

# 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:

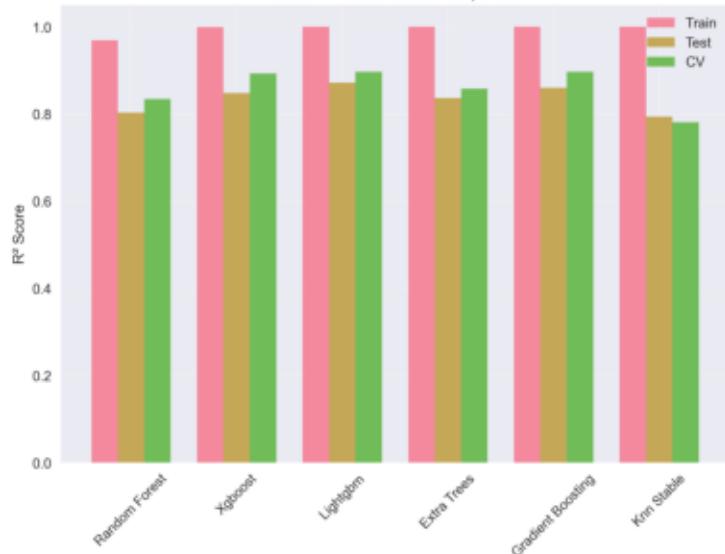
- Training samples: 759
- Test samples: 190
- Total features: 30
- SOAP features: 15

Best Model: Lightgbm

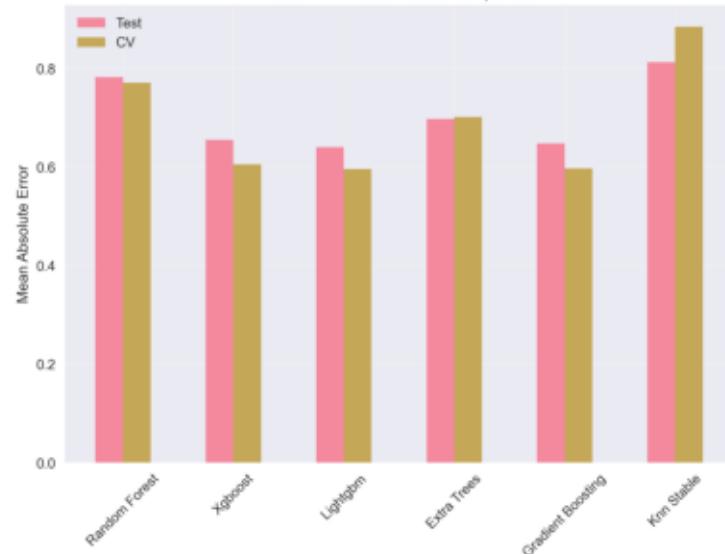
Best Test R<sup>2</sup>: 0.8717

# Combined Model Comparison

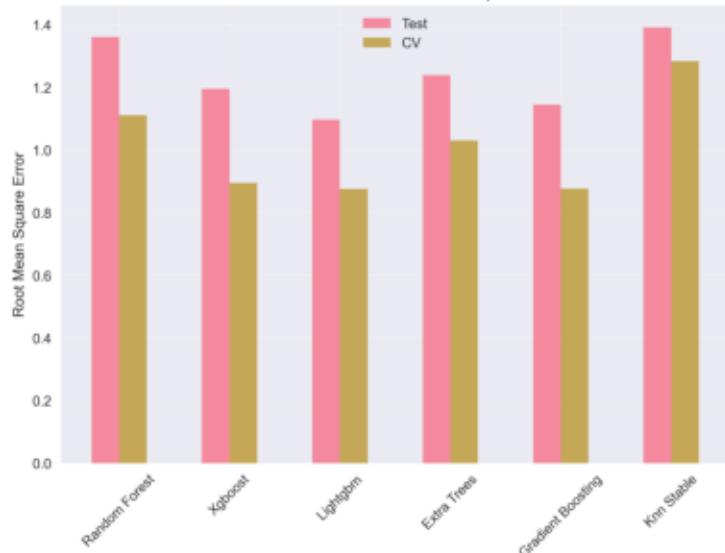
Model R<sup>2</sup> Performance Comparison



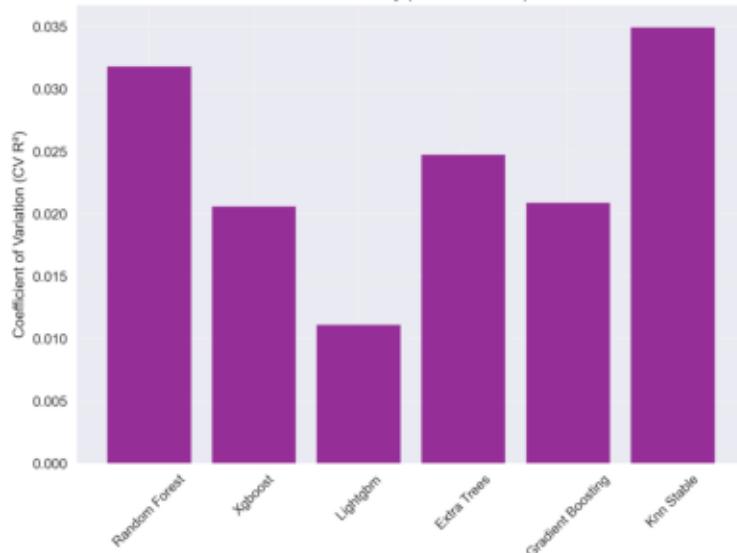
Model MAE Performance Comparison



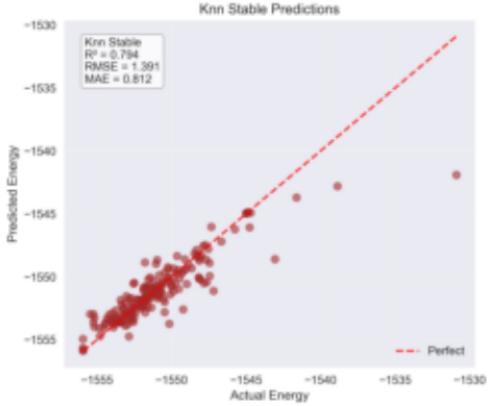
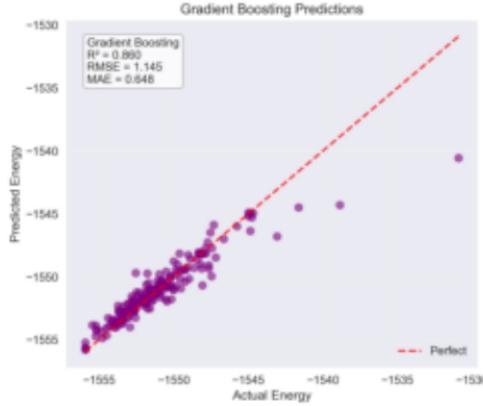
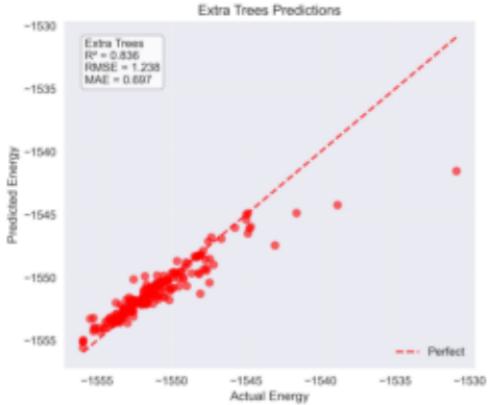
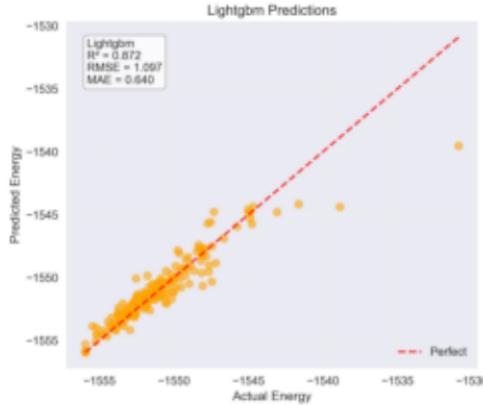
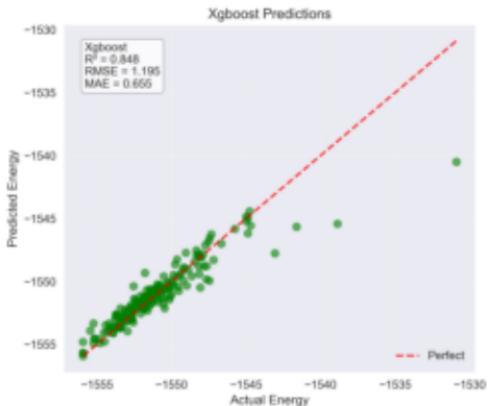
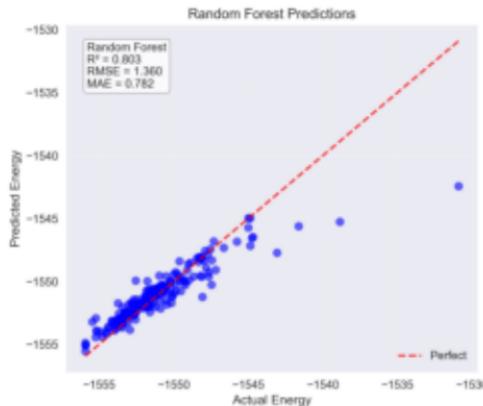
Model RMSE Performance Comparison



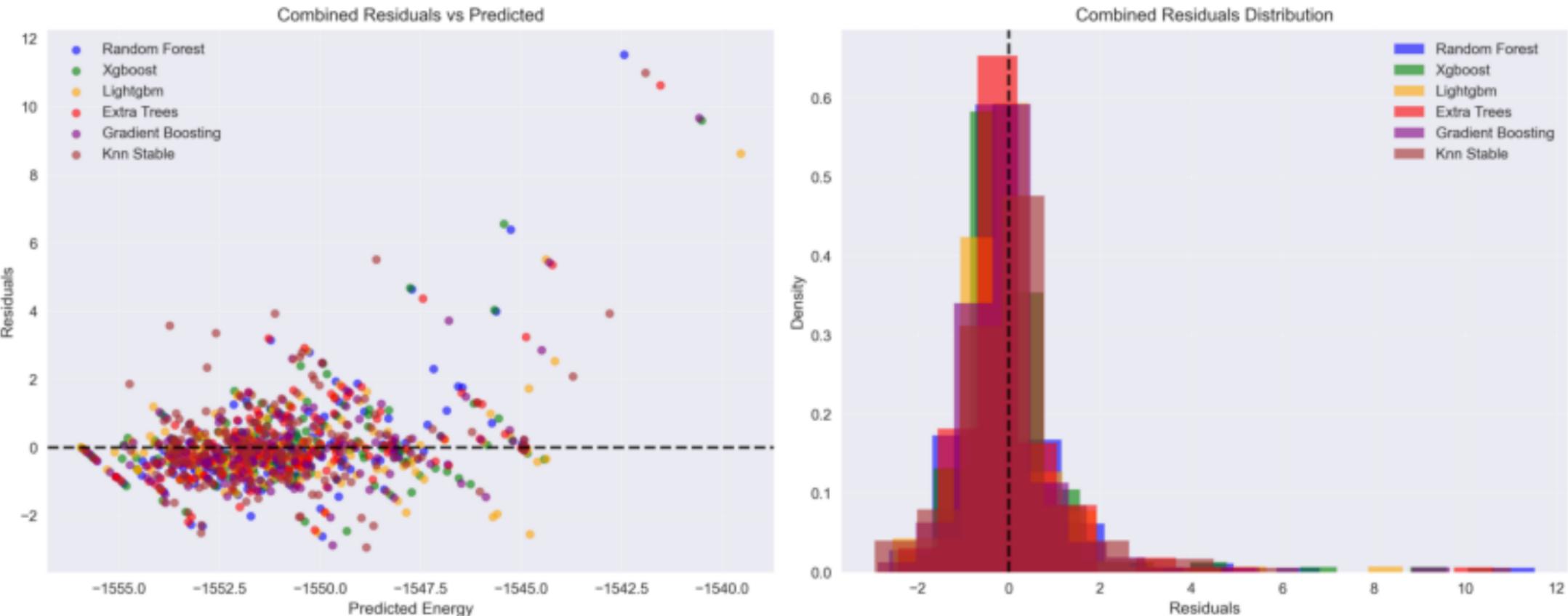
Model Stability (Lower is Better)



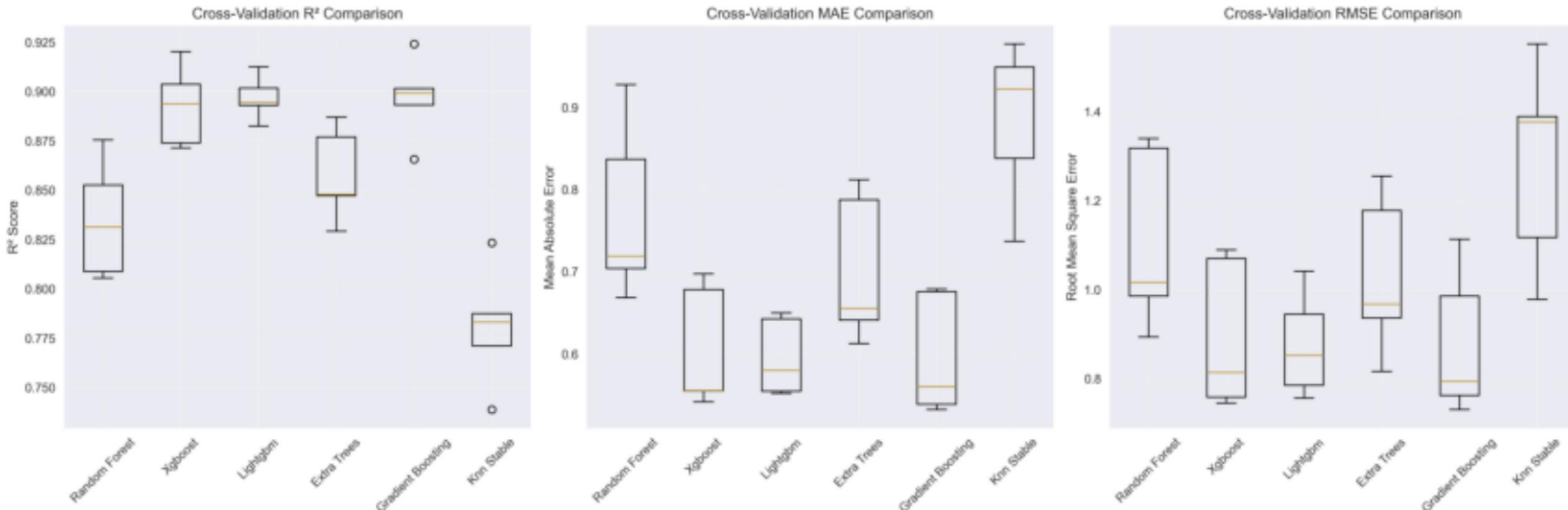
# Combined Predictions Vs Actual



# Combined Residual Analysis

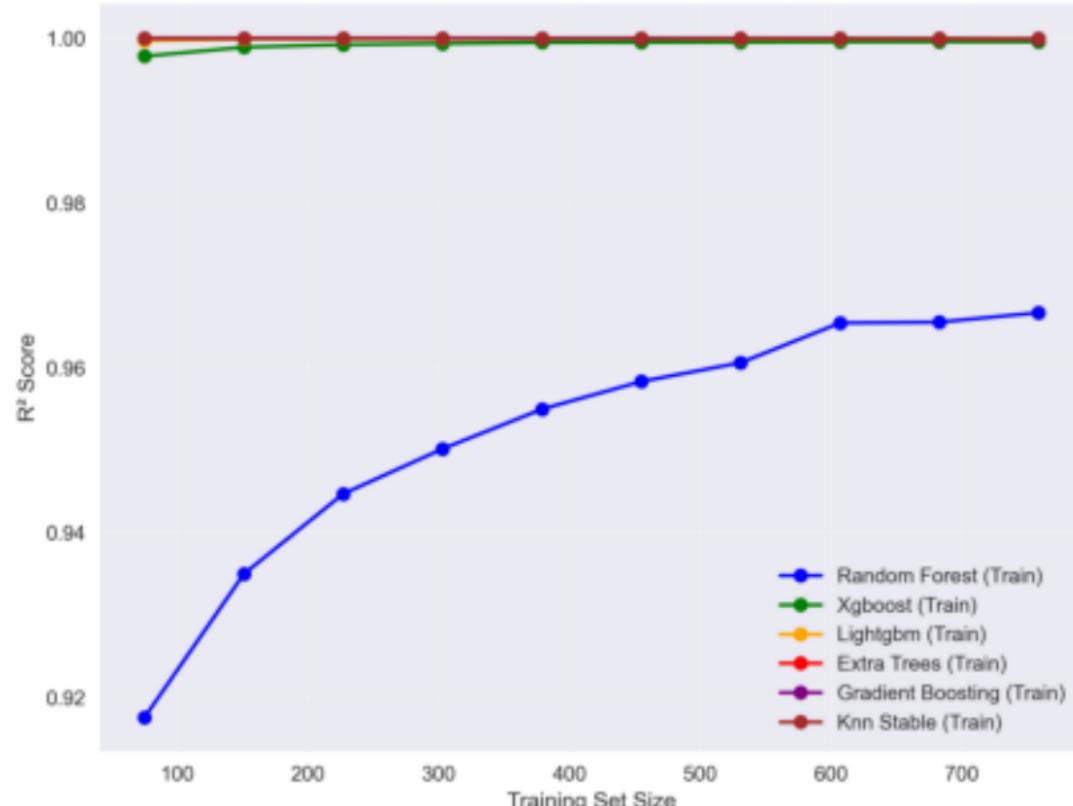


# Combined Cv Comparison

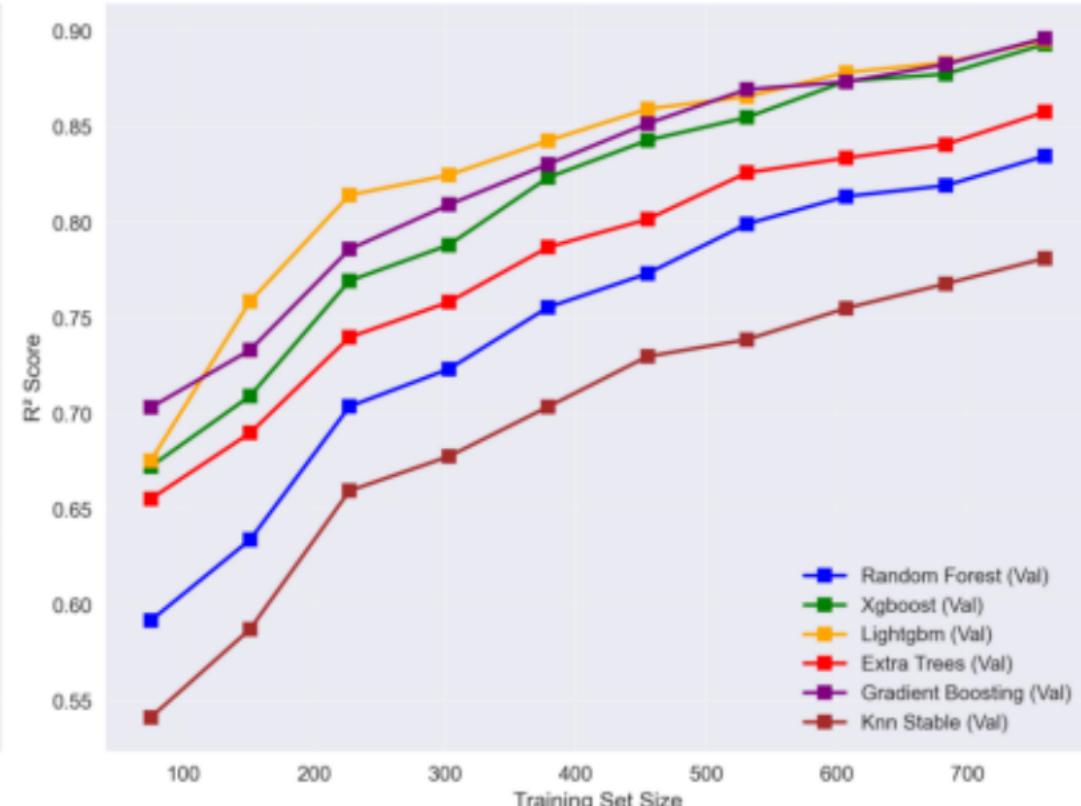


# Combined Learning Curves

Combined Learning Curves - Training



Combined Learning Curves - Validation



# Feature Importance Comparison

