

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:

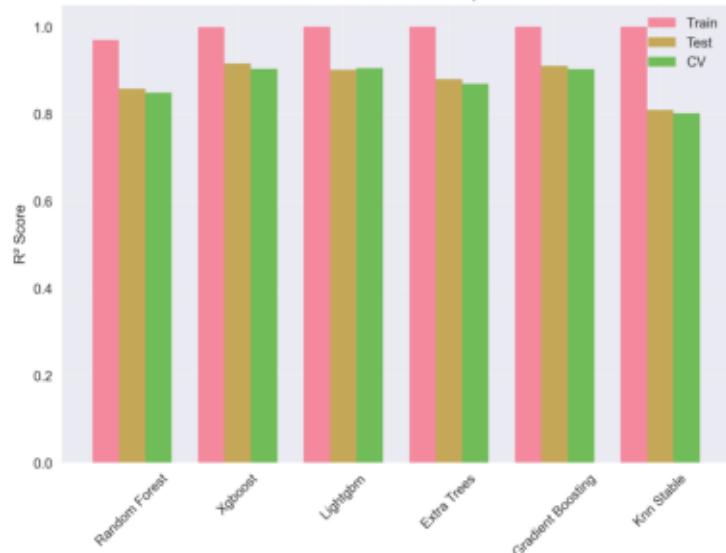
- Training samples: 799
- Test samples: 200
- Total features: 30
- SOAP features: 15

Best Model: Xgboost

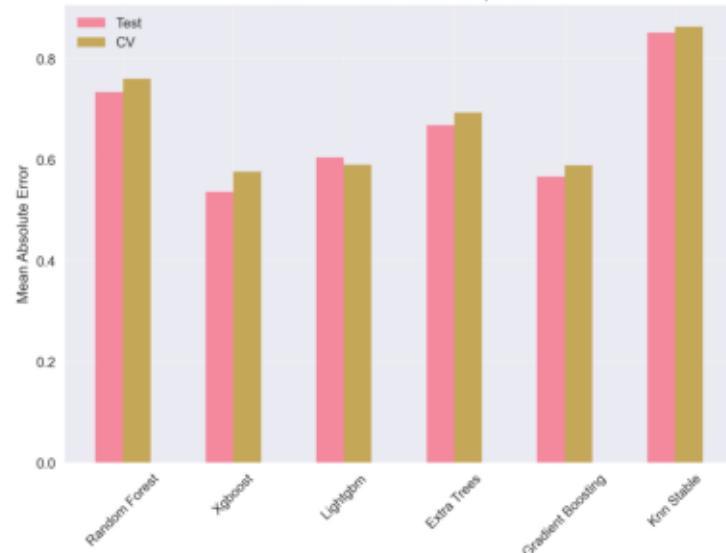
Best Test R²: 0.9156

Combined Model Comparison

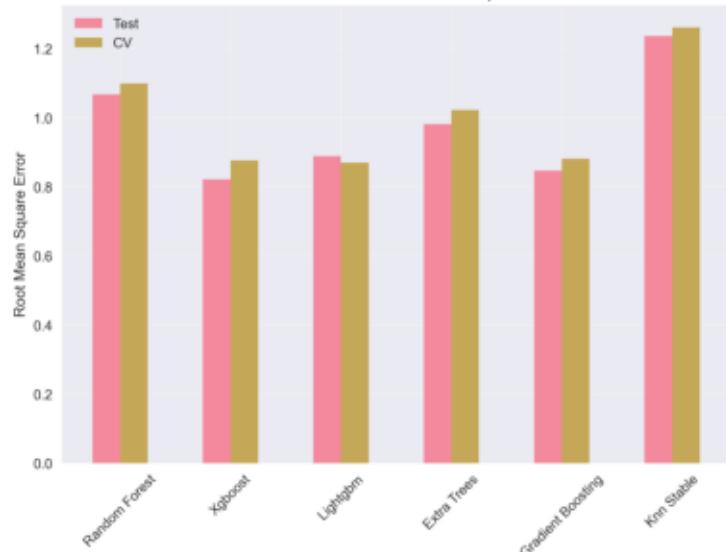
Model R² Performance Comparison



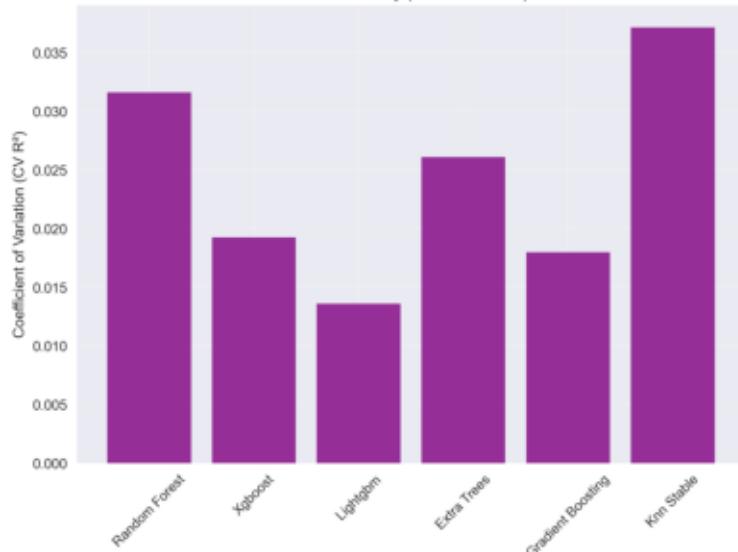
Model MAE Performance Comparison



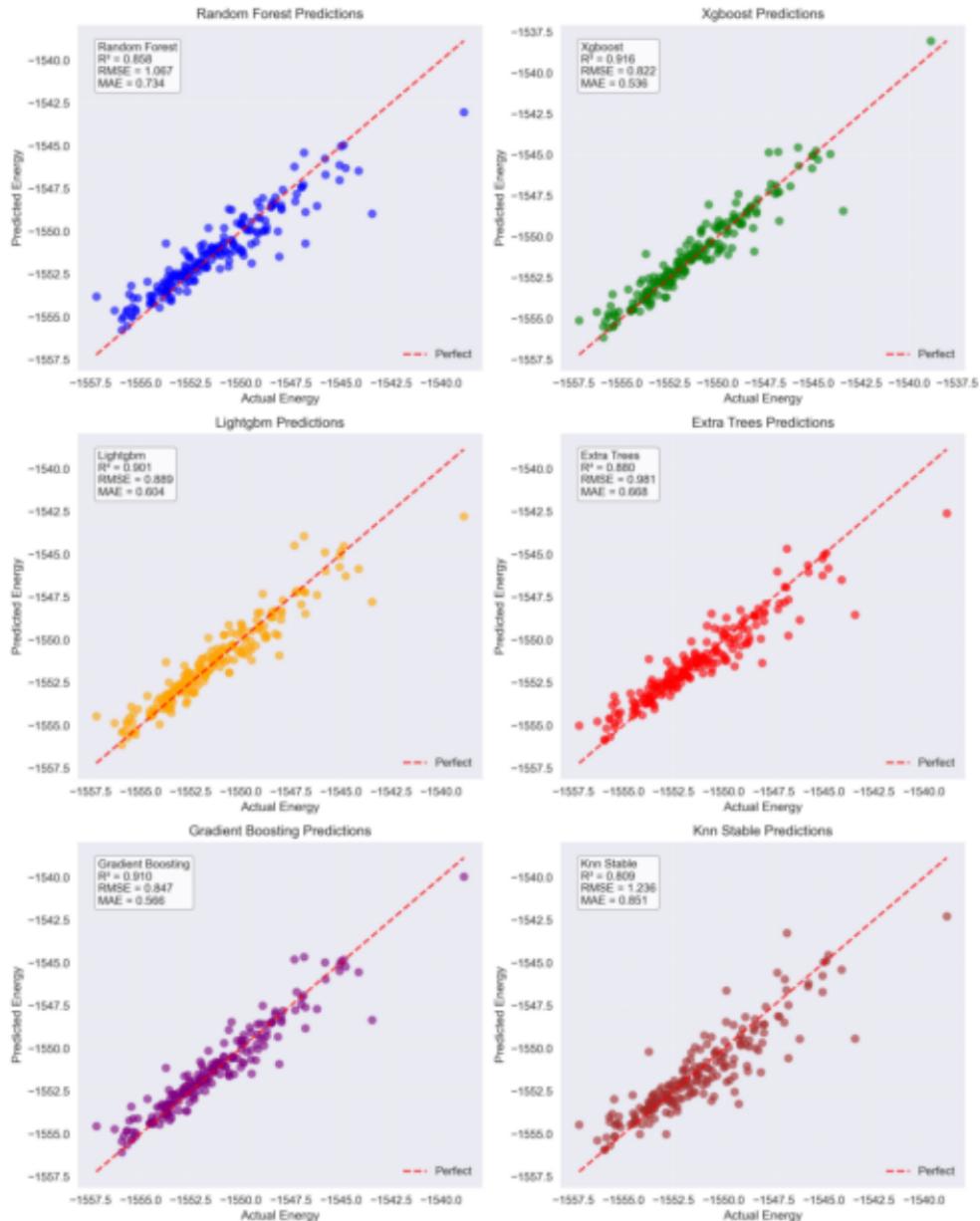
Model RMSE Performance Comparison



Model Stability (Lower is Better)

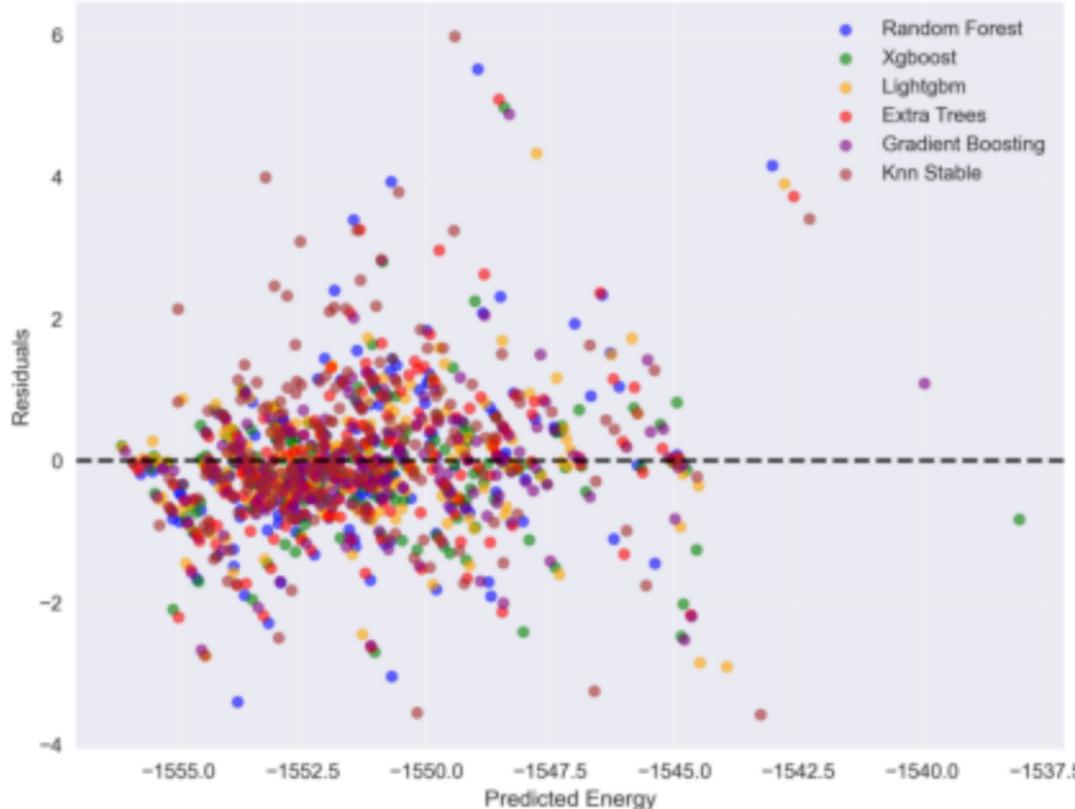


Combined Predictions Vs Actual

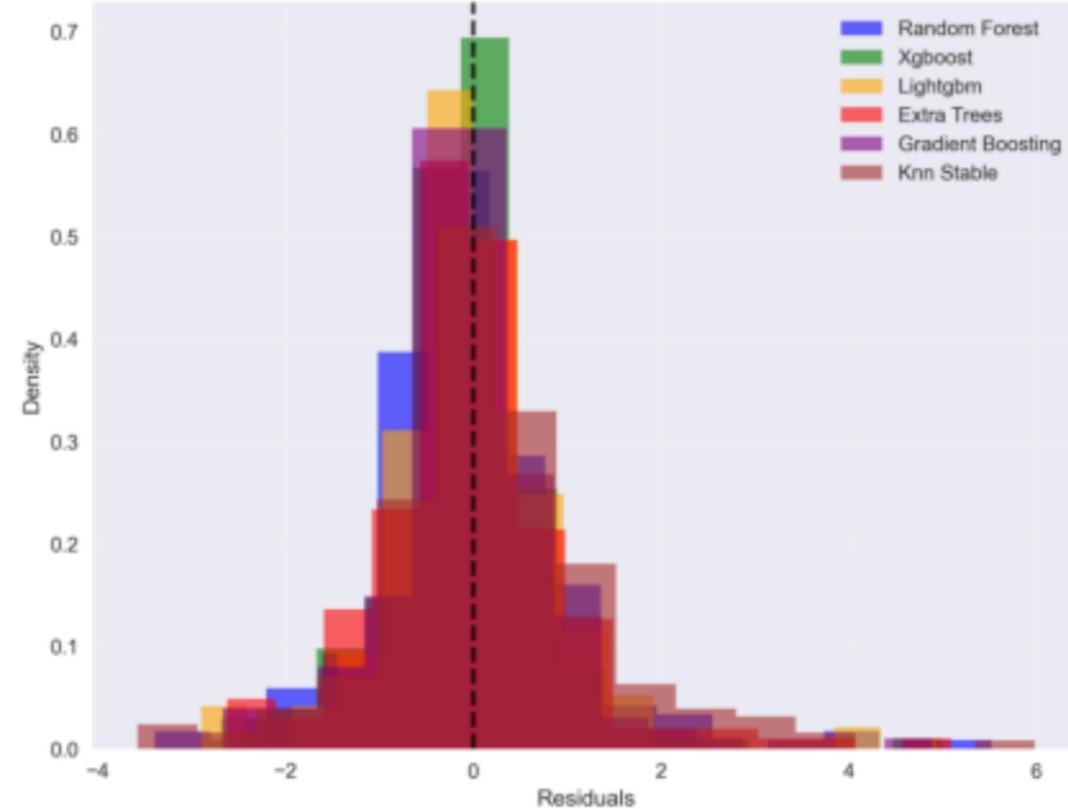


Combined Residual Analysis

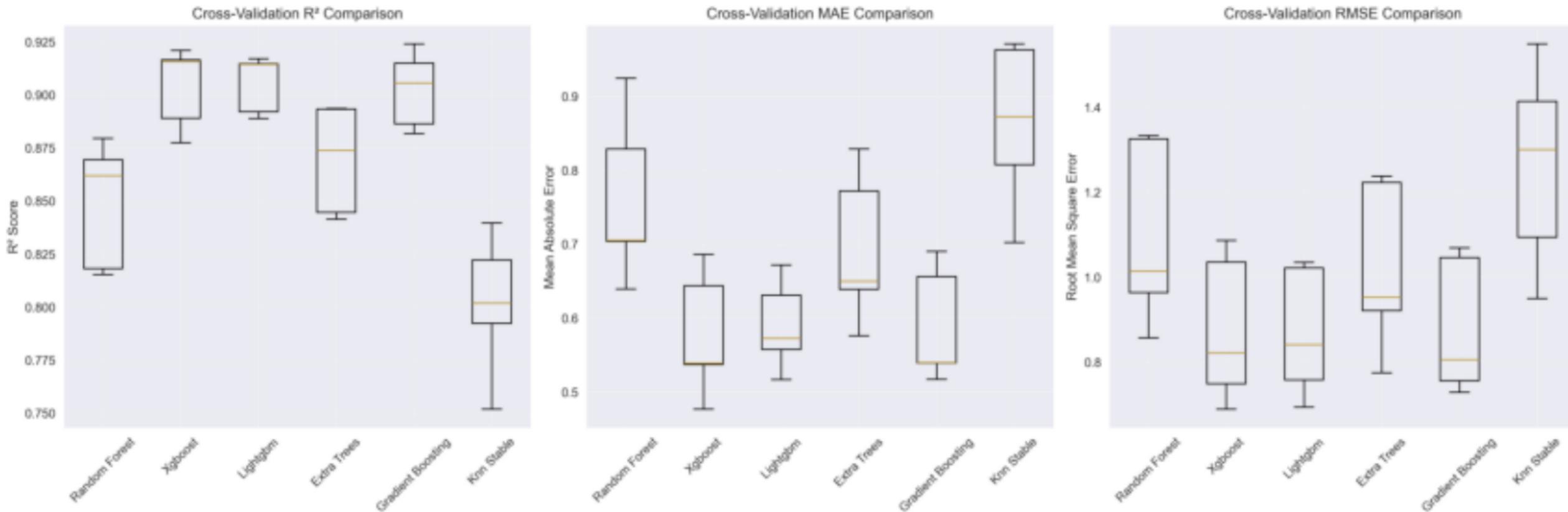
Combined Residuals vs Predicted



Combined Residuals Distribution

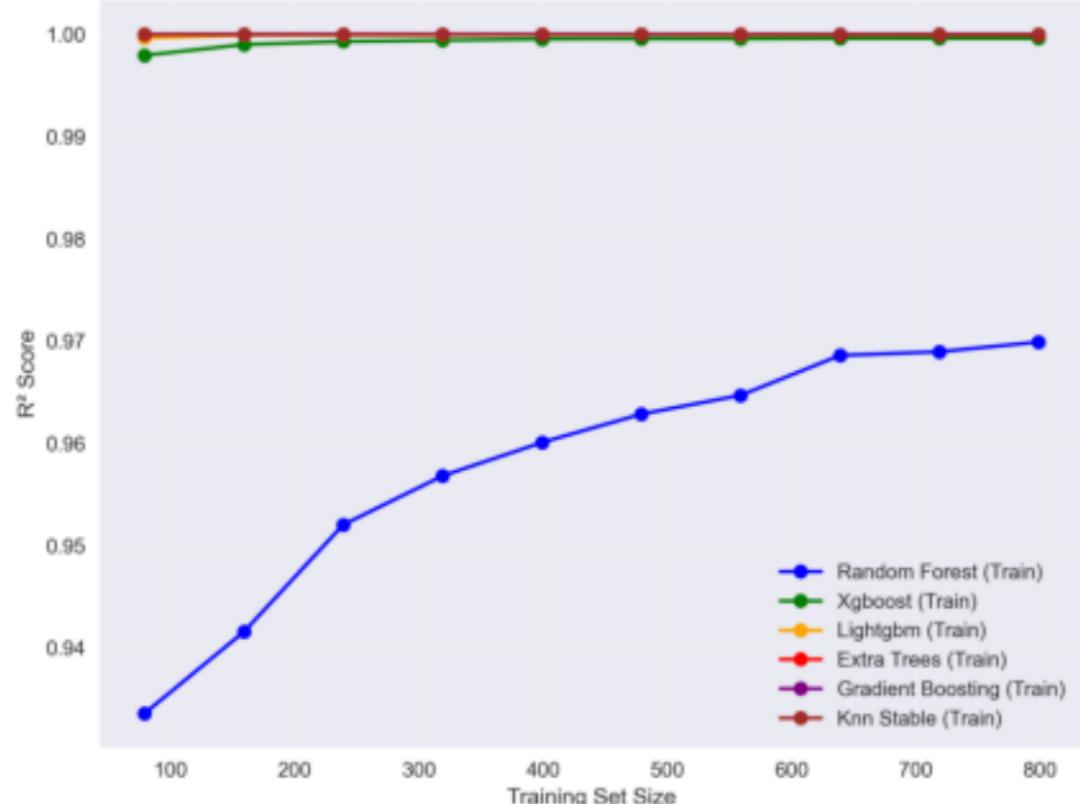


Combined Cv Comparison

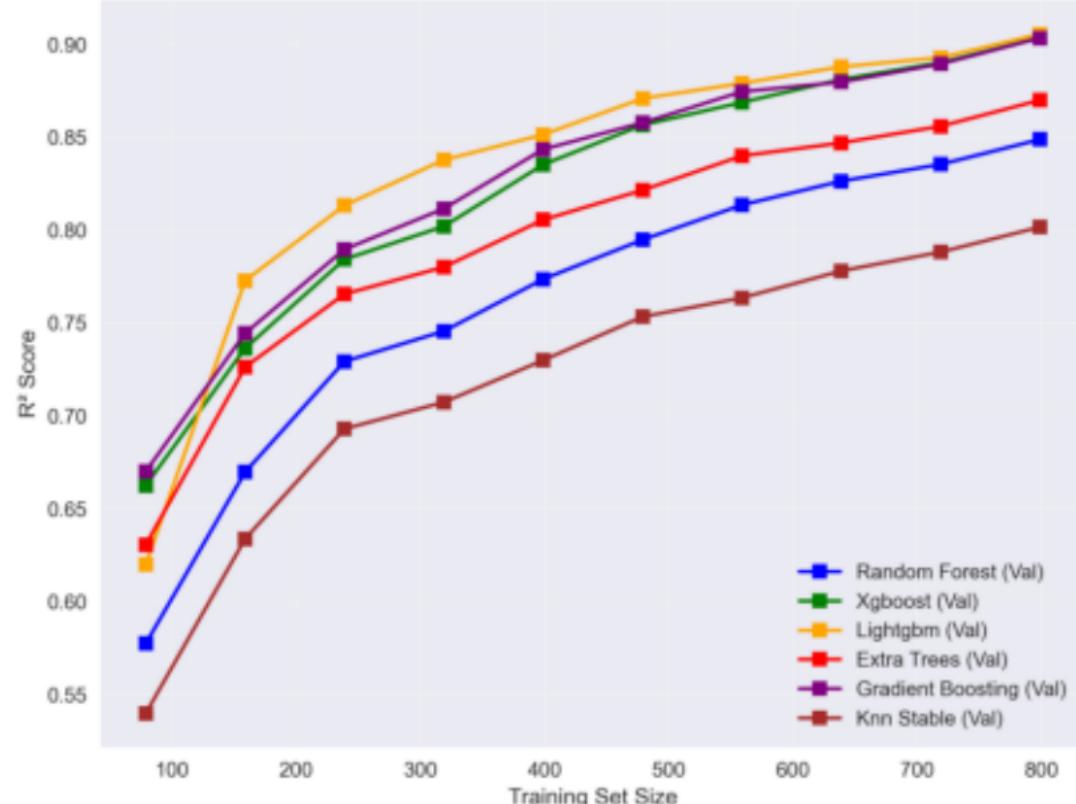


Combined Learning Curves

Combined Learning Curves - Training



Combined Learning Curves - Validation



Feature Importance Comparison

