

Tree-Based Models Analysis for Au Cluster Energy Prediction

Comprehensive Performance Report

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Models Analyzed:

- Random Forest (Ensemble Bagging)
- XGBoost (Gradient Boosting) - Available
- LightGBM (Fast Gradient Boosting) - Available

Dataset Information:

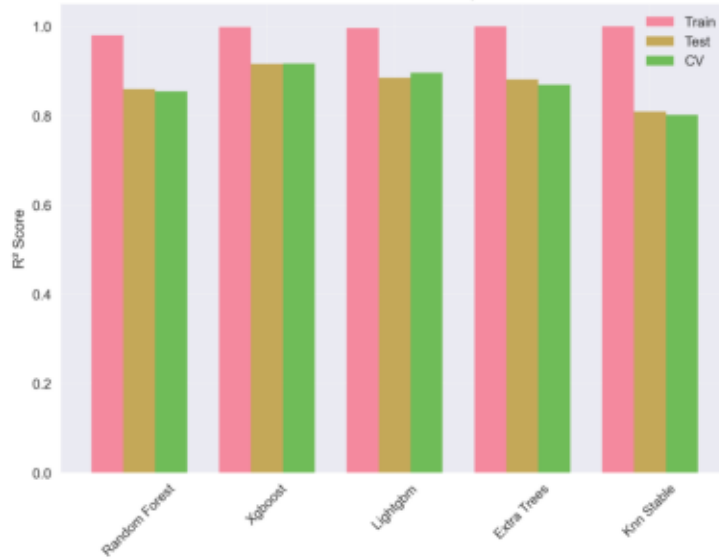
- Training samples: 799
- Test samples: 200
- Total features: 30
- SOAP features: 15

Best Model: Xgboost

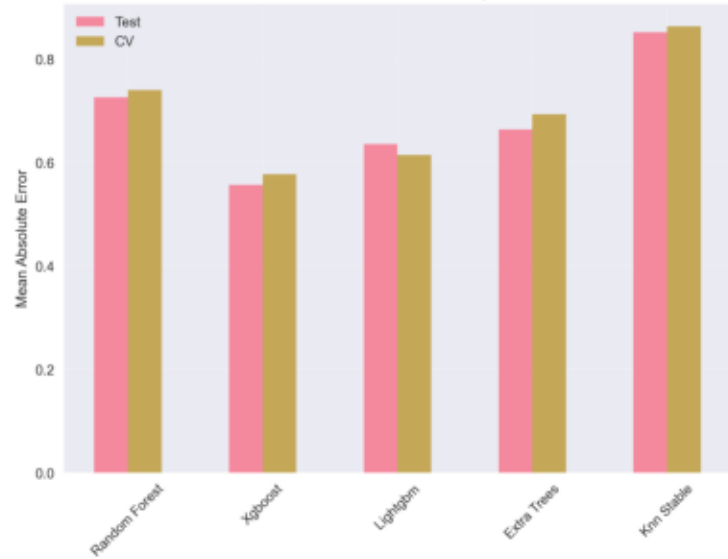
Best Test R^2 : 0.9162

Combined Model Comparison

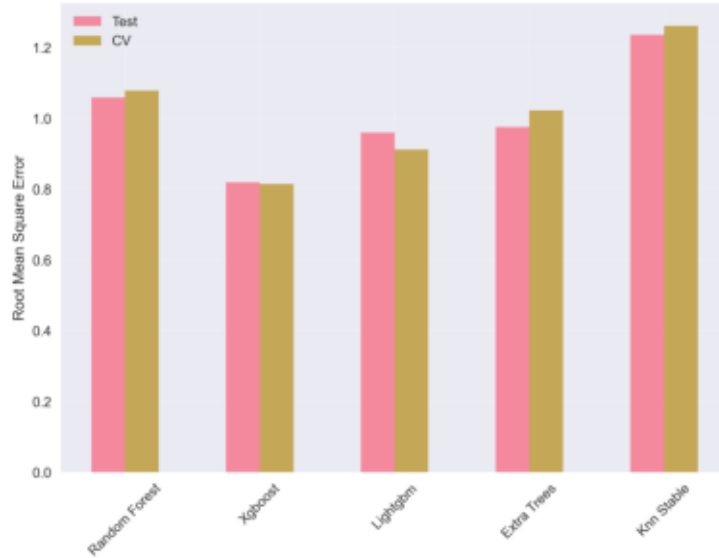
Model R² Performance Comparison



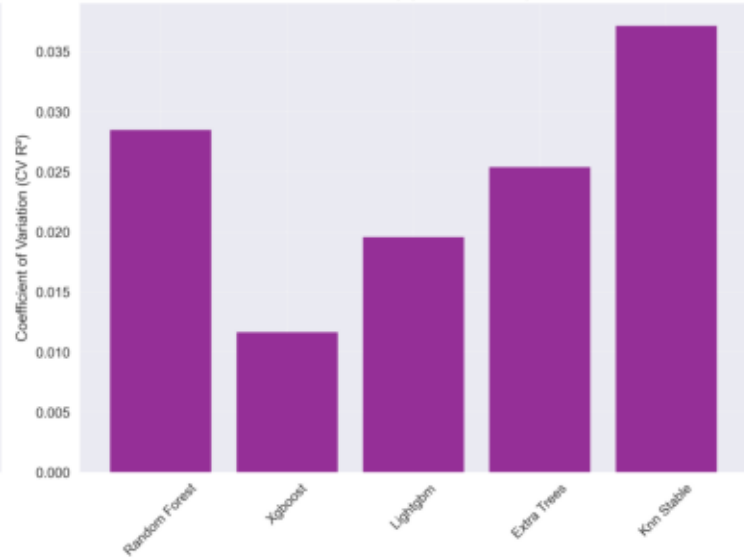
Model MAE Performance Comparison



Model RMSE Performance Comparison

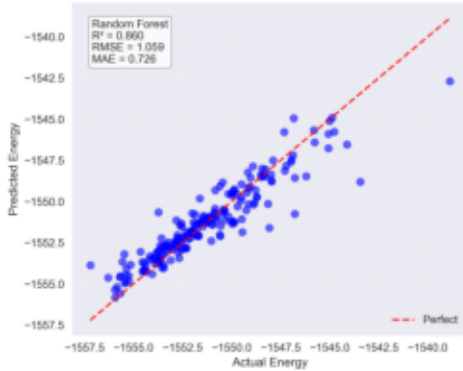


Model Stability (Lower is Better)

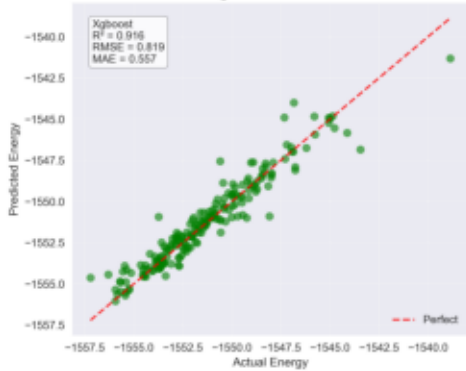


Combined Predictions Vs Actual

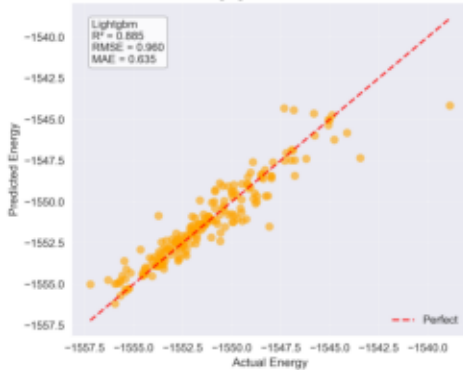
Random Forest Predictions



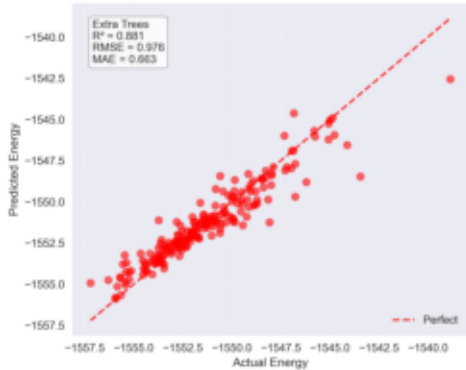
Xgboost Predictions



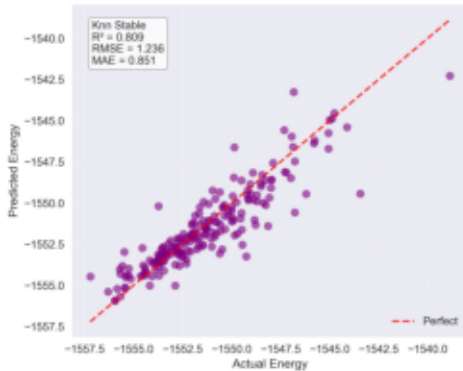
Lightgbm Predictions



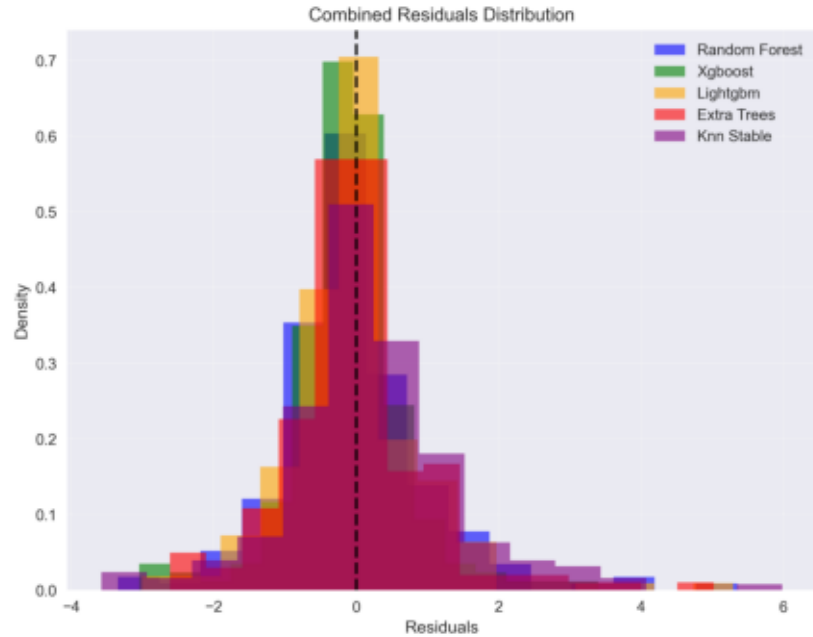
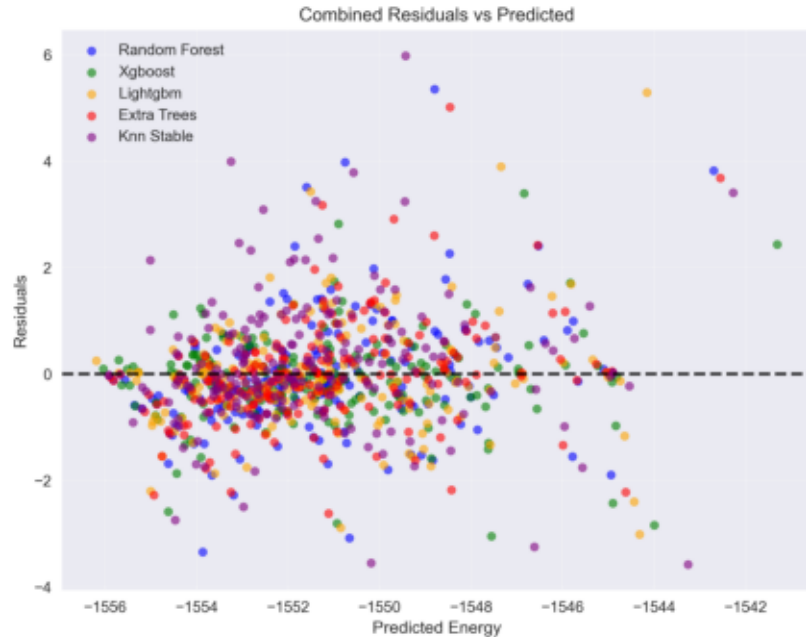
Extra Trees Predictions



Knn Stable Predictions

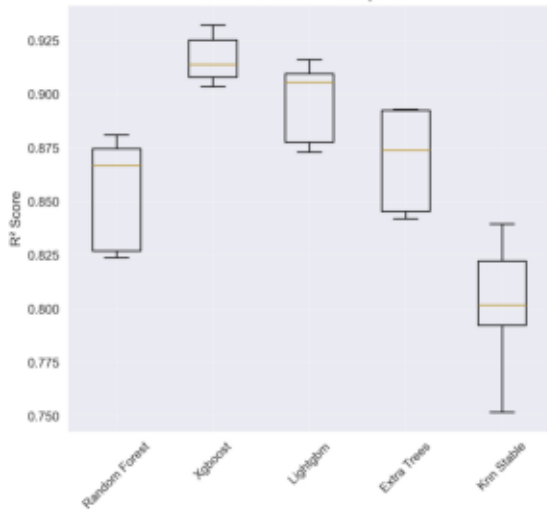


Combined Residual Analysis

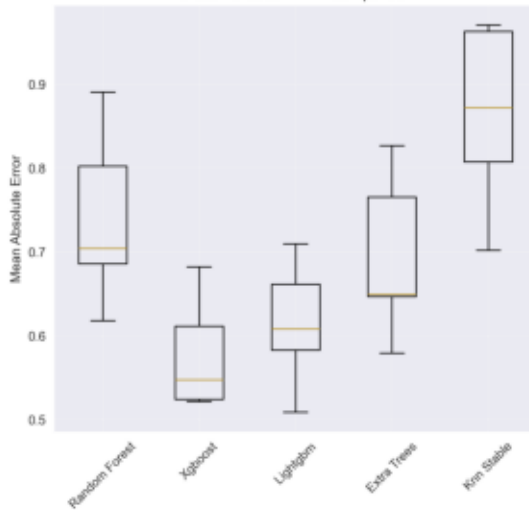


Combined Cv Comparison

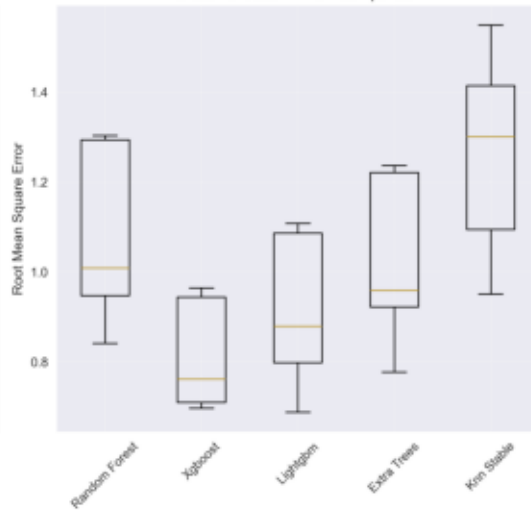
Cross-Validation R^2 Comparison



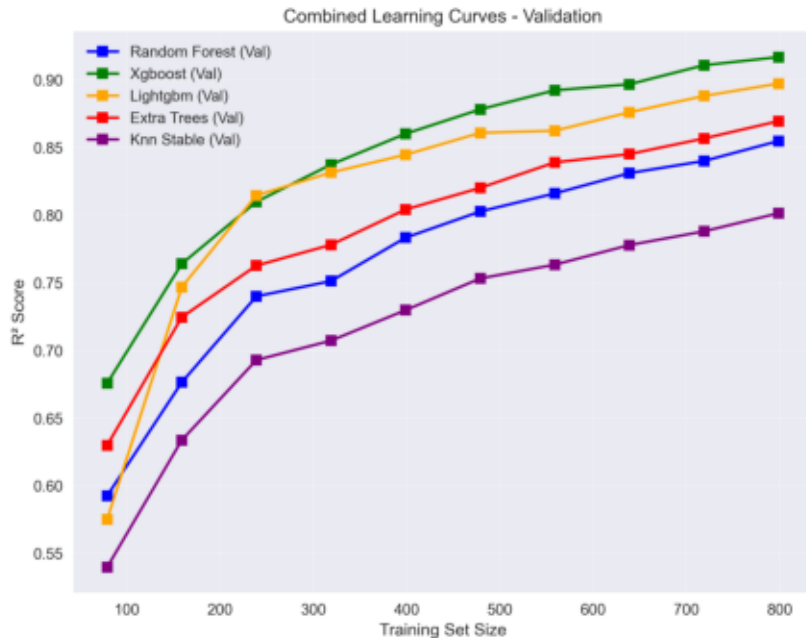
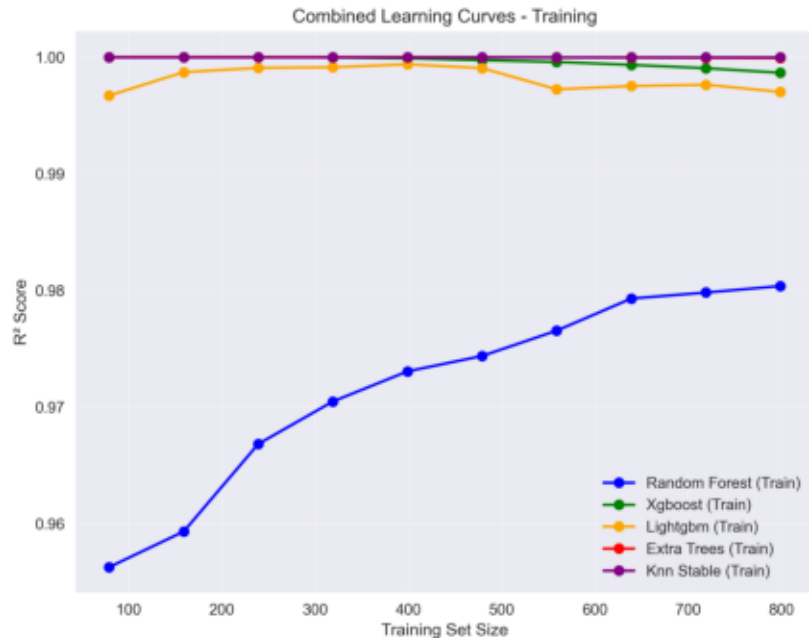
Cross-Validation MAE Comparison



Cross-Validation RMSE Comparison



Combined Learning Curves



Feature Importance Comparison

