 0.1],  
    'min_child_weight': [1, 2, 4]  
}
```

Testing different parameter combinations on the normalized dataset:

R²

R² with n_estimators=10, max_depth=3, learning_rate=0.01, min_child_weight=1: 0.0375

R² with n_estimators=10, max_depth=3, learning_rate=0.01, min_child_weight=2: 0.0375

R² with n_estimators=10, max_depth=3, learning_rate=0.01, min_child_weight=4: 0.0375

R² with n_estimators=10, max_depth=3, learning_rate=0.05, min_child_weight=1: 0.1418

R² with n_estimators=10, max_depth=3, learning_rate=0.05, min_child_weight=2: 0.1418

R² with n_estimators=10, max_depth=3, learning_rate=0.05, min_child_weight=4: 0.1418

R² with n_estimators=10, max_depth=3, learning_rate=0.1, min_child_weight=1: 0.2137

R² with n_estimators=10, max_depth=3, learning_rate=0.1, min_child_weight=2: 0.2137

R² with n_estimators=10, max_depth=3, learning_rate=0.1, min_child_weight=4: 0.2137

R² with n_estimators=10, max_depth=5, learning_rate=0.01, min_child_weight=1: 0.0575

R² with n_estimators=10, max_depth=5, learning_rate=0.01, min_child_weight=2: 0.0575

R² with n_estimators=10, max_depth=5, learning_rate=0.01, min_child_weight=4: 0.0574
R² with n_estimators=10, max_depth=5, learning_rate=0.05, min_child_weight=1: 0.2107
R² with n_estimators=10, max_depth=5, learning_rate=0.05, min_child_weight=2: 0.2106
R² with n_estimators=10, max_depth=5, learning_rate=0.05, min_child_weight=4: 0.2109
R² with n_estimators=10, max_depth=5, learning_rate=0.1, min_child_weight=1: 0.3215
R² with n_estimators=10, max_depth=5, learning_rate=0.1, min_child_weight=2: 0.3205
R² with n_estimators=10, max_depth=5, learning_rate=0.1, min_child_weight=4: 0.3204
R² with n_estimators=10, max_depth=7, learning_rate=0.01, min_child_weight=1: 0.0798
R² with n_estimators=10, max_depth=7, learning_rate=0.01, min_child_weight=2: 0.0798
R² with n_estimators=10, max_depth=7, learning_rate=0.01, min_child_weight=4: 0.0790
R² with n_estimators=10, max_depth=7, learning_rate=0.05, min_child_weight=1: 0.2909
R² with n_estimators=10, max_depth=7, learning_rate=0.05, min_child_weight=2: 0.2904
R² with n_estimators=10, max_depth=7, learning_rate=0.05, min_child_weight=4: 0.2891
R² with n_estimators=10, max_depth=7, learning_rate=0.1, min_child_weight=1: 0.4315
R² with n_estimators=10, max_depth=7, learning_rate=0.1, min_child_weight=2: 0.4329
R² with n_estimators=10, max_depth=7, learning_rate=0.1, min_child_weight=4: 0.4332
R² with n_estimators=10, max_depth=10, learning_rate=0.01, min_child_weight=1: 0.1015
R² with n_estimators=10, max_depth=10, learning_rate=0.01, min_child_weight=2: 0.1016
R² with n_estimators=10, max_depth=10, learning_rate=0.01, min_child_weight=4: 0.1003
R² with n_estimators=10, max_depth=10, learning_rate=0.05, min_child_weight=1: 0.3767
R² with n_estimators=10, max_depth=10, learning_rate=0.05, min_child_weight=2: 0.3764
R² with n_estimators=10, max_depth=10, learning_rate=0.05, min_child_weight=4: 0.3731
R² with n_estimators=10, max_depth=10, learning_rate=0.1, min_child_weight=1: 0.5472
R² with n_estimators=10, max_depth=10, learning_rate=0.1, min_child_weight=2: 0.5512
R² with n_estimators=10, max_depth=10, learning_rate=0.1, min_child_weight=4: 0.5474
R² with n_estimators=10, max_depth=15, learning_rate=0.01, min_child_weight=1: 0.1189
R² with n_estimators=10, max_depth=15, learning_rate=0.01, min_child_weight=2: 0.1189
R² with n_estimators=10, max_depth=15, learning_rate=0.01, min_child_weight=4: 0.1172
R² with n_estimators=10, max_depth=15, learning_rate=0.05, min_child_weight=1: 0.4408
R² with n_estimators=10, max_depth=15, learning_rate=0.05, min_child_weight=2: 0.4400
R² with n_estimators=10, max_depth=15, learning_rate=0.05, min_child_weight=4: 0.4334
R² with n_estimators=10, max_depth=15, learning_rate=0.1, min_child_weight=1: 0.6217

R² with n_estimators=10, max_depth=15, learning_rate=0.1, min_child_weight=2: 0.6231
R² with n_estimators=10, max_depth=15, learning_rate=0.1, min_child_weight=4: 0.6144
R² with n_estimators=50, max_depth=3, learning_rate=0.01, min_child_weight=1: 0.1397
R² with n_estimators=50, max_depth=3, learning_rate=0.01, min_child_weight=2: 0.1397
R² with n_estimators=50, max_depth=3, learning_rate=0.01, min_child_weight=4: 0.1397
R² with n_estimators=50, max_depth=3, learning_rate=0.05, min_child_weight=1: 0.3186
R² with n_estimators=50, max_depth=3, learning_rate=0.05, min_child_weight=2: 0.3186
R² with n_estimators=50, max_depth=3, learning_rate=0.05, min_child_weight=4: 0.3186
R² with n_estimators=50, max_depth=3, learning_rate=0.1, min_child_weight=1: 0.3885
R² with n_estimators=50, max_depth=3, learning_rate=0.1, min_child_weight=2: 0.3885
R² with n_estimators=50, max_depth=3, learning_rate=0.1, min_child_weight=4: 0.3884
R² with n_estimators=50, max_depth=5, learning_rate=0.01, min_child_weight=1: 0.2074
R² with n_estimators=50, max_depth=5, learning_rate=0.01, min_child_weight=2: 0.2074
R² with n_estimators=50, max_depth=5, learning_rate=0.01, min_child_weight=4: 0.2075
R² with n_estimators=50, max_depth=5, learning_rate=0.05, min_child_weight=1: 0.4695
R² with n_estimators=50, max_depth=5, learning_rate=0.05, min_child_weight=2: 0.4694
R² with n_estimators=50, max_depth=5, learning_rate=0.05, min_child_weight=4: 0.4725
R² with n_estimators=50, max_depth=5, learning_rate=0.1, min_child_weight=1: 0.5505
R² with n_estimators=50, max_depth=5, learning_rate=0.1, min_child_weight=2: 0.5478
R² with n_estimators=50, max_depth=5, learning_rate=0.1, min_child_weight=4: 0.5503
R² with n_estimators=50, max_depth=7, learning_rate=0.01, min_child_weight=1: 0.2867
R² with n_estimators=50, max_depth=7, learning_rate=0.01, min_child_weight=2: 0.2889
R² with n_estimators=50, max_depth=7, learning_rate=0.01, min_child_weight=4: 0.2880
R² with n_estimators=50, max_depth=7, learning_rate=0.05, min_child_weight=1: 0.5925
R² with n_estimators=50, max_depth=7, learning_rate=0.05, min_child_weight=2: 0.5935
R² with n_estimators=50, max_depth=7, learning_rate=0.05, min_child_weight=4: 0.5865
R² with n_estimators=50, max_depth=7, learning_rate=0.1, min_child_weight=1: 0.6655
R² with n_estimators=50, max_depth=7, learning_rate=0.1, min_child_weight=2: 0.6643
R² with n_estimators=50, max_depth=7, learning_rate=0.1, min_child_weight=4: 0.6600
R² with n_estimators=50, max_depth=10, learning_rate=0.01, min_child_weight=1: 0.3733
R² with n_estimators=50, max_depth=10, learning_rate=0.01, min_child_weight=2: 0.3729
R² with n_estimators=50, max_depth=10, learning_rate=0.01, min_child_weight=4: 0.3702

R² with n_estimators=50, max_depth=10, learning_rate=0.05, min_child_weight=1: 0.7004
R² with n_estimators=50, max_depth=10, learning_rate=0.05, min_child_weight=2: 0.6996
R² with n_estimators=50, max_depth=10, learning_rate=0.05, min_child_weight=4: 0.6970
R² with n_estimators=50, max_depth=10, learning_rate=0.1, min_child_weight=1: 0.7482
R² with n_estimators=50, max_depth=10, learning_rate=0.1, min_child_weight=2: 0.7468
R² with n_estimators=50, max_depth=10, learning_rate=0.1, min_child_weight=4: 0.7488
R² with n_estimators=50, max_depth=15, learning_rate=0.01, min_child_weight=1: 0.4347
R² with n_estimators=50, max_depth=15, learning_rate=0.01, min_child_weight=2: 0.4338
R² with n_estimators=50, max_depth=15, learning_rate=0.01, min_child_weight=4: 0.4273
R² with n_estimators=50, max_depth=15, learning_rate=0.05, min_child_weight=1: 0.7474
R² with n_estimators=50, max_depth=15, learning_rate=0.05, min_child_weight=2: 0.7489
R² with n_estimators=50, max_depth=15, learning_rate=0.05, min_child_weight=4: 0.7438
R² with n_estimators=50, max_depth=15, learning_rate=0.1, min_child_weight=1: 0.7562
R² with n_estimators=50, max_depth=15, learning_rate=0.1, min_child_weight=2: 0.7615
R² with n_estimators=50, max_depth=15, learning_rate=0.1, min_child_weight=4: 0.7586
R² with n_estimators=100, max_depth=3, learning_rate=0.01, min_child_weight=1: 0.2122
R² with n_estimators=100, max_depth=3, learning_rate=0.01, min_child_weight=2: 0.2122
R² with n_estimators=100, max_depth=3, learning_rate=0.01, min_child_weight=4: 0.2122
R² with n_estimators=100, max_depth=3, learning_rate=0.05, min_child_weight=1: 0.3904
R² with n_estimators=100, max_depth=3, learning_rate=0.05, min_child_weight=2: 0.3904
R² with n_estimators=100, max_depth=3, learning_rate=0.05, min_child_weight=4: 0.3903
R² with n_estimators=100, max_depth=3, learning_rate=0.1, min_child_weight=1: 0.4677
R² with n_estimators=100, max_depth=3, learning_rate=0.1, min_child_weight=2: 0.4677
R² with n_estimators=100, max_depth=3, learning_rate=0.1, min_child_weight=4: 0.4679
R² with n_estimators=100, max_depth=5, learning_rate=0.01, min_child_weight=1: 0.3169
R² with n_estimators=100, max_depth=5, learning_rate=0.01, min_child_weight=2: 0.3173
R² with n_estimators=100, max_depth=5, learning_rate=0.01, min_child_weight=4: 0.3170
R² with n_estimators=100, max_depth=5, learning_rate=0.05, min_child_weight=1: 0.5447
R² with n_estimators=100, max_depth=5, learning_rate=0.05, min_child_weight=2: 0.5480
R² with n_estimators=100, max_depth=5, learning_rate=0.05, min_child_weight=4: 0.5492
R² with n_estimators=100, max_depth=5, learning_rate=0.1, min_child_weight=1: 0.6222
R² with n_estimators=100, max_depth=5, learning_rate=0.1, min_child_weight=2: 0.6232

R² with n_estimators=100, max_depth=5, learning_rate=0.1, min_child_weight=4: 0.6216
R² with n_estimators=100, max_depth=7, learning_rate=0.01, min_child_weight=1: 0.4265
R² with n_estimators=100, max_depth=7, learning_rate=0.01, min_child_weight=2: 0.4276
R² with n_estimators=100, max_depth=7, learning_rate=0.01, min_child_weight=4: 0.4262
R² with n_estimators=100, max_depth=7, learning_rate=0.05, min_child_weight=1: 0.6672
R² with n_estimators=100, max_depth=7, learning_rate=0.05, min_child_weight=2: 0.6650
R² with n_estimators=100, max_depth=7, learning_rate=0.05, min_child_weight=4: 0.6624
R² with n_estimators=100, max_depth=7, learning_rate=0.1, min_child_weight=1: 0.7171
R² with n_estimators=100, max_depth=7, learning_rate=0.1, min_child_weight=2: 0.7204
R² with n_estimators=100, max_depth=7, learning_rate=0.1, min_child_weight=4: 0.7169
R² with n_estimators=100, max_depth=10, learning_rate=0.01, min_child_weight=1: 0.5435
R² with n_estimators=100, max_depth=10, learning_rate=0.01, min_child_weight=2: 0.5415
R² with n_estimators=100, max_depth=10, learning_rate=0.01, min_child_weight=4: 0.5401
R² with n_estimators=100, max_depth=10, learning_rate=0.05, min_child_weight=1: 0.7533
R² with n_estimators=100, max_depth=10, learning_rate=0.05, min_child_weight=2: 0.7526
R² with n_estimators=100, max_depth=10, learning_rate=0.05, min_child_weight=4: 0.7483
R² with n_estimators=100, max_depth=10, learning_rate=0.1, min_child_weight=1: 0.7670
R² with n_estimators=100, max_depth=10, learning_rate=0.1, min_child_weight=2: 0.7665
R² with n_estimators=100, max_depth=10, learning_rate=0.1, min_child_weight=4: 0.7695
R² with n_estimators=100, max_depth=15, learning_rate=0.01, min_child_weight=1: 0.6153
R² with n_estimators=100, max_depth=15, learning_rate=0.01, min_child_weight=2: 0.6129
R² with n_estimators=100, max_depth=15, learning_rate=0.01, min_child_weight=4: 0.6097
R² with n_estimators=100, max_depth=15, learning_rate=0.05, min_child_weight=1: 0.7621
R² with n_estimators=100, max_depth=15, learning_rate=0.05, min_child_weight=2: 0.7635
R² with n_estimators=100, max_depth=15, learning_rate=0.05, min_child_weight=4: 0.7619
R² with n_estimators=100, max_depth=15, learning_rate=0.1, min_child_weight=1: 0.7557
R² with n_estimators=100, max_depth=15, learning_rate=0.1, min_child_weight=2: 0.7612
R² with n_estimators=100, max_depth=15, learning_rate=0.1, min_child_weight=4: 0.7592
R² with n_estimators=110, max_depth=3, learning_rate=0.01, min_child_weight=1: 0.2230
R² with n_estimators=110, max_depth=3, learning_rate=0.01, min_child_weight=2: 0.2230
R² with n_estimators=110, max_depth=3, learning_rate=0.01, min_child_weight=4: 0.2230
R² with n_estimators=110, max_depth=3, learning_rate=0.05, min_child_weight=1: 0.3998

R² with n_estimators=110, max_depth=3, learning_rate=0.05, min_child_weight=2: 0.3998
R² with n_estimators=110, max_depth=3, learning_rate=0.05, min_child_weight=4: 0.3996
R² with n_estimators=110, max_depth=3, learning_rate=0.1, min_child_weight=1: 0.4782
R² with n_estimators=110, max_depth=3, learning_rate=0.1, min_child_weight=2: 0.4783
R² with n_estimators=110, max_depth=3, learning_rate=0.1, min_child_weight=4: 0.4781
R² with n_estimators=110, max_depth=5, learning_rate=0.01, min_child_weight=1: 0.3335
R² with n_estimators=110, max_depth=5, learning_rate=0.01, min_child_weight=2: 0.3335
R² with n_estimators=110, max_depth=5, learning_rate=0.01, min_child_weight=4: 0.3337
R² with n_estimators=110, max_depth=5, learning_rate=0.05, min_child_weight=1: 0.5553
R² with n_estimators=110, max_depth=5, learning_rate=0.05, min_child_weight=2: 0.5573
R² with n_estimators=110, max_depth=5, learning_rate=0.05, min_child_weight=4: 0.5605
R² with n_estimators=110, max_depth=5, learning_rate=0.1, min_child_weight=1: 0.6323
R² with n_estimators=110, max_depth=5, learning_rate=0.1, min_child_weight=2: 0.6334
R² with n_estimators=110, max_depth=5, learning_rate=0.1, min_child_weight=4: 0.6302
R² with n_estimators=110, max_depth=7, learning_rate=0.01, min_child_weight=1: 0.4465
R² with n_estimators=110, max_depth=7, learning_rate=0.01, min_child_weight=2: 0.4478
R² with n_estimators=110, max_depth=7, learning_rate=0.01, min_child_weight=4: 0.4468
R² with n_estimators=110, max_depth=7, learning_rate=0.05, min_child_weight=1: 0.6740
R² with n_estimators=110, max_depth=7, learning_rate=0.05, min_child_weight=2: 0.6751
R² with n_estimators=110, max_depth=7, learning_rate=0.05, min_child_weight=4: 0.6726
R² with n_estimators=110, max_depth=7, learning_rate=0.1, min_child_weight=1: 0.7237
R² with n_estimators=110, max_depth=7, learning_rate=0.1, min_child_weight=2: 0.7259
R² with n_estimators=110, max_depth=7, learning_rate=0.1, min_child_weight=4: 0.7220
R² with n_estimators=110, max_depth=10, learning_rate=0.01, min_child_weight=1: 0.5664
R² with n_estimators=110, max_depth=10, learning_rate=0.01, min_child_weight=2: 0.5644
R² with n_estimators=110, max_depth=10, learning_rate=0.01, min_child_weight=4: 0.5629
R² with n_estimators=110, max_depth=10, learning_rate=0.05, min_child_weight=1: 0.7579
R² with n_estimators=110, max_depth=10, learning_rate=0.05, min_child_weight=2: 0.7553
R² with n_estimators=110, max_depth=10, learning_rate=0.05, min_child_weight=4: 0.7525
R² with n_estimators=110, max_depth=10, learning_rate=0.1, min_child_weight=1: 0.7684
R² with n_estimators=110, max_depth=10, learning_rate=0.1, min_child_weight=2: 0.7679
R² with n_estimators=110, max_depth=10, learning_rate=0.1, min_child_weight=4: 0.7715

R² with n_estimators=110, max_depth=15, learning_rate=0.01, min_child_weight=1: 0.6361
R² with n_estimators=110, max_depth=15, learning_rate=0.01, min_child_weight=2: 0.6337
R² with n_estimators=110, max_depth=15, learning_rate=0.01, min_child_weight=4: 0.6309
R² with n_estimators=110, max_depth=15, learning_rate=0.05, min_child_weight=1: 0.7623
R² with n_estimators=110, max_depth=15, learning_rate=0.05, min_child_weight=2: 0.7640
R² with n_estimators=110, max_depth=15, learning_rate=0.05, min_child_weight=4: 0.7623
R² with n_estimators=110, max_depth=15, learning_rate=0.1, min_child_weight=1: 0.7554
R² with n_estimators=110, max_depth=15, learning_rate=0.1, min_child_weight=2: 0.7610
R² with n_estimators=110, max_depth=15, learning_rate=0.1, min_child_weight=4: 0.7590
R² with n_estimators=150, max_depth=3, learning_rate=0.01, min_child_weight=1: 0.2591
R² with n_estimators=150, max_depth=3, learning_rate=0.01, min_child_weight=2: 0.2591
R² with n_estimators=150, max_depth=3, learning_rate=0.01, min_child_weight=4: 0.2591
R² with n_estimators=150, max_depth=3, learning_rate=0.05, min_child_weight=1: 0.4329
R² with n_estimators=150, max_depth=3, learning_rate=0.05, min_child_weight=2: 0.4329
R² with n_estimators=150, max_depth=3, learning_rate=0.05, min_child_weight=4: 0.4317
R² with n_estimators=150, max_depth=3, learning_rate=0.1, min_child_weight=1: 0.5158
R² with n_estimators=150, max_depth=3, learning_rate=0.1, min_child_weight=2: 0.5180
R² with n_estimators=150, max_depth=3, learning_rate=0.1, min_child_weight=4: 0.5120
R² with n_estimators=150, max_depth=5, learning_rate=0.01, min_child_weight=1: 0.3850
R² with n_estimators=150, max_depth=5, learning_rate=0.01, min_child_weight=2: 0.3855
R² with n_estimators=150, max_depth=5, learning_rate=0.01, min_child_weight=4: 0.3844
R² with n_estimators=150, max_depth=5, learning_rate=0.05, min_child_weight=1: 0.5884
R² with n_estimators=150, max_depth=5, learning_rate=0.05, min_child_weight=2: 0.5910
R² with n_estimators=150, max_depth=5, learning_rate=0.05, min_child_weight=4: 0.5906
R² with n_estimators=150, max_depth=5, learning_rate=0.1, min_child_weight=1: 0.6589
R² with n_estimators=150, max_depth=5, learning_rate=0.1, min_child_weight=2: 0.6619
R² with n_estimators=150, max_depth=5, learning_rate=0.1, min_child_weight=4: 0.6581
R² with n_estimators=150, max_depth=7, learning_rate=0.01, min_child_weight=1: 0.5015
R² with n_estimators=150, max_depth=7, learning_rate=0.01, min_child_weight=2: 0.5024
R² with n_estimators=150, max_depth=7, learning_rate=0.01, min_child_weight=4: 0.5003
R² with n_estimators=150, max_depth=7, learning_rate=0.05, min_child_weight=1: 0.6974
R² with n_estimators=150, max_depth=7, learning_rate=0.05, min_child_weight=2: 0.7009

R² with n_estimators=150, max_depth=7, learning_rate=0.05, min_child_weight=4: 0.6973
R² with n_estimators=150, max_depth=7, learning_rate=0.1, min_child_weight=1: 0.7399
R² with n_estimators=150, max_depth=7, learning_rate=0.1, min_child_weight=2: 0.7433
R² with n_estimators=150, max_depth=7, learning_rate=0.1, min_child_weight=4: 0.7398
R² with n_estimators=150, max_depth=10, learning_rate=0.01, min_child_weight=1: 0.6282
R² with n_estimators=150, max_depth=10, learning_rate=0.01, min_child_weight=2: 0.6265
R² with n_estimators=150, max_depth=10, learning_rate=0.01, min_child_weight=4: 0.6268
R² with n_estimators=150, max_depth=10, learning_rate=0.05, min_child_weight=1: 0.7661
R² with n_estimators=150, max_depth=10, learning_rate=0.05, min_child_weight=2: 0.7654
R² with n_estimators=150, max_depth=10, learning_rate=0.05, min_child_weight=4: 0.7627
R² with n_estimators=150, max_depth=10, learning_rate=0.1, min_child_weight=1: 0.7716
R² with n_estimators=150, max_depth=10, learning_rate=0.1, min_child_weight=2: 0.7713
R² with n_estimators=150, max_depth=10, learning_rate=0.1, min_child_weight=4: 0.7754
R² with n_estimators=150, max_depth=15, learning_rate=0.01, min_child_weight=1: 0.6930
R² with n_estimators=150, max_depth=15, learning_rate=0.01, min_child_weight=2: 0.6910
R² with n_estimators=150, max_depth=15, learning_rate=0.01, min_child_weight=4: 0.6890
R² with n_estimators=150, max_depth=15, learning_rate=0.05, min_child_weight=1: 0.7621
R² with n_estimators=150, max_depth=15, learning_rate=0.05, min_child_weight=2: 0.7637
R² with n_estimators=150, max_depth=15, learning_rate=0.05, min_child_weight=4: 0.7628
R² with n_estimators=150, max_depth=15, learning_rate=0.1, min_child_weight=1: 0.7545
R² with n_estimators=150, max_depth=15, learning_rate=0.1, min_child_weight=2: 0.7598
R² with n_estimators=150, max_depth=15, learning_rate=0.1, min_child_weight=4: 0.7586
R² with n_estimators=300, max_depth=3, learning_rate=0.01, min_child_weight=1: 0.3370
R² with n_estimators=300, max_depth=3, learning_rate=0.01, min_child_weight=2: 0.3370
R² with n_estimators=300, max_depth=3, learning_rate=0.01, min_child_weight=4: 0.3370
R² with n_estimators=300, max_depth=3, learning_rate=0.05, min_child_weight=1: 0.5142
R² with n_estimators=300, max_depth=3, learning_rate=0.05, min_child_weight=2: 0.5124
R² with n_estimators=300, max_depth=3, learning_rate=0.05, min_child_weight=4: 0.5122
R² with n_estimators=300, max_depth=3, learning_rate=0.1, min_child_weight=1: 0.5875
R² with n_estimators=300, max_depth=3, learning_rate=0.1, min_child_weight=2: 0.5933
R² with n_estimators=300, max_depth=3, learning_rate=0.1, min_child_weight=4: 0.5931
R² with n_estimators=300, max_depth=5, learning_rate=0.01, min_child_weight=1: 0.4951

R² with n_estimators=300, max_depth=5, learning_rate=0.01, min_child_weight=2: 0.4948
R² with n_estimators=300, max_depth=5, learning_rate=0.01, min_child_weight=4: 0.4942
R² with n_estimators=300, max_depth=5, learning_rate=0.05, min_child_weight=1: 0.6593
R² with n_estimators=300, max_depth=5, learning_rate=0.05, min_child_weight=2: 0.6586
R² with n_estimators=300, max_depth=5, learning_rate=0.05, min_child_weight=4: 0.6558
R² with n_estimators=300, max_depth=5, learning_rate=0.1, min_child_weight=1: 0.7159
R² with n_estimators=300, max_depth=5, learning_rate=0.1, min_child_weight=2: 0.7173
R² with n_estimators=300, max_depth=5, learning_rate=0.1, min_child_weight=4: 0.7176
R² with n_estimators=300, max_depth=7, learning_rate=0.01, min_child_weight=1: 0.6134
R² with n_estimators=300, max_depth=7, learning_rate=0.01, min_child_weight=2: 0.6146
R² with n_estimators=300, max_depth=7, learning_rate=0.01, min_child_weight=4: 0.6135
R² with n_estimators=300, max_depth=7, learning_rate=0.05, min_child_weight=1: 0.7399
R² with n_estimators=300, max_depth=7, learning_rate=0.05, min_child_weight=2: 0.7426
R² with n_estimators=300, max_depth=7, learning_rate=0.05, min_child_weight=4: 0.7450
R² with n_estimators=300, max_depth=7, learning_rate=0.1, min_child_weight=1: 0.7671
R² with n_estimators=300, max_depth=7, learning_rate=0.1, min_child_weight=2: 0.7678
R² with n_estimators=300, max_depth=7, learning_rate=0.1, min_child_weight=4: 0.7680
R² with n_estimators=300, max_depth=10, learning_rate=0.01, min_child_weight=1: 0.7174
R² with n_estimators=300, max_depth=10, learning_rate=0.01, min_child_weight=2: 0.7183
R² with n_estimators=300, max_depth=10, learning_rate=0.01, min_child_weight=4: 0.7171
R² with n_estimators=300, max_depth=10, learning_rate=0.05, min_child_weight=1: 0.7776
R² with n_estimators=300, max_depth=10, learning_rate=0.05, min_child_weight=2: 0.7780
R² with n_estimators=300, max_depth=10, learning_rate=0.05, min_child_weight=4: 0.7759
R² with n_estimators=300, max_depth=10, learning_rate=0.1, min_child_weight=1: 0.7722
R² with n_estimators=300, max_depth=10, learning_rate=0.1, min_child_weight=2: 0.7719
R² with n_estimators=300, max_depth=10, learning_rate=0.1, min_child_weight=4: 0.7773
R² with n_estimators=300, max_depth=15, learning_rate=0.01, min_child_weight=1: 0.7556
R² with n_estimators=300, max_depth=15, learning_rate=0.01, min_child_weight=2: 0.7525
R² with n_estimators=300, max_depth=15, learning_rate=0.01, min_child_weight=4: 0.7529
R² with n_estimators=300, max_depth=15, learning_rate=0.05, min_child_weight=1: 0.7603
R² with n_estimators=300, max_depth=15, learning_rate=0.05, min_child_weight=2: 0.7615
R² with n_estimators=300, max_depth=15, learning_rate=0.05, min_child_weight=4: 0.7617

R² with n_estimators=300, max_depth=15, learning_rate=0.1, min_child_weight=1: 0.7538
R² with n_estimators=300, max_depth=15, learning_rate=0.1, min_child_weight=2: 0.7590
R² with n_estimators=300, max_depth=15, learning_rate=0.1, min_child_weight=4: 0.7561
R² with n_estimators=500, max_depth=3, learning_rate=0.01, min_child_weight=1: 0.3895
R² with n_estimators=500, max_depth=3, learning_rate=0.01, min_child_weight=2: 0.3895
R² with n_estimators=500, max_depth=3, learning_rate=0.01, min_child_weight=4: 0.3892
R² with n_estimators=500, max_depth=3, learning_rate=0.05, min_child_weight=1: 0.5735
R² with n_estimators=500, max_depth=3, learning_rate=0.05, min_child_weight=2: 0.5684
R² with n_estimators=500, max_depth=3, learning_rate=0.05, min_child_weight=4: 0.5709
R² with n_estimators=500, max_depth=3, learning_rate=0.1, min_child_weight=1: 0.6362
R² with n_estimators=500, max_depth=3, learning_rate=0.1, min_child_weight=2: 0.6445
R² with n_estimators=500, max_depth=3, learning_rate=0.1, min_child_weight=4: 0.6442
R² with n_estimators=500, max_depth=5, learning_rate=0.01, min_child_weight=1: 0.5490
R² with n_estimators=500, max_depth=5, learning_rate=0.01, min_child_weight=2: 0.5487
R² with n_estimators=500, max_depth=5, learning_rate=0.01, min_child_weight=4: 0.5479
R² with n_estimators=500, max_depth=5, learning_rate=0.05, min_child_weight=1: 0.7021
R² with n_estimators=500, max_depth=5, learning_rate=0.05, min_child_weight=2: 0.6986
R² with n_estimators=500, max_depth=5, learning_rate=0.05, min_child_weight=4: 0.6993
R² with n_estimators=500, max_depth=5, learning_rate=0.1, min_child_weight=1: 0.7468
R² with n_estimators=500, max_depth=5, learning_rate=0.1, min_child_weight=2: 0.7484
R² with n_estimators=500, max_depth=5, learning_rate=0.1, min_child_weight=4: 0.7470
R² with n_estimators=500, max_depth=7, learning_rate=0.01, min_child_weight=1: 0.6660
R² with n_estimators=500, max_depth=7, learning_rate=0.01, min_child_weight=2: 0.6641
R² with n_estimators=500, max_depth=7, learning_rate=0.01, min_child_weight=4: 0.6641
R² with n_estimators=500, max_depth=7, learning_rate=0.05, min_child_weight=1: 0.7626
R² with n_estimators=500, max_depth=7, learning_rate=0.05, min_child_weight=2: 0.7648
R² with n_estimators=500, max_depth=7, learning_rate=0.05, min_child_weight=4: 0.7661
R² with n_estimators=500, max_depth=7, learning_rate=0.1, min_child_weight=1: 0.7753
R² with n_estimators=500, max_depth=7, learning_rate=0.1, min_child_weight=2: 0.7739
R² with n_estimators=500, max_depth=7, learning_rate=0.1, min_child_weight=4: 0.7752
R² with n_estimators=500, max_depth=10, learning_rate=0.01, min_child_weight=1: 0.7505
R² with n_estimators=500, max_depth=10, learning_rate=0.01, min_child_weight=2: 0.7521

R² with n_estimators=500, max_depth=10, learning_rate=0.01, min_child_weight=4: 0.7512
R² with n_estimators=500, max_depth=10, learning_rate=0.05, min_child_weight=1: 0.7786
R² with n_estimators=500, max_depth=10, learning_rate=0.05, min_child_weight=2: 0.7800
R² with n_estimators=500, max_depth=10, learning_rate=0.05, min_child_weight=4: 0.7791
R² with n_estimators=500, max_depth=10, learning_rate=0.1, min_child_weight=1: 0.7703
R² with n_estimators=500, max_depth=10, learning_rate=0.1, min_child_weight=2: 0.7701
R² with n_estimators=500, max_depth=10, learning_rate=0.1, min_child_weight=4: 0.7754
R² with n_estimators=500, max_depth=15, learning_rate=0.01, min_child_weight=1: 0.7632
R² with n_estimators=500, max_depth=15, learning_rate=0.01, min_child_weight=2: 0.7611
R² with n_estimators=500, max_depth=15, learning_rate=0.01, min_child_weight=4: 0.7621
R² with n_estimators=500, max_depth=15, learning_rate=0.05, min_child_weight=1: 0.7595
R² with n_estimators=500, max_depth=15, learning_rate=0.05, min_child_weight=2: 0.7605
R² with n_estimators=500, max_depth=15, learning_rate=0.05, min_child_weight=4: 0.7602
R² with n_estimators=500, max_depth=15, learning_rate=0.1, min_child_weight=1: 0.7538
R² with n_estimators=500, max_depth=15, learning_rate=0.1, min_child_weight=2: 0.7590
R² with n_estimators=500, max_depth=15, learning_rate=0.1, min_child_weight=4: 0.7555
R² with n_estimators=1000, max_depth=3, learning_rate=0.01, min_child_weight=1: 0.4656
R² with n_estimators=1000, max_depth=3, learning_rate=0.01, min_child_weight=2: 0.4652
R² with n_estimators=1000, max_depth=3, learning_rate=0.01, min_child_weight=4: 0.4660
R² with n_estimators=1000, max_depth=3, learning_rate=0.05, min_child_weight=1: 0.6391
R² with n_estimators=1000, max_depth=3, learning_rate=0.05, min_child_weight=2: 0.6391
R² with n_estimators=1000, max_depth=3, learning_rate=0.05, min_child_weight=4: 0.6432
R² with n_estimators=1000, max_depth=3, learning_rate=0.1, min_child_weight=1: 0.6938
R² with n_estimators=1000, max_depth=3, learning_rate=0.1, min_child_weight=2: 0.6960
R² with n_estimators=1000, max_depth=3, learning_rate=0.1, min_child_weight=4: 0.6978
R² with n_estimators=1000, max_depth=5, learning_rate=0.01, min_child_weight=1: 0.6172
R² with n_estimators=1000, max_depth=5, learning_rate=0.01, min_child_weight=2: 0.6175
R² with n_estimators=1000, max_depth=5, learning_rate=0.01, min_child_weight=4: 0.6189
R² with n_estimators=1000, max_depth=5, learning_rate=0.05, min_child_weight=1: 0.7469
R² with n_estimators=1000, max_depth=5, learning_rate=0.05, min_child_weight=2: 0.7432
R² with n_estimators=1000, max_depth=5, learning_rate=0.05, min_child_weight=4: 0.7456
R² with n_estimators=1000, max_depth=5, learning_rate=0.1, min_child_weight=1: 0.7701

R² with n_estimators=1000, max_depth=5, learning_rate=0.1, min_child_weight=2: 0.7705
R² with n_estimators=1000, max_depth=5, learning_rate=0.1, min_child_weight=4: 0.7700
R² with n_estimators=1000, max_depth=7, learning_rate=0.01, min_child_weight=1: 0.7174
R² with n_estimators=1000, max_depth=7, learning_rate=0.01, min_child_weight=2: 0.7183
R² with n_estimators=1000, max_depth=7, learning_rate=0.01, min_child_weight=4: 0.7184
R² with n_estimators=1000, max_depth=7, learning_rate=0.05, min_child_weight=1: 0.7782
R² with n_estimators=1000, max_depth=7, learning_rate=0.05, min_child_weight=2: 0.7782
R² with n_estimators=1000, max_depth=7, learning_rate=0.05, min_child_weight=4: 0.7777
R² with n_estimators=1000, max_depth=7, learning_rate=0.1, min_child_weight=1: 0.7769
R² with n_estimators=1000, max_depth=7, learning_rate=0.1, min_child_weight=2: 0.7750
R² with n_estimators=1000, max_depth=7, learning_rate=0.1, min_child_weight=4: 0.7774
R² with n_estimators=1000, max_depth=10, learning_rate=0.01, min_child_weight=1: 0.7687
R² with n_estimators=1000, max_depth=10, learning_rate=0.01, min_child_weight=2: 0.7713
R² with n_estimators=1000, max_depth=10, learning_rate=0.01, min_child_weight=4: 0.7712
R² with n_estimators=1000, max_depth=10, learning_rate=0.05, min_child_weight=1: 0.7766
R² with n_estimators=1000, max_depth=10, learning_rate=0.05, min_child_weight=2: 0.7779
R² with n_estimators=1000, max_depth=10, learning_rate=0.05, min_child_weight=4: 0.7774
R² with n_estimators=1000, max_depth=10, learning_rate=0.1, min_child_weight=1: 0.7687
R² with n_estimators=1000, max_depth=10, learning_rate=0.1, min_child_weight=2: 0.7688
R² with n_estimators=1000, max_depth=10, learning_rate=0.1, min_child_weight=4: 0.7736
R² with n_estimators=1000, max_depth=15, learning_rate=0.01, min_child_weight=1: 0.7624
R² with n_estimators=1000, max_depth=15, learning_rate=0.01, min_child_weight=2: 0.7607
R² with n_estimators=1000, max_depth=15, learning_rate=0.01, min_child_weight=4: 0.7640
R² with n_estimators=1000, max_depth=15, learning_rate=0.05, min_child_weight=1: 0.7595
R² with n_estimators=1000, max_depth=15, learning_rate=0.05, min_child_weight=2: 0.7604
R² with n_estimators=1000, max_depth=15, learning_rate=0.05, min_child_weight=4: 0.7594
R² with n_estimators=1000, max_depth=15, learning_rate=0.1, min_child_weight=1: 0.7538
R² with n_estimators=1000, max_depth=15, learning_rate=0.1, min_child_weight=2: 0.7590
R² with n_estimators=1000, max_depth=15, learning_rate=0.1, min_child_weight=4: 0.7555

Best parameters found in the normalized dataset.:

{'n_estimators': 500, 'max_depth': 10, 'learning_rate': 0.05, 'min_child_weight': 2} 0.7800

1.5 LightGBM

Testing different parameter combinations for LightGBM on the normalized dataset (test set 15%)

```
param_grid_normalized = {  
    'n_estimators': [10, 50, 100, 110, 150],  
    'max_depth': [3, 5, 7, 10],  
    'learning_rate': [0.01, 0.05, 0.1],  
    'min_child_samples': [1, 5, 10]  
}
```

R²

```
R2 with n_estimators=10, max_depth=3, learning_rate=0.01, min_child_samples=1: 0.0374  
R2 with n_estimators=10, max_depth=3, learning_rate=0.01, min_child_samples=5: 0.0374  
R2 with n_estimators=10, max_depth=3, learning_rate=0.01, min_child_samples=10: 0.0374  
R2 with n_estimators=10, max_depth=3, learning_rate=0.05, min_child_samples=1: 0.1404  
R2 with n_estimators=10, max_depth=3, learning_rate=0.05, min_child_samples=5: 0.1404  
R2 with n_estimators=10, max_depth=3, learning_rate=0.05, min_child_samples=10: 0.1404  
R2 with n_estimators=10, max_depth=3, learning_rate=0.1, min_child_samples=1: 0.2108  
R2 with n_estimators=10, max_depth=3, learning_rate=0.1, min_child_samples=5: 0.2108  
R2 with n_estimators=10, max_depth=3, learning_rate=0.1, min_child_samples=10: 0.2108  
R2 with n_estimators=10, max_depth=5, learning_rate=0.01, min_child_samples=1: 0.0567  
R2 with n_estimators=10, max_depth=5, learning_rate=0.01, min_child_samples=5: 0.0567  
R2 with n_estimators=10, max_depth=5, learning_rate=0.01, min_child_samples=10: 0.0567  
R2 with n_estimators=10, max_depth=5, learning_rate=0.05, min_child_samples=1: 0.2053  
R2 with n_estimators=10, max_depth=5, learning_rate=0.05, min_child_samples=5: 0.2061  
R2 with n_estimators=10, max_depth=5, learning_rate=0.05, min_child_samples=10: 0.2054  
R2 with n_estimators=10, max_depth=5, learning_rate=0.1, min_child_samples=1: 0.3134  
R2 with n_estimators=10, max_depth=5, learning_rate=0.1, min_child_samples=5: 0.3135  
R2 with n_estimators=10, max_depth=5, learning_rate=0.1, min_child_samples=10: 0.3161  
R2 with n_estimators=10, max_depth=7, learning_rate=0.01, min_child_samples=1: 0.0634  
R2 with n_estimators=10, max_depth=7, learning_rate=0.01, min_child_samples=5: 0.0634
```

R² with n_estimators=10, max_depth=7, learning_rate=0.01, min_child_samples=10: 0.0631
R² with n_estimators=10, max_depth=7, learning_rate=0.05, min_child_samples=1: 0.2349
R² with n_estimators=10, max_depth=7, learning_rate=0.05, min_child_samples=5: 0.2349
R² with n_estimators=10, max_depth=7, learning_rate=0.05, min_child_samples=10: 0.2342
R² with n_estimators=10, max_depth=7, learning_rate=0.1, min_child_samples=1: 0.3559
R² with n_estimators=10, max_depth=7, learning_rate=0.1, min_child_samples=5: 0.3559
R² with n_estimators=10, max_depth=7, learning_rate=0.1, min_child_samples=10: 0.3566
R² with n_estimators=10, max_depth=10, learning_rate=0.01, min_child_samples=1: 0.0629
R² with n_estimators=10, max_depth=10, learning_rate=0.01, min_child_samples=5: 0.0629
R² with n_estimators=10, max_depth=10, learning_rate=0.01, min_child_samples=10: 0.0629
R² with n_estimators=10, max_depth=10, learning_rate=0.05, min_child_samples=1: 0.2401
R² with n_estimators=10, max_depth=10, learning_rate=0.05, min_child_samples=5: 0.2401
R² with n_estimators=10, max_depth=10, learning_rate=0.05, min_child_samples=10: 0.2406
R² with n_estimators=10, max_depth=10, learning_rate=0.1, min_child_samples=1: 0.3599
R² with n_estimators=10, max_depth=10, learning_rate=0.1, min_child_samples=5: 0.3599
R² with n_estimators=10, max_depth=10, learning_rate=0.1, min_child_samples=10: 0.3619
R² with n_estimators=10, max_depth=15, learning_rate=0.01, min_child_samples=1: 0.0629
R² with n_estimators=10, max_depth=15, learning_rate=0.01, min_child_samples=5: 0.0629
R² with n_estimators=10, max_depth=15, learning_rate=0.01, min_child_samples=10: 0.0629
R² with n_estimators=10, max_depth=15, learning_rate=0.05, min_child_samples=1: 0.2407
R² with n_estimators=10, max_depth=15, learning_rate=0.05, min_child_samples=5: 0.2407
R² with n_estimators=10, max_depth=15, learning_rate=0.05, min_child_samples=10: 0.2409
R² with n_estimators=10, max_depth=15, learning_rate=0.1, min_child_samples=1: 0.3599
R² with n_estimators=10, max_depth=15, learning_rate=0.1, min_child_samples=5: 0.3599
R² with n_estimators=10, max_depth=15, learning_rate=0.1, min_child_samples=10: 0.3597
R² with n_estimators=50, max_depth=3, learning_rate=0.01, min_child_samples=1: 0.1384
R² with n_estimators=50, max_depth=3, learning_rate=0.01, min_child_samples=5: 0.1384
R² with n_estimators=50, max_depth=3, learning_rate=0.01, min_child_samples=10: 0.1384
R² with n_estimators=50, max_depth=3, learning_rate=0.05, min_child_samples=1: 0.3173
R² with n_estimators=50, max_depth=3, learning_rate=0.05, min_child_samples=5: 0.3173
R² with n_estimators=50, max_depth=3, learning_rate=0.05, min_child_samples=10: 0.3166
R² with n_estimators=50, max_depth=3, learning_rate=0.1, min_child_samples=1: 0.3819

R² with n_estimators=50, max_depth=3, learning_rate=0.1, min_child_samples=5: 0.3863
R² with n_estimators=50, max_depth=3, learning_rate=0.1, min_child_samples=10: 0.3834
R² with n_estimators=50, max_depth=5, learning_rate=0.01, min_child_samples=1: 0.2048
R² with n_estimators=50, max_depth=5, learning_rate=0.01, min_child_samples=5: 0.2047
R² with n_estimators=50, max_depth=5, learning_rate=0.01, min_child_samples=10: 0.2040
R² with n_estimators=50, max_depth=5, learning_rate=0.05, min_child_samples=1: 0.4687
R² with n_estimators=50, max_depth=5, learning_rate=0.05, min_child_samples=5: 0.4669
R² with n_estimators=50, max_depth=5, learning_rate=0.05, min_child_samples=10: 0.4670
R² with n_estimators=50, max_depth=5, learning_rate=0.1, min_child_samples=1: 0.5416
R² with n_estimators=50, max_depth=5, learning_rate=0.1, min_child_samples=5: 0.5516
R² with n_estimators=50, max_depth=5, learning_rate=0.1, min_child_samples=10: 0.5474
R² with n_estimators=50, max_depth=7, learning_rate=0.01, min_child_samples=1: 0.2331
R² with n_estimators=50, max_depth=7, learning_rate=0.01, min_child_samples=5: 0.2332
R² with n_estimators=50, max_depth=7, learning_rate=0.01, min_child_samples=10: 0.2328
R² with n_estimators=50, max_depth=7, learning_rate=0.05, min_child_samples=1: 0.5050
R² with n_estimators=50, max_depth=7, learning_rate=0.05, min_child_samples=5: 0.5030
R² with n_estimators=50, max_depth=7, learning_rate=0.05, min_child_samples=10: 0.5049
R² with n_estimators=50, max_depth=7, learning_rate=0.1, min_child_samples=1: 0.5879
R² with n_estimators=50, max_depth=7, learning_rate=0.1, min_child_samples=5: 0.5886
R² with n_estimators=50, max_depth=7, learning_rate=0.1, min_child_samples=10: 0.5896
R² with n_estimators=50, max_depth=10, learning_rate=0.01, min_child_samples=1: 0.2373
R² with n_estimators=50, max_depth=10, learning_rate=0.01, min_child_samples=5: 0.2373
R² with n_estimators=50, max_depth=10, learning_rate=0.01, min_child_samples=10: 0.2379
R² with n_estimators=50, max_depth=10, learning_rate=0.05, min_child_samples=1: 0.5066
R² with n_estimators=50, max_depth=10, learning_rate=0.05, min_child_samples=5: 0.5049
R² with n_estimators=50, max_depth=10, learning_rate=0.05, min_child_samples=10: 0.5084
R² with n_estimators=50, max_depth=10, learning_rate=0.1, min_child_samples=1: 0.5939
R² with n_estimators=50, max_depth=10, learning_rate=0.1, min_child_samples=5: 0.5992
R² with n_estimators=50, max_depth=10, learning_rate=0.1, min_child_samples=10: 0.5998
R² with n_estimators=50, max_depth=15, learning_rate=0.01, min_child_samples=1: 0.2370
R² with n_estimators=50, max_depth=15, learning_rate=0.01, min_child_samples=5: 0.2370
R² with n_estimators=50, max_depth=15, learning_rate=0.01, min_child_samples=10: 0.2376

R² with n_estimators=50, max_depth=15, learning_rate=0.05, min_child_samples=1: 0.5089
R² with n_estimators=50, max_depth=15, learning_rate=0.05, min_child_samples=5: 0.5068
R² with n_estimators=50, max_depth=15, learning_rate=0.05, min_child_samples=10: 0.5094
R² with n_estimators=50, max_depth=15, learning_rate=0.1, min_child_samples=1: 0.5966
R² with n_estimators=50, max_depth=15, learning_rate=0.1, min_child_samples=5: 0.5989
R² with n_estimators=50, max_depth=15, learning_rate=0.1, min_child_samples=10: 0.6001
R² with n_estimators=100, max_depth=3, learning_rate=0.01, min_child_samples=1: 0.2086
R² with n_estimators=100, max_depth=3, learning_rate=0.01, min_child_samples=5: 0.2086
R² with n_estimators=100, max_depth=3, learning_rate=0.01, min_child_samples=10: 0.2086
R² with n_estimators=100, max_depth=3, learning_rate=0.05, min_child_samples=1: 0.3892
R² with n_estimators=100, max_depth=3, learning_rate=0.05, min_child_samples=5: 0.3894
R² with n_estimators=100, max_depth=3, learning_rate=0.05, min_child_samples=10: 0.3892
R² with n_estimators=100, max_depth=3, learning_rate=0.1, min_child_samples=1: 0.4659
R² with n_estimators=100, max_depth=3, learning_rate=0.1, min_child_samples=5: 0.4642
R² with n_estimators=100, max_depth=3, learning_rate=0.1, min_child_samples=10: 0.4659
R² with n_estimators=100, max_depth=5, learning_rate=0.01, min_child_samples=1: 0.3118
R² with n_estimators=100, max_depth=5, learning_rate=0.01, min_child_samples=5: 0.3123
R² with n_estimators=100, max_depth=5, learning_rate=0.01, min_child_samples=10: 0.3105
R² with n_estimators=100, max_depth=5, learning_rate=0.05, min_child_samples=1: 0.5473
R² with n_estimators=100, max_depth=5, learning_rate=0.05, min_child_samples=5: 0.5473
R² with n_estimators=100, max_depth=5, learning_rate=0.05, min_child_samples=10: 0.5492
R² with n_estimators=100, max_depth=5, learning_rate=0.1, min_child_samples=1: 0.6167
R² with n_estimators=100, max_depth=5, learning_rate=0.1, min_child_samples=5: 0.6209
R² with n_estimators=100, max_depth=5, learning_rate=0.1, min_child_samples=10: 0.6215
R² with n_estimators=100, max_depth=7, learning_rate=0.01, min_child_samples=1: 0.3516
R² with n_estimators=100, max_depth=7, learning_rate=0.01, min_child_samples=5: 0.3516
R² with n_estimators=100, max_depth=7, learning_rate=0.01, min_child_samples=10: 0.3509
R² with n_estimators=100, max_depth=7, learning_rate=0.05, min_child_samples=1: 0.5894
R² with n_estimators=100, max_depth=7, learning_rate=0.05, min_child_samples=5: 0.5931
R² with n_estimators=100, max_depth=7, learning_rate=0.05, min_child_samples=10: 0.5933
R² with n_estimators=100, max_depth=7, learning_rate=0.1, min_child_samples=1: 0.6585
R² with n_estimators=100, max_depth=7, learning_rate=0.1, min_child_samples=5: 0.6580

R² with n_estimators=100, max_depth=7, learning_rate=0.1, min_child_samples=10: 0.6602
R² with n_estimators=100, max_depth=10, learning_rate=0.01, min_child_samples=1: 0.3550
R² with n_estimators=100, max_depth=10, learning_rate=0.01, min_child_samples=5: 0.3550
R² with n_estimators=100, max_depth=10, learning_rate=0.01, min_child_samples=10: 0.3553
R² with n_estimators=100, max_depth=10, learning_rate=0.05, min_child_samples=1: 0.5964
R² with n_estimators=100, max_depth=10, learning_rate=0.05, min_child_samples=5: 0.5953
R² with n_estimators=100, max_depth=10, learning_rate=0.05, min_child_samples=10: 0.5998
R² with n_estimators=100, max_depth=10, learning_rate=0.1, min_child_samples=1: 0.6628
R² with n_estimators=100, max_depth=10, learning_rate=0.1, min_child_samples=5: 0.6656
R² with n_estimators=100, max_depth=10, learning_rate=0.1, min_child_samples=10: 0.6624
R² with n_estimators=100, max_depth=15, learning_rate=0.01, min_child_samples=1: 0.3543
R² with n_estimators=100, max_depth=15, learning_rate=0.01, min_child_samples=5: 0.3547
R² with n_estimators=100, max_depth=15, learning_rate=0.01, min_child_samples=10: 0.3558
R² with n_estimators=100, max_depth=15, learning_rate=0.05, min_child_samples=1: 0.6011
R² with n_estimators=100, max_depth=15, learning_rate=0.05, min_child_samples=5: 0.6003
R² with n_estimators=100, max_depth=15, learning_rate=0.05, min_child_samples=10: 0.6016
R² with n_estimators=100, max_depth=15, learning_rate=0.1, min_child_samples=1: 0.6603
R² with n_estimators=100, max_depth=15, learning_rate=0.1, min_child_samples=5: 0.6661
R² with n_estimators=100, max_depth=15, learning_rate=0.1, min_child_samples=10: 0.6666
R² with n_estimators=110, max_depth=3, learning_rate=0.01, min_child_samples=1: 0.2192
R² with n_estimators=110, max_depth=3, learning_rate=0.01, min_child_samples=5: 0.2192
R² with n_estimators=110, max_depth=3, learning_rate=0.01, min_child_samples=10: 0.2192
R² with n_estimators=110, max_depth=3, learning_rate=0.05, min_child_samples=1: 0.3994
R² with n_estimators=110, max_depth=3, learning_rate=0.05, min_child_samples=5: 0.4001
R² with n_estimators=110, max_depth=3, learning_rate=0.05, min_child_samples=10: 0.3998
R² with n_estimators=110, max_depth=3, learning_rate=0.1, min_child_samples=1: 0.4776
R² with n_estimators=110, max_depth=3, learning_rate=0.1, min_child_samples=5: 0.4750
R² with n_estimators=110, max_depth=3, learning_rate=0.1, min_child_samples=10: 0.4734
R² with n_estimators=110, max_depth=5, learning_rate=0.01, min_child_samples=1: 0.3269

R² with n_estimators=110, max_depth=5, learning_rate=0.01, min_child_samples=5: 0.3278
R² with n_estimators=110, max_depth=5, learning_rate=0.01, min_child_samples=10: 0.3261
R² with n_estimators=110, max_depth=5, learning_rate=0.05, min_child_samples=1: 0.5598
R² with n_estimators=110, max_depth=5, learning_rate=0.05, min_child_samples=5: 0.5571
R² with n_estimators=110, max_depth=5, learning_rate=0.05, min_child_samples=10: 0.5626
R² with n_estimators=110, max_depth=5, learning_rate=0.1, min_child_samples=1: 0.6261
R² with n_estimators=110, max_depth=5, learning_rate=0.1, min_child_samples=5: 0.6314
R² with n_estimators=110, max_depth=5, learning_rate=0.1, min_child_samples=10: 0.6294
R² with n_estimators=110, max_depth=7, learning_rate=0.01, min_child_samples=1: 0.3676
R² with n_estimators=110, max_depth=7, learning_rate=0.01, min_child_samples=5: 0.3680
R² with n_estimators=110, max_depth=7, learning_rate=0.01, min_child_samples=10: 0.3671
R² with n_estimators=110, max_depth=7, learning_rate=0.05, min_child_samples=1: 0.6013
R² with n_estimators=110, max_depth=7, learning_rate=0.05, min_child_samples=5: 0.6032
R² with n_estimators=110, max_depth=7, learning_rate=0.05, min_child_samples=10: 0.6044
R² with n_estimators=110, max_depth=7, learning_rate=0.1, min_child_samples=1: 0.6655
R² with n_estimators=110, max_depth=7, learning_rate=0.1, min_child_samples=5: 0.6643
R² with n_estimators=110, max_depth=7, learning_rate=0.1, min_child_samples=10: 0.6674
R² with n_estimators=110, max_depth=10, learning_rate=0.01, min_child_samples=1: 0.3713
R² with n_estimators=110, max_depth=10, learning_rate=0.01, min_child_samples=5: 0.3713
R² with n_estimators=110, max_depth=10, learning_rate=0.01, min_child_samples=10: 0.3711
R² with n_estimators=110, max_depth=10, learning_rate=0.05, min_child_samples=1: 0.6059
R² with n_estimators=110, max_depth=10, learning_rate=0.05, min_child_samples=5: 0.6064
R² with n_estimators=110, max_depth=10, learning_rate=0.05, min_child_samples=10: 0.6098
R² with n_estimators=110, max_depth=10, learning_rate=0.1, min_child_samples=1: 0.6713
R² with n_estimators=110, max_depth=10, learning_rate=0.1, min_child_samples=5: 0.6739
R² with n_estimators=110, max_depth=10, learning_rate=0.1, min_child_samples=10: 0.6703
R² with n_estimators=110, max_depth=15, learning_rate=0.01, min_child_samples=1: 0.3702
R² with n_estimators=110, max_depth=15, learning_rate=0.01, min_child_samples=5: 0.3703
R² with n_estimators=110, max_depth=15, learning_rate=0.01, min_child_samples=10: 0.3716
R² with n_estimators=110, max_depth=15, learning_rate=0.05, min_child_samples=1: 0.6114

R² with n_estimators=110, max_depth=15, learning_rate=0.05, min_child_samples=5: 0.6095
R² with n_estimators=110, max_depth=15, learning_rate=0.05, min_child_samples=10: 0.6125
R² with n_estimators=110, max_depth=15, learning_rate=0.1, min_child_samples=1: 0.6682
R² with n_estimators=110, max_depth=15, learning_rate=0.1, min_child_samples=5: 0.6737
R² with n_estimators=110, max_depth=15, learning_rate=0.1, min_child_samples=10: 0.6751
R² with n_estimators=150, max_depth=3, learning_rate=0.01, min_child_samples=1: 0.2570
R² with n_estimators=150, max_depth=3, learning_rate=0.01, min_child_samples=5: 0.2570
R² with n_estimators=150, max_depth=3, learning_rate=0.01, min_child_samples=10: 0.2567
R² with n_estimators=150, max_depth=3, learning_rate=0.05, min_child_samples=1: 0.4339
R² with n_estimators=150, max_depth=3, learning_rate=0.05, min_child_samples=5: 0.4364
R² with n_estimators=150, max_depth=3, learning_rate=0.05, min_child_samples=10: 0.4360
R² with n_estimators=150, max_depth=3, learning_rate=0.1, min_child_samples=1: 0.5150
R² with n_estimators=150, max_depth=3, learning_rate=0.1, min_child_samples=5: 0.5148
R² with n_estimators=150, max_depth=3, learning_rate=0.1, min_child_samples=10: 0.5116
R² with n_estimators=150, max_depth=5, learning_rate=0.01, min_child_samples=1: 0.3813
R² with n_estimators=150, max_depth=5, learning_rate=0.01, min_child_samples=5: 0.3818
R² with n_estimators=150, max_depth=5, learning_rate=0.01, min_child_samples=10: 0.3800
R² with n_estimators=150, max_depth=5, learning_rate=0.05, min_child_samples=1: 0.5908
R² with n_estimators=150, max_depth=5, learning_rate=0.05, min_child_samples=5: 0.5860
R² with n_estimators=150, max_depth=5, learning_rate=0.05, min_child_samples=10: 0.5925
R² with n_estimators=150, max_depth=5, learning_rate=0.1, min_child_samples=1: 0.6587
R² with n_estimators=150, max_depth=5, learning_rate=0.1, min_child_samples=5: 0.6617
R² with n_estimators=150, max_depth=5, learning_rate=0.1, min_child_samples=10: 0.6586
R² with n_estimators=150, max_depth=7, learning_rate=0.01, min_child_samples=1: 0.4196
R² with n_estimators=150, max_depth=7, learning_rate=0.01, min_child_samples=5: 0.4205
R² with n_estimators=150, max_depth=7, learning_rate=0.01, min_child_samples=10: 0.4189
R² with n_estimators=150, max_depth=7, learning_rate=0.05, min_child_samples=1: 0.6329
R² with n_estimators=150, max_depth=7, learning_rate=0.05, min_child_samples=5: 0.6343
R² with n_estimators=150, max_depth=7, learning_rate=0.05, min_child_samples=10: 0.6352
R² with n_estimators=150, max_depth=7, learning_rate=0.1, min_child_samples=1: 0.6888
R² with n_estimators=150, max_depth=7, learning_rate=0.1, min_child_samples=5: 0.6910

R² with n_estimators=150, max_depth=7, learning_rate=0.1, min_child_samples=10: 0.6922
R² with n_estimators=150, max_depth=10, learning_rate=0.01, min_child_samples=1: 0.4228
R² with n_estimators=150, max_depth=10, learning_rate=0.01, min_child_samples=5: 0.4228
R² with n_estimators=150, max_depth=10, learning_rate=0.01, min_child_samples=10: 0.4220
R² with n_estimators=150, max_depth=10, learning_rate=0.05, min_child_samples=1: 0.6387
R² with n_estimators=150, max_depth=10, learning_rate=0.05, min_child_samples=5: 0.6375
R² with n_estimators=150, max_depth=10, learning_rate=0.05, min_child_samples=10: 0.6409
R² with n_estimators=150, max_depth=10, learning_rate=0.1, min_child_samples=1: 0.6941
R² with n_estimators=150, max_depth=10, learning_rate=0.1, min_child_samples=5: 0.6999
R² with n_estimators=150, max_depth=10, learning_rate=0.1, min_child_samples=10: 0.6953
R² with n_estimators=150, max_depth=15, learning_rate=0.01, min_child_samples=1: 0.4218
R² with n_estimators=150, max_depth=15, learning_rate=0.01, min_child_samples=5: 0.4220
R² with n_estimators=150, max_depth=15, learning_rate=0.01, min_child_samples=10: 0.4227
R² with n_estimators=150, max_depth=15, learning_rate=0.05, min_child_samples=1: 0.6420
R² with n_estimators=150, max_depth=15, learning_rate=0.05, min_child_samples=5: 0.6422
R² with n_estimators=150, max_depth=15, learning_rate=0.05, min_child_samples=10: 0.6424
R² with n_estimators=150, max_depth=15, learning_rate=0.1, min_child_samples=1: 0.6907
R² with n_estimators=150, max_depth=15, learning_rate=0.1, min_child_samples=5: 0.6961
R² with n_estimators=150, max_depth=15, learning_rate=0.1, min_child_samples=10: 0.6983
R² with n_estimators=300, max_depth=3, learning_rate=0.01, min_child_samples=1: 0.3338
R² with n_estimators=300, max_depth=3, learning_rate=0.01, min_child_samples=5: 0.3338
R² with n_estimators=300, max_depth=3, learning_rate=0.01, min_child_samples=10: 0.3333
R² with n_estimators=300, max_depth=3, learning_rate=0.05, min_child_samples=1: 0.5126
R² with n_estimators=300, max_depth=3, learning_rate=0.05, min_child_samples=5: 0.5155
R² with n_estimators=300, max_depth=3, learning_rate=0.05, min_child_samples=10: 0.5126
R² with n_estimators=300, max_depth=3, learning_rate=0.1, min_child_samples=1: 0.5909
R² with n_estimators=300, max_depth=3, learning_rate=0.1, min_child_samples=5: 0.5917
R² with n_estimators=300, max_depth=3, learning_rate=0.1, min_child_samples=10: 0.5896
R² with n_estimators=300, max_depth=5, learning_rate=0.01, min_child_samples=1: 0.4888

R² with n_estimators=300, max_depth=5, learning_rate=0.01, min_child_samples=5: 0.4907
R² with n_estimators=300, max_depth=5, learning_rate=0.01, min_child_samples=10: 0.4892
R² with n_estimators=300, max_depth=5, learning_rate=0.05, min_child_samples=1: 0.6658
R² with n_estimators=300, max_depth=5, learning_rate=0.05, min_child_samples=5: 0.6592
R² with n_estimators=300, max_depth=5, learning_rate=0.05, min_child_samples=10: 0.6599
R² with n_estimators=300, max_depth=5, learning_rate=0.1, min_child_samples=1: 0.7145
R² with n_estimators=300, max_depth=5, learning_rate=0.1, min_child_samples=5: 0.7165
R² with n_estimators=300, max_depth=5, learning_rate=0.1, min_child_samples=10: 0.7136
R² with n_estimators=300, max_depth=7, learning_rate=0.01, min_child_samples=1: 0.5273
R² with n_estimators=300, max_depth=7, learning_rate=0.01, min_child_samples=5: 0.5293
R² with n_estimators=300, max_depth=7, learning_rate=0.01, min_child_samples=10: 0.5288
R² with n_estimators=300, max_depth=7, learning_rate=0.05, min_child_samples=1: 0.6871
R² with n_estimators=300, max_depth=7, learning_rate=0.05, min_child_samples=5: 0.6916
R² with n_estimators=300, max_depth=7, learning_rate=0.05, min_child_samples=10: 0.6942
R² with n_estimators=300, max_depth=7, learning_rate=0.1, min_child_samples=1: 0.7320
R² with n_estimators=300, max_depth=7, learning_rate=0.1, min_child_samples=5: 0.7327
R² with n_estimators=300, max_depth=7, learning_rate=0.1, min_child_samples=10: 0.7402
R² with n_estimators=300, max_depth=10, learning_rate=0.01, min_child_samples=1: 0.5326
R² with n_estimators=300, max_depth=10, learning_rate=0.01, min_child_samples=5: 0.5332
R² with n_estimators=300, max_depth=10, learning_rate=0.01, min_child_samples=10: 0.5317
R² with n_estimators=300, max_depth=10, learning_rate=0.05, min_child_samples=1: 0.6987
R² with n_estimators=300, max_depth=10, learning_rate=0.05, min_child_samples=5: 0.6968
R² with n_estimators=300, max_depth=10, learning_rate=0.05, min_child_samples=10: 0.6998
R² with n_estimators=300, max_depth=10, learning_rate=0.1, min_child_samples=1: 0.7354
R² with n_estimators=300, max_depth=10, learning_rate=0.1, min_child_samples=5: 0.7447
R² with n_estimators=300, max_depth=10, learning_rate=0.1, min_child_samples=10: 0.7406
R² with n_estimators=300, max_depth=15, learning_rate=0.01, min_child_samples=1: 0.5336
R² with n_estimators=300, max_depth=15, learning_rate=0.01, min_child_samples=5: 0.5328
R² with n_estimators=300, max_depth=15, learning_rate=0.01, min_child_samples=10: 0.5336
R² with n_estimators=300, max_depth=15, learning_rate=0.05, min_child_samples=1: 0.6996

R² with n_estimators=300, max_depth=15, learning_rate=0.05, min_child_samples=5: 0.7003
R² with n_estimators=300, max_depth=15, learning_rate=0.05, min_child_samples=10: 0.6987
R² with n_estimators=300, max_depth=15, learning_rate=0.1, min_child_samples=1: 0.7356
R² with n_estimators=300, max_depth=15, learning_rate=0.1, min_child_samples=5: 0.7382
R² with n_estimators=300, max_depth=15, learning_rate=0.1, min_child_samples=10: 0.7438
R² with n_estimators=500, max_depth=3, learning_rate=0.01, min_child_samples=1: 0.3876
R² with n_estimators=500, max_depth=3, learning_rate=0.01, min_child_samples=5: 0.3883
R² with n_estimators=500, max_depth=3, learning_rate=0.01, min_child_samples=10: 0.3881
R² with n_estimators=500, max_depth=3, learning_rate=0.05, min_child_samples=1: 0.5680
R² with n_estimators=500, max_depth=3, learning_rate=0.05, min_child_samples=5: 0.5678
R² with n_estimators=500, max_depth=3, learning_rate=0.05, min_child_samples=10: 0.5723
R² with n_estimators=500, max_depth=3, learning_rate=0.1, min_child_samples=1: 0.6402
R² with n_estimators=500, max_depth=3, learning_rate=0.1, min_child_samples=5: 0.6412
R² with n_estimators=500, max_depth=3, learning_rate=0.1, min_child_samples=10: 0.6415
R² with n_estimators=500, max_depth=5, learning_rate=0.01, min_child_samples=1: 0.5496
R² with n_estimators=500, max_depth=5, learning_rate=0.01, min_child_samples=5: 0.5514
R² with n_estimators=500, max_depth=5, learning_rate=0.01, min_child_samples=10: 0.5495
R² with n_estimators=500, max_depth=5, learning_rate=0.05, min_child_samples=1: 0.7052
R² with n_estimators=500, max_depth=5, learning_rate=0.05, min_child_samples=5: 0.7063
R² with n_estimators=500, max_depth=5, learning_rate=0.05, min_child_samples=10: 0.7065
R² with n_estimators=500, max_depth=5, learning_rate=0.1, min_child_samples=1: 0.7448
R² with n_estimators=500, max_depth=5, learning_rate=0.1, min_child_samples=5: 0.7441
R² with n_estimators=500, max_depth=5, learning_rate=0.1, min_child_samples=10: 0.7414
R² with n_estimators=500, max_depth=7, learning_rate=0.01, min_child_samples=1: 0.5923
R² with n_estimators=500, max_depth=7, learning_rate=0.01, min_child_samples=5: 0.5936
R² with n_estimators=500, max_depth=7, learning_rate=0.01, min_child_samples=10: 0.5933
R² with n_estimators=500, max_depth=7, learning_rate=0.05, min_child_samples=1: 0.7221
R² with n_estimators=500, max_depth=7, learning_rate=0.05, min_child_samples=5: 0.7271
R² with n_estimators=500, max_depth=7, learning_rate=0.05, min_child_samples=10: 0.7268
R² with n_estimators=500, max_depth=7, learning_rate=0.1, min_child_samples=1: 0.7562
R² with n_estimators=500, max_depth=7, learning_rate=0.1, min_child_samples=5: 0.7556

R² with n_estimators=500, max_depth=7, learning_rate=0.1, min_child_samples=10: 0.7620
R² with n_estimators=500, max_depth=10, learning_rate=0.01, min_child_samples=1: 0.5979
R² with n_estimators=500, max_depth=10, learning_rate=0.01, min_child_samples=5: 0.5996
R² with n_estimators=500, max_depth=10, learning_rate=0.01, min_child_samples=10: 0.5984
R² with n_estimators=500, max_depth=10, learning_rate=0.05, min_child_samples=1: 0.7300
R² with n_estimators=500, max_depth=10, learning_rate=0.05, min_child_samples=5: 0.7316
R² with n_estimators=500, max_depth=10, learning_rate=0.05, min_child_samples=10: 0.7336
R² with n_estimators=500, max_depth=10, learning_rate=0.1, min_child_samples=1: 0.7568
R² with n_estimators=500, max_depth=10, learning_rate=0.1, min_child_samples=5: 0.7650
R² with n_estimators=500, max_depth=10, learning_rate=0.1, min_child_samples=10: 0.7615
R² with n_estimators=500, max_depth=15, learning_rate=0.01, min_child_samples=1: 0.6000
R² with n_estimators=500, max_depth=15, learning_rate=0.01, min_child_samples=5: 0.6004
R² with n_estimators=500, max_depth=15, learning_rate=0.01, min_child_samples=10: 0.6002
R² with n_estimators=500, max_depth=15, learning_rate=0.05, min_child_samples=1: 0.7320
R² with n_estimators=500, max_depth=15, learning_rate=0.05, min_child_samples=5: 0.7313
R² with n_estimators=500, max_depth=15, learning_rate=0.05, min_child_samples=10: 0.7331
R² with n_estimators=500, max_depth=15, learning_rate=0.1, min_child_samples=1: 0.7570
R² with n_estimators=500, max_depth=15, learning_rate=0.1, min_child_samples=5: 0.7619
R² with n_estimators=500, max_depth=15, learning_rate=0.1, min_child_samples=10: 0.7648
R² with n_estimators=1000, max_depth=3, learning_rate=0.01, min_child_samples=1: 0.4666
R² with n_estimators=1000, max_depth=3, learning_rate=0.01, min_child_samples=5: 0.4689
R² with n_estimators=1000, max_depth=3, learning_rate=0.01, min_child_samples=10: 0.4676
R² with n_estimators=1000, max_depth=3, learning_rate=0.05, min_child_samples=1: 0.6344
R² with n_estimators=1000, max_depth=3, learning_rate=0.05, min_child_samples=5: 0.6372
R² with n_estimators=1000, max_depth=3, learning_rate=0.05, min_child_samples=10: 0.6404
R² with n_estimators=1000, max_depth=3, learning_rate=0.1, min_child_samples=1: 0.6942
R² with n_estimators=1000, max_depth=3, learning_rate=0.1, min_child_samples=5: 0.6947
R² with n_estimators=1000, max_depth=3, learning_rate=0.1, min_child_samples=10: 0.6961

R² with n_estimators=1000, max_depth=5, learning_rate=0.01, min_child_samples=1: 0.6200
R² with n_estimators=1000, max_depth=5, learning_rate=0.01, min_child_samples=5: 0.6246
R² with n_estimators=1000, max_depth=5, learning_rate=0.01, min_child_samples=10: 0.6238
R² with n_estimators=1000, max_depth=5, learning_rate=0.05, min_child_samples=1: 0.7449
R² with n_estimators=1000, max_depth=5, learning_rate=0.05, min_child_samples=5: 0.7497
R² with n_estimators=1000, max_depth=5, learning_rate=0.05, min_child_samples=10: 0.7474
R² with n_estimators=1000, max_depth=5, learning_rate=0.1, min_child_samples=1: 0.7690
R² with n_estimators=1000, max_depth=5, learning_rate=0.1, min_child_samples=5: 0.7657
R² with n_estimators=1000, max_depth=5, learning_rate=0.1, min_child_samples=10: 0.7678
R² with n_estimators=1000, max_depth=7, learning_rate=0.01, min_child_samples=1: 0.6614
R² with n_estimators=1000, max_depth=7, learning_rate=0.01, min_child_samples=5: 0.6615
R² with n_estimators=1000, max_depth=7, learning_rate=0.01, min_child_samples=10: 0.6611
R² with n_estimators=1000, max_depth=7, learning_rate=0.05, min_child_samples=1: 0.7545
R² with n_estimators=1000, max_depth=7, learning_rate=0.05, min_child_samples=5: 0.7600
R² with n_estimators=1000, max_depth=7, learning_rate=0.05, min_child_samples=10: 0.7582
R² with n_estimators=1000, max_depth=7, learning_rate=0.1, min_child_samples=1: 0.7744
R² with n_estimators=1000, max_depth=7, learning_rate=0.1, min_child_samples=5: 0.7726
R² with n_estimators=1000, max_depth=7, learning_rate=0.1, min_child_samples=10: 0.7750
R² with n_estimators=1000, max_depth=10, learning_rate=0.01, min_child_samples=1: 0.6655
R² with n_estimators=1000, max_depth=10, learning_rate=0.01, min_child_samples=5: 0.6672
R² with n_estimators=1000, max_depth=10, learning_rate=0.01, min_child_samples=10: 0.6656
R² with n_estimators=1000, max_depth=10, learning_rate=0.05, min_child_samples=1: 0.7599
R² with n_estimators=1000, max_depth=10, learning_rate=0.05, min_child_samples=5: 0.7647
R² with n_estimators=1000, max_depth=10, learning_rate=0.05, min_child_samples=10: 0.7647
R² with n_estimators=1000, max_depth=10, learning_rate=0.1, min_child_samples=1: 0.7713
R² with n_estimators=1000, max_depth=10, learning_rate=0.1, min_child_samples=5: 0.7781

R² with n_estimators=1000, max_depth=10, learning_rate=0.1, min_child_samples=10: 0.7759

R² with n_estimators=1000, max_depth=15, learning_rate=0.01, min_child_samples=1: 0.6682

R² with n_estimators=1000, max_depth=15, learning_rate=0.01, min_child_samples=5: 0.6671

R² with n_estimators=1000, max_depth=15, learning_rate=0.01, min_child_samples=10: 0.6685

R² with n_estimators=1000, max_depth=15, learning_rate=0.05, min_child_samples=1: 0.7625

R² with n_estimators=1000, max_depth=15, learning_rate=0.05, min_child_samples=5: 0.7627

R² with n_estimators=1000, max_depth=15, learning_rate=0.05, min_child_samples=10: 0.7624

R² with n_estimators=1000, max_depth=15, learning_rate=0.1, min_child_samples=1: 0.7709

R² with n_estimators=1000, max_depth=15, learning_rate=0.1, min_child_samples=5: 0.7803

R² with n_estimators=1000, max_depth=15, learning_rate=0.1, min_child_samples=10: 0.7796

Best parameters found in the normalized dataset:

{'n_estimators': 1000, 'max_depth': 15, 'learning_rate': 0.1, 'min_child_samples': 5} 0.7803

2 General Benchmarks

```
=====
TROPOL BOITATÁ - RADIUS BENCHMARK
=====
  Radius  Name  R2_Mean  R2_Std
  2       3  ECFP6   0.783401 0.012422
  1       2  ECFP4   0.781211 0.009154
  0       1  ECFP2   0.767296 0.010752
-----
```

```
=====
TROPOL BOITATÁ - BIT DENSITY REPORT
=====
Total Valid Molecules: 16388
Fingerprint Size:      2048
-----
Average ON Bits:      49.74
Bit Density:          2.4285%
=====
STATUS: OPTIMAL. (Low risk of collision)
```

```
--- ANOTHER STATISTICAL PARAMETERS (30% test set) ---
Q2: 0.7370
-----
k (predicted vs. observed slope): 0.9993
k' (observed vs. predicted slope): 0.9859
-----
r2m (average): 0.5791
Δr2m: 0.3115
```