

# Tree-Based Models Analysis for Au Cluster Energy Prediction

## Comprehensive Performance Report

Generated: 2025-10-01 23:05:19

### Models Analyzed:

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

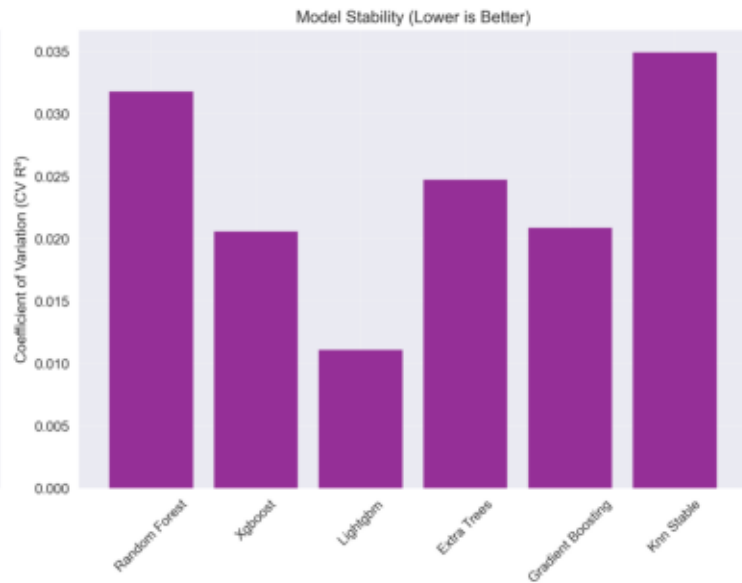
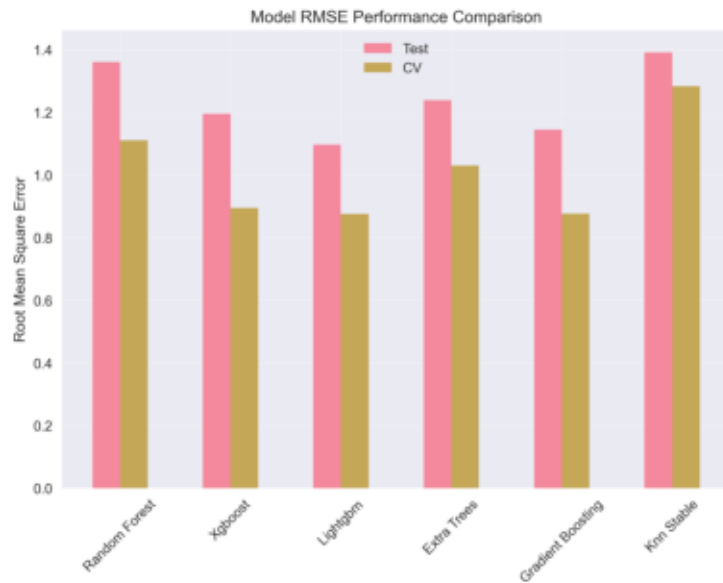
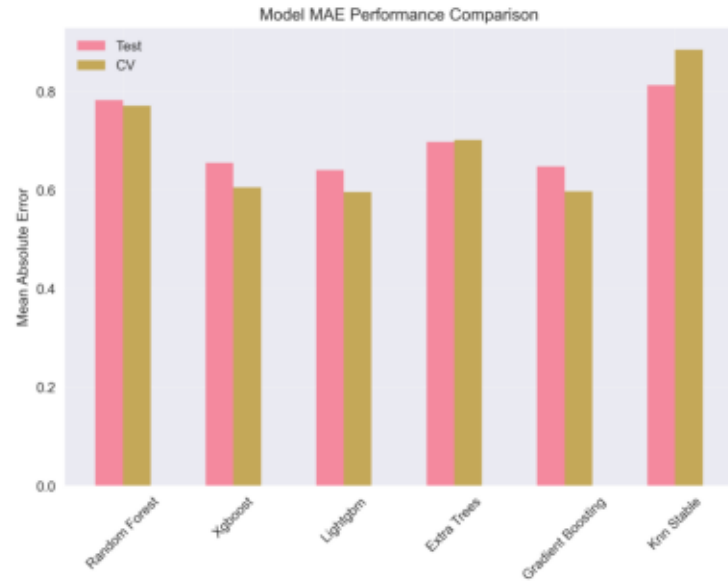
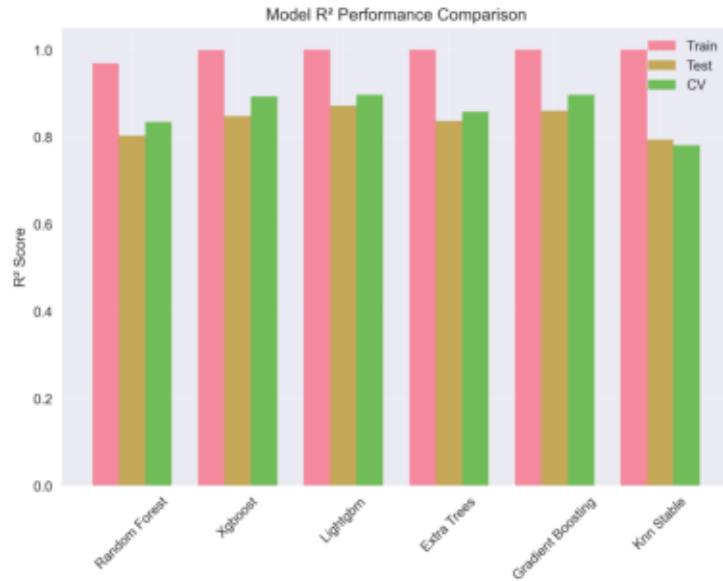
### Dataset Information:

- Training samples: 759
- Test samples: 190
- Total features: 30
- SOAP features: 15

Best Model: Lightgbm

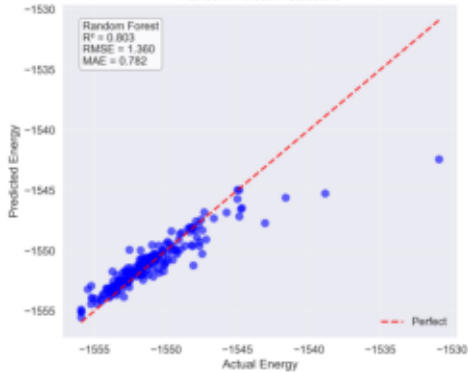
Best Test  $R^2$ : 0.8717

# Combined Model Comparison

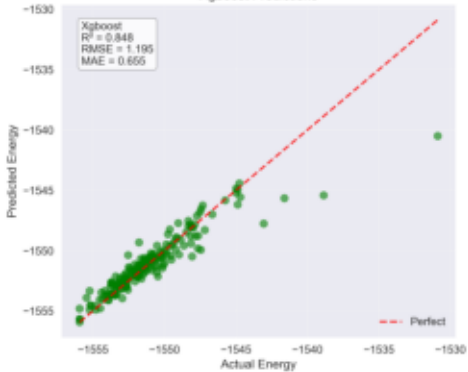


# Combined Predictions Vs Actual

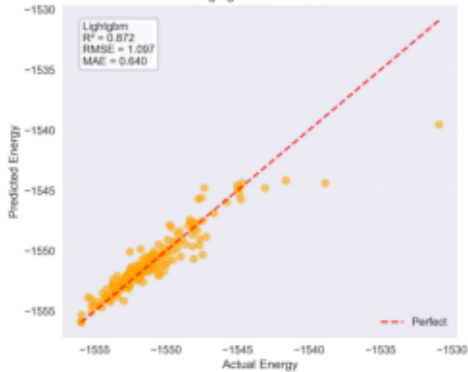
Random Forest Predictions



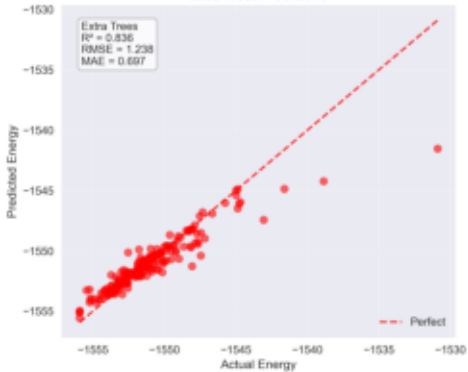
Xgboost Predictions



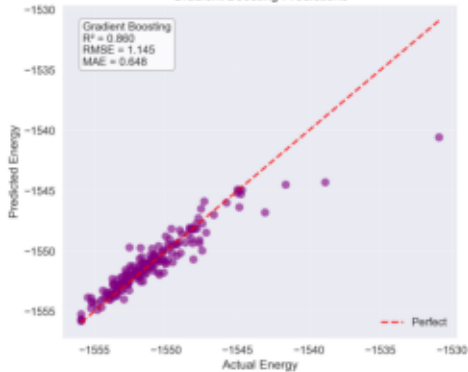
Lightgbm Predictions



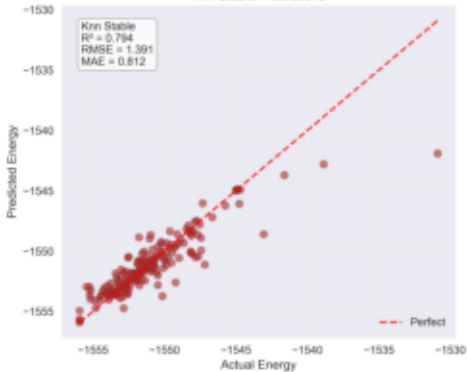
Extra Trees Predictions



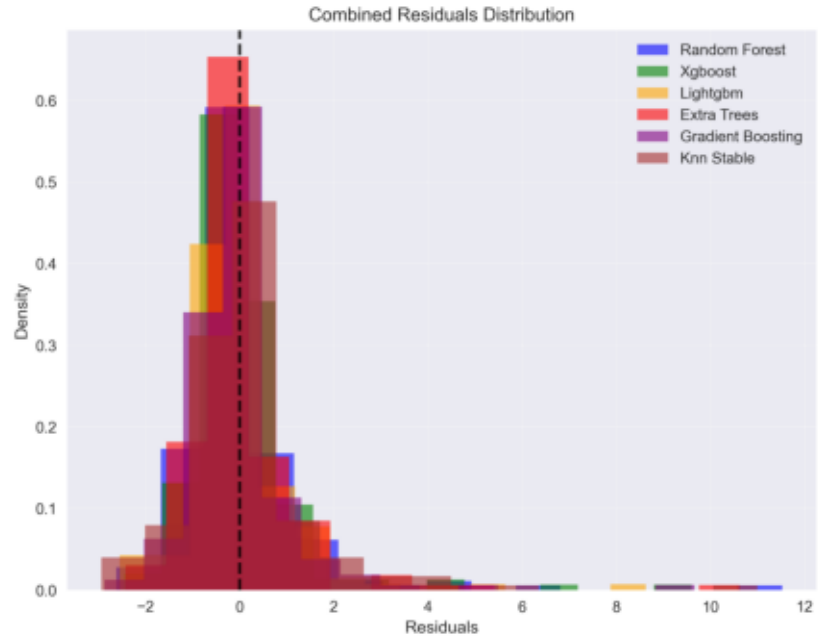
Gradient Boosting Predictions



Knn Stable Predictions

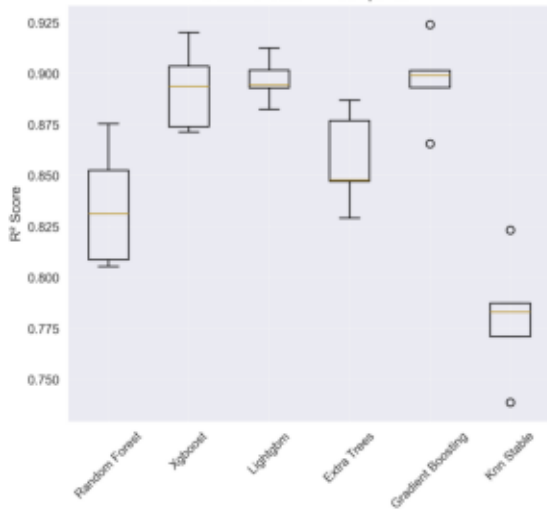


# Combined Residual Analysis

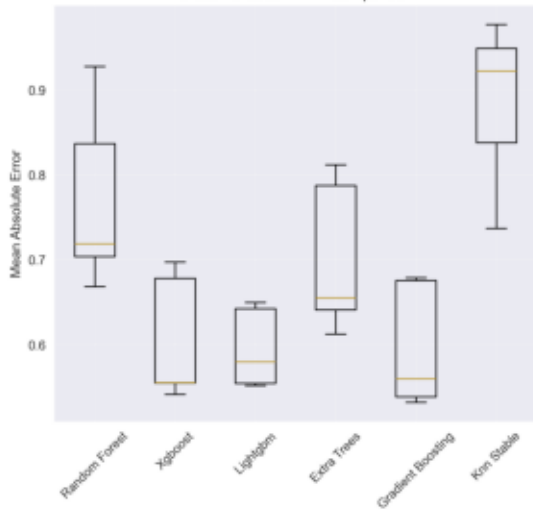


# Combined Cv Comparison

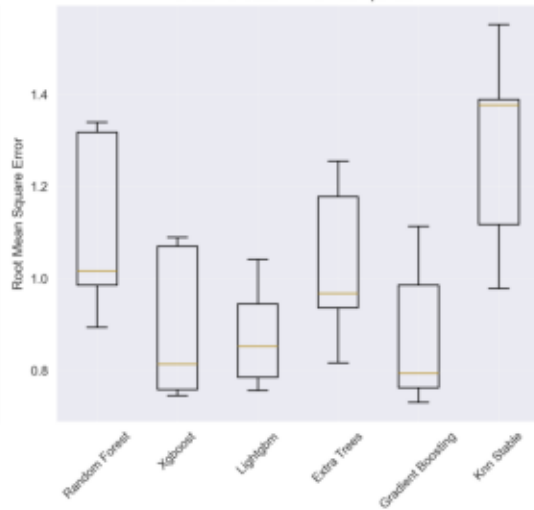
Cross-Validation  $R^2$  Comparison



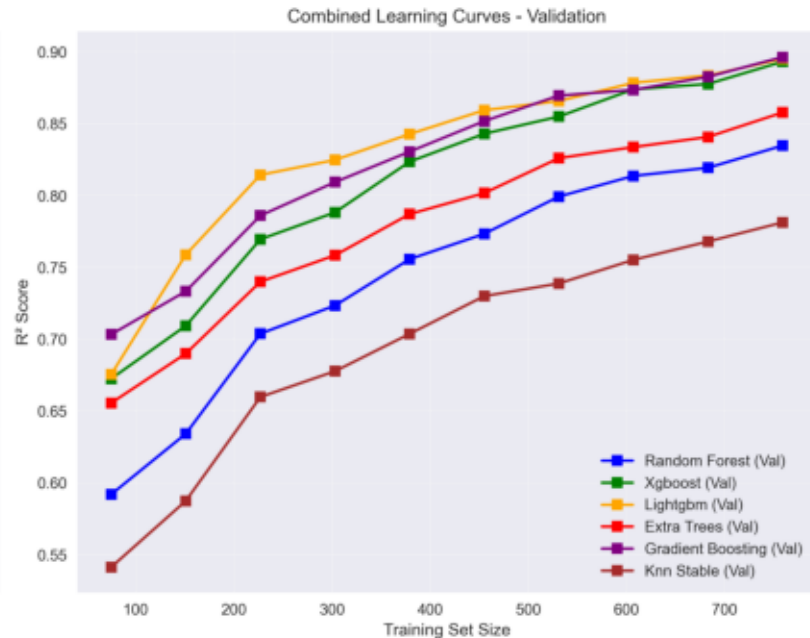
Cross-Validation MAE Comparison



Cross-Validation RMSE Comparison



# Combined Learning Curves



# Feature Importance Comparison

