Linear Models Analysis for Au Cluster Energy Prediction

Comprehensive Performance Report

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Models Analyzed:
• Linear Regression (Baseline)
• Ridge Regression (L2 Regularization)
• Lasso Regression (L1 Regularization + Feature Selection)
• Elastic Net (L1+L2 Regularization)

Dataset Information:
• Training samples: 799
• Test samples: 200
• Total features: 15
• SOAP features: 0
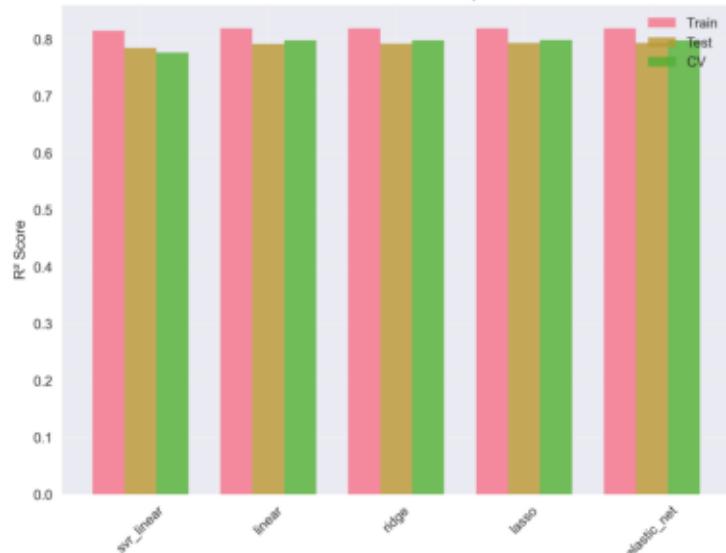
Best Model: Elastic_Net
Best Test R^2: 0.7930
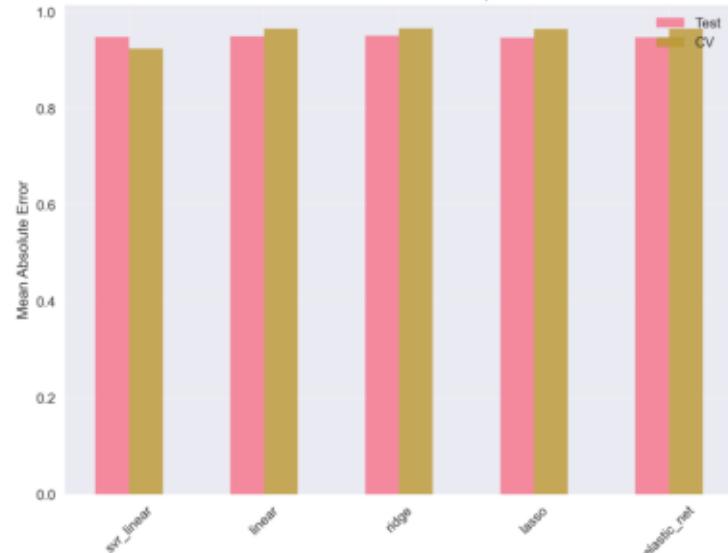
Combined Model Comparison
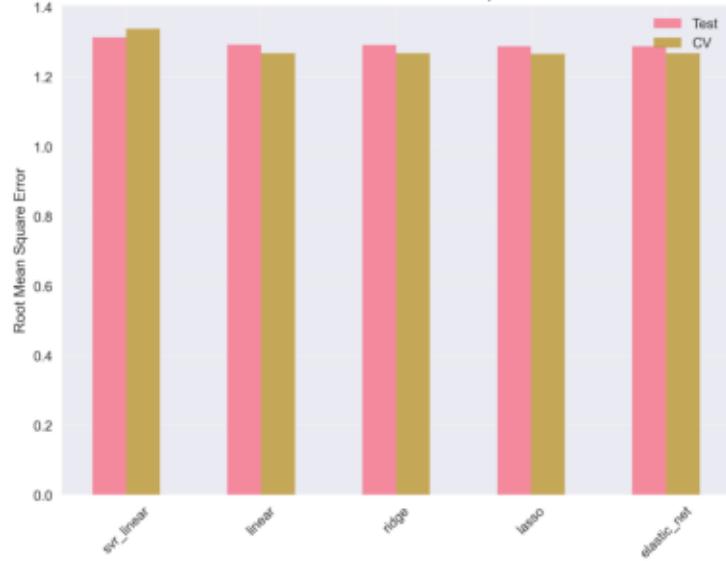

Model R² Performance Comparison — R² Score for svr_linear, linear, ridge, lasso, elastic_net (Train, Test, CV)
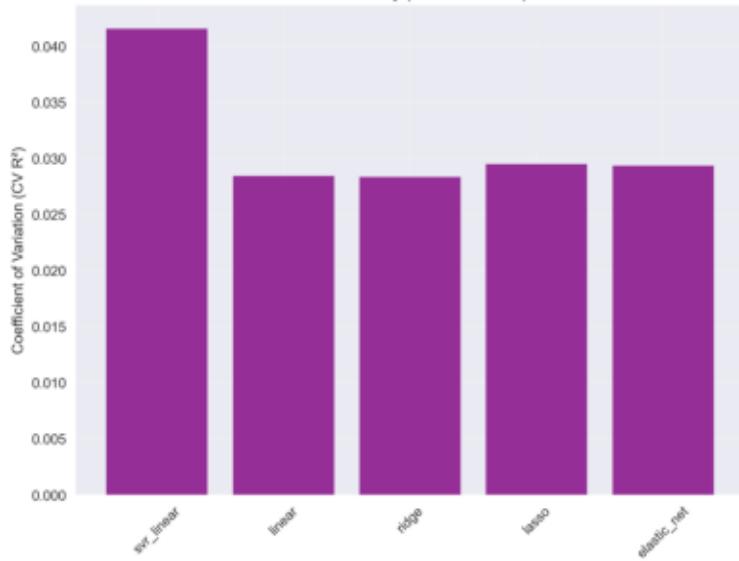
Model MAE Performance Comparison — Mean Absolute Error for svr_linear, linear, ridge, lasso, elastic_net (Test, CV)

Model RMSE Performance Comparison — Root Mean Square Error for svr_linear, linear, ridge, lasso, elastic_net (Test, CV)
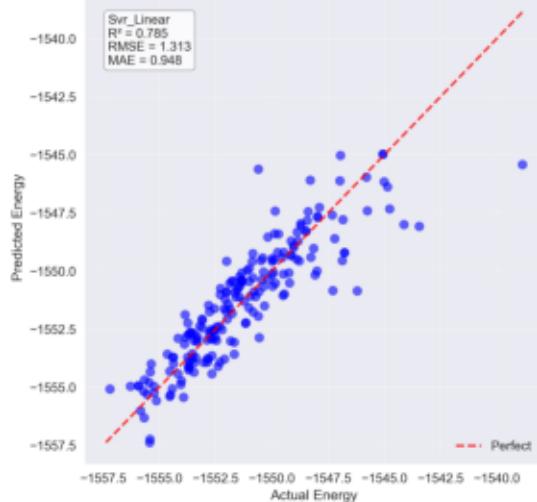
Model Stability (Lower is Better) — Coefficient of Variation (CV R²) for svr_linear, linear, ridge, lasso, elastic_net
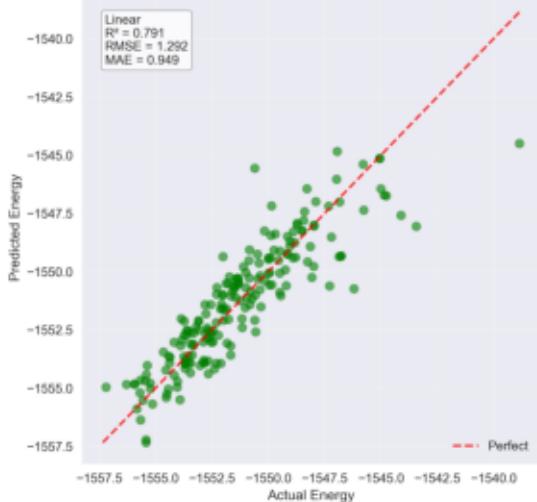
Combined Predictions Vs Actual
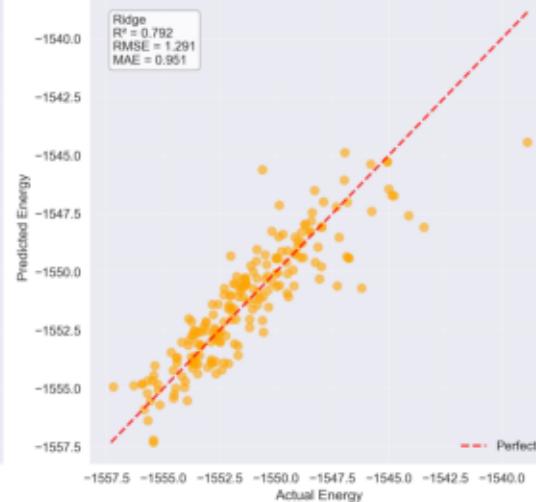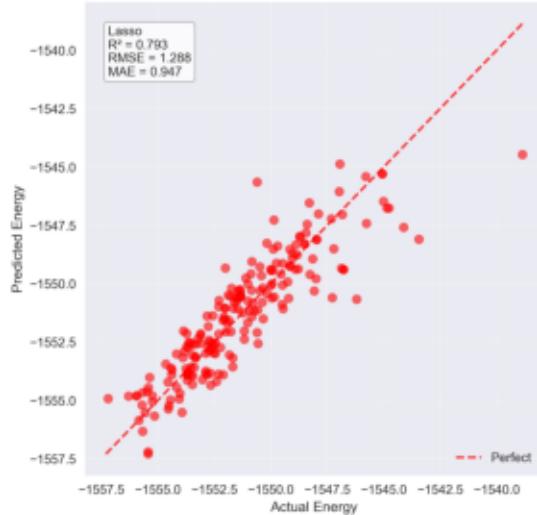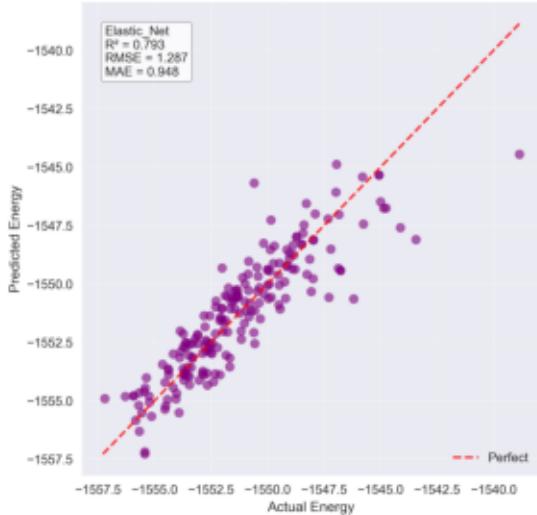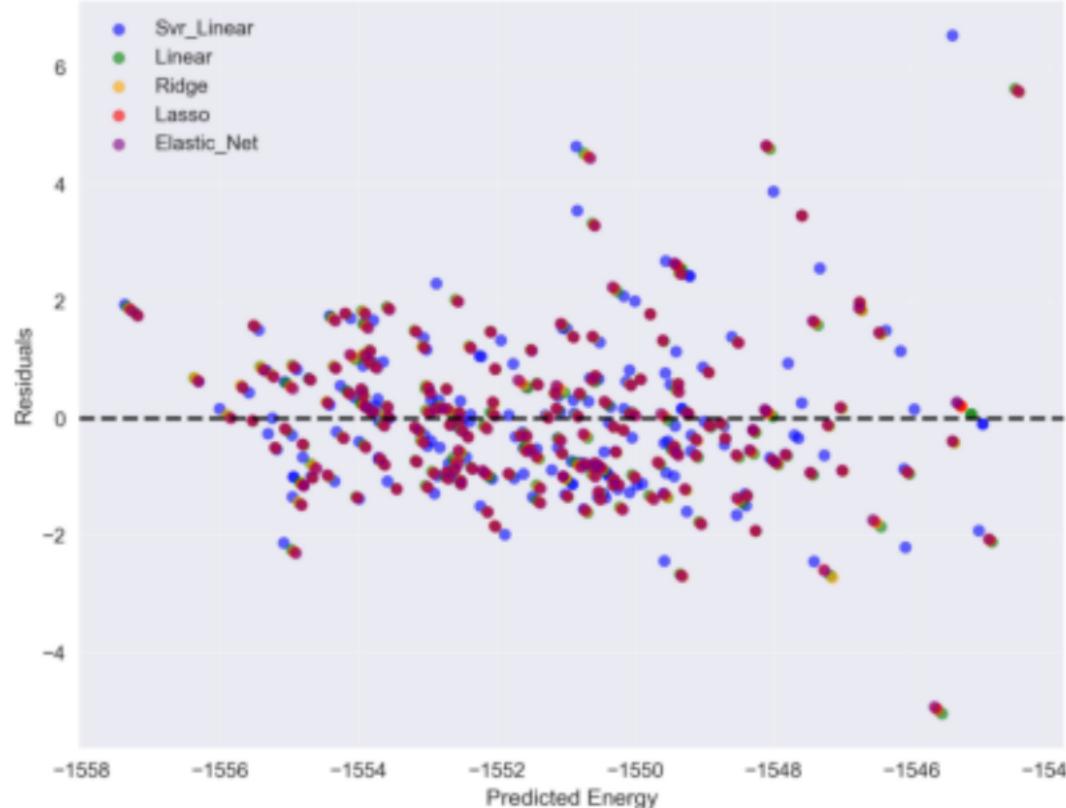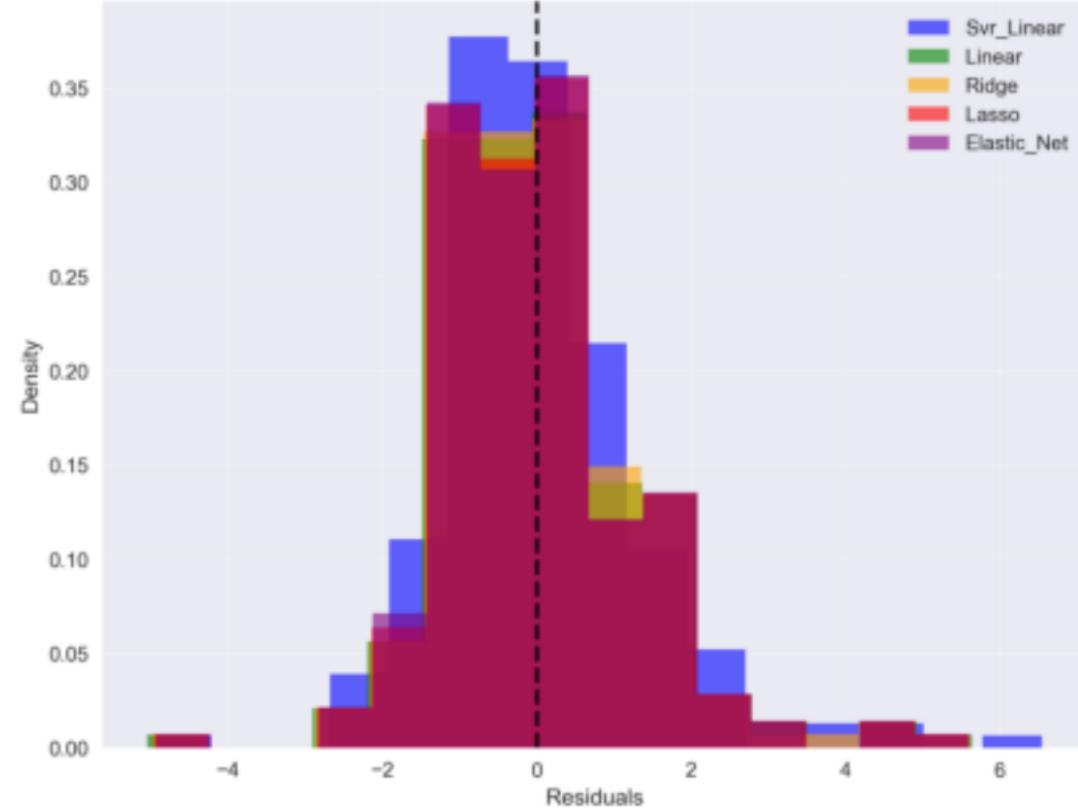
Combined Residual Analysis
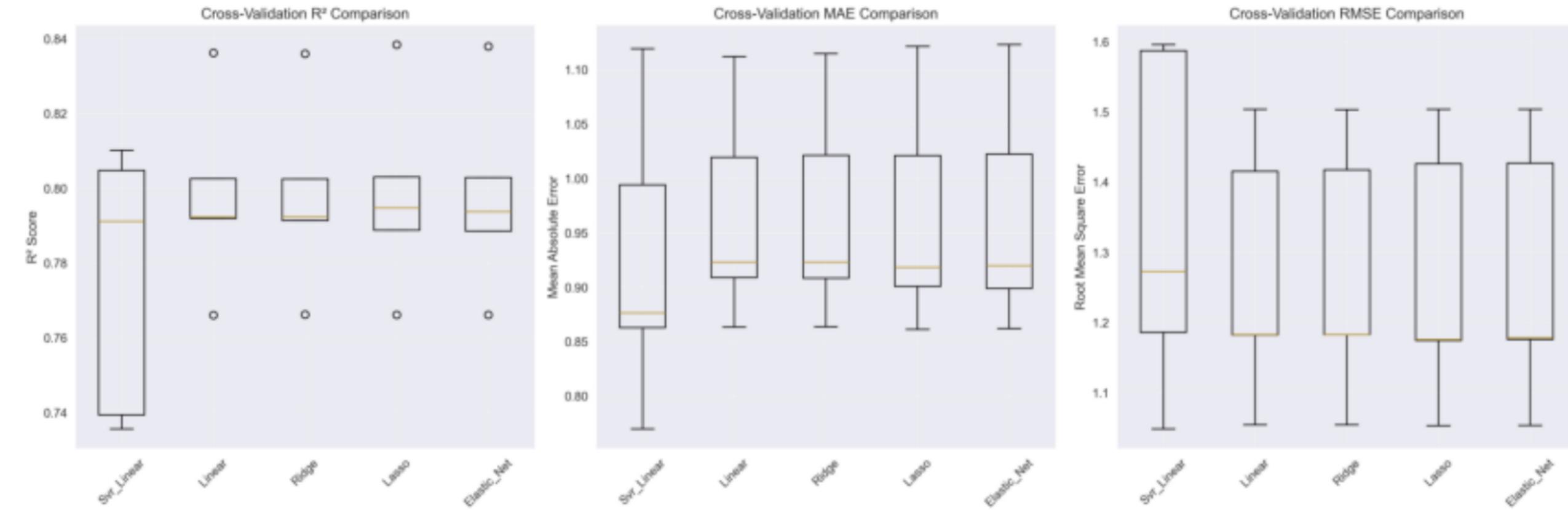

Combined Residuals vs Predicted — Combined Residuals Distribution
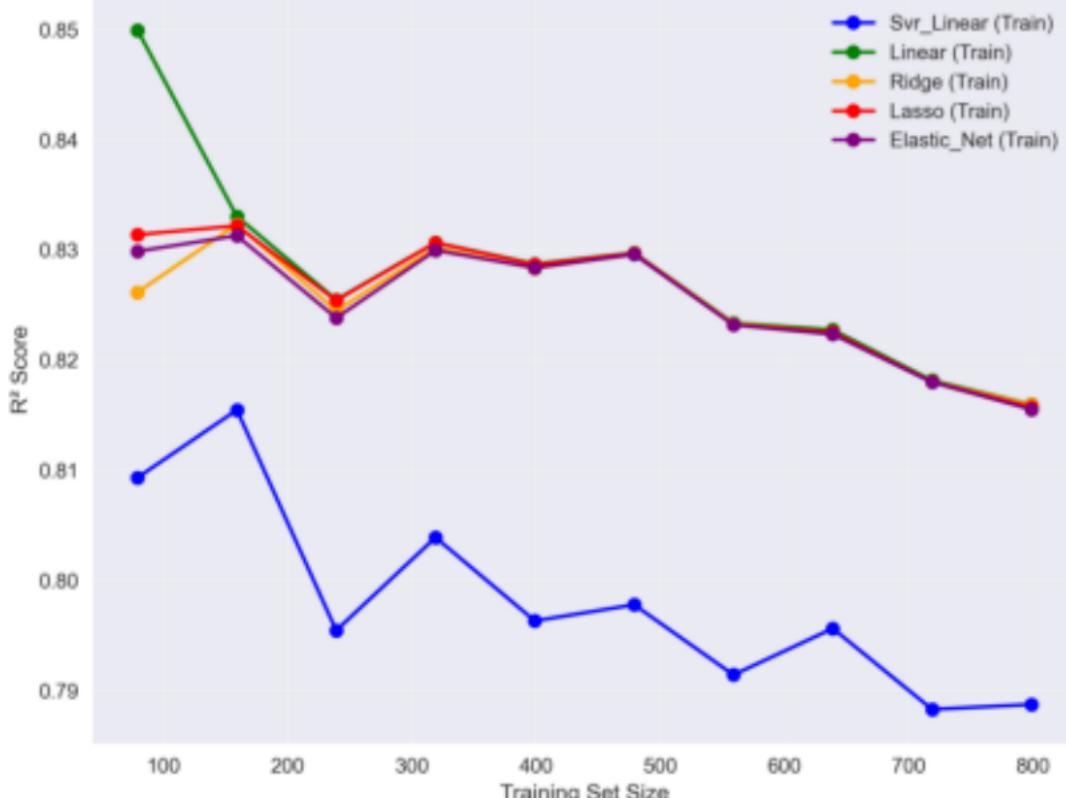
Combined Cv Comparison

Cross-Validation R² Comparison   Cross-Validation MAE Comparison   Cross-Validation RMSE Comparison
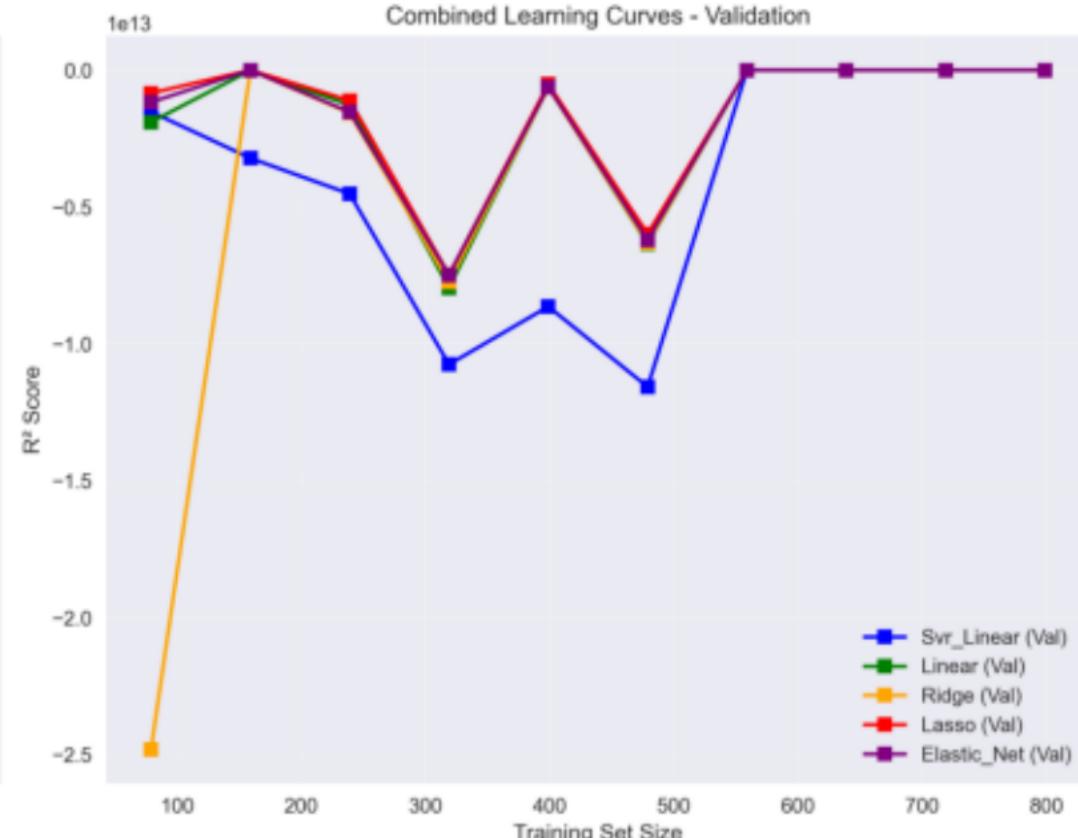
Combined Learning Curves

Combined Learning Curves - Training | Combined Learning Curves - Validation
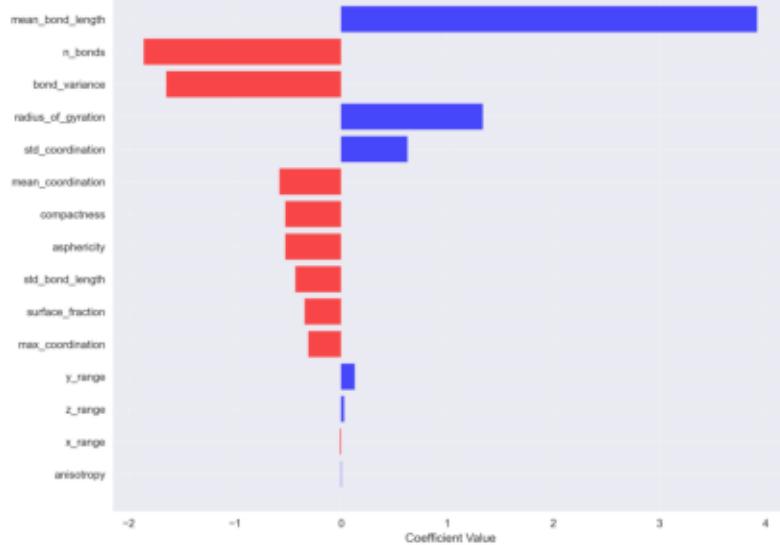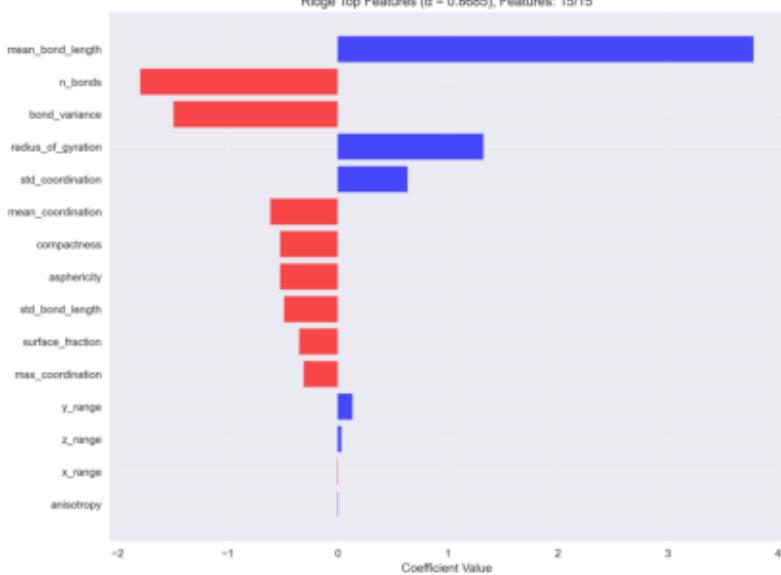
Feature Importance Comparison