

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:

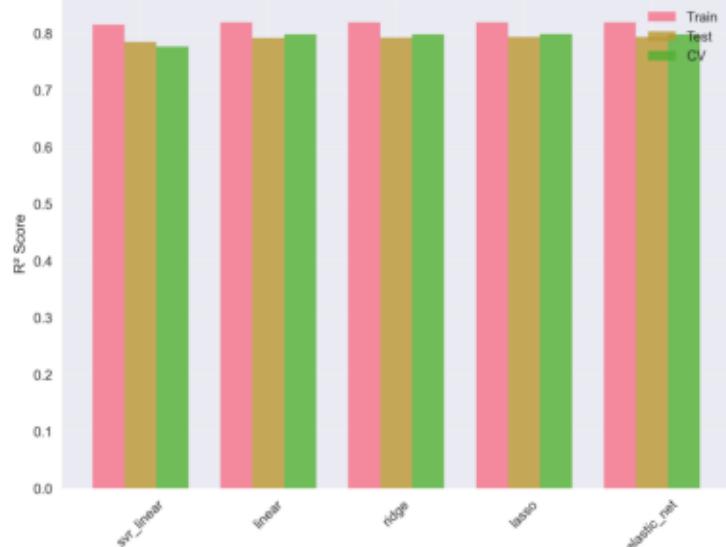
- Training samples: 799
- Test samples: 200
- Total features: 15
- SOAP features: 0

Best Model: Elastic_Net

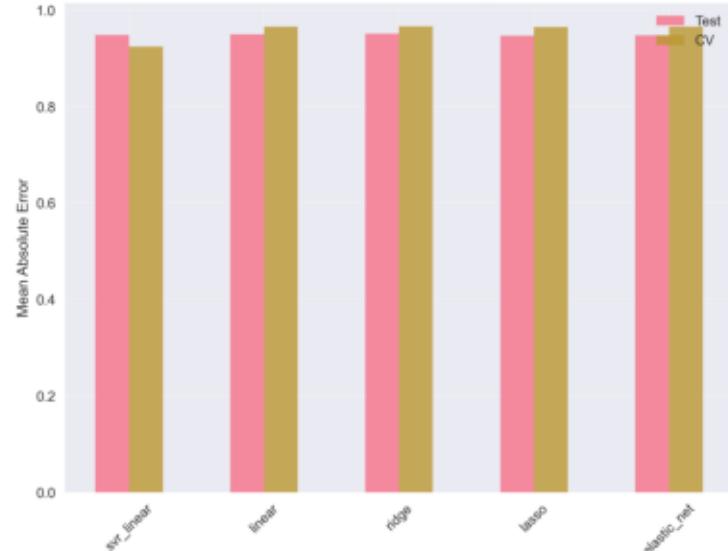
Best Test R²: 0.7930

Combined Model Comparison

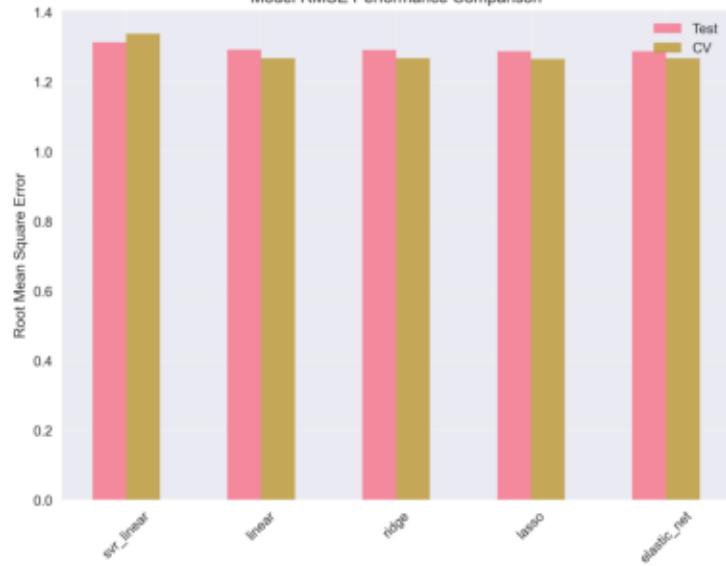
Model R² Performance Comparison



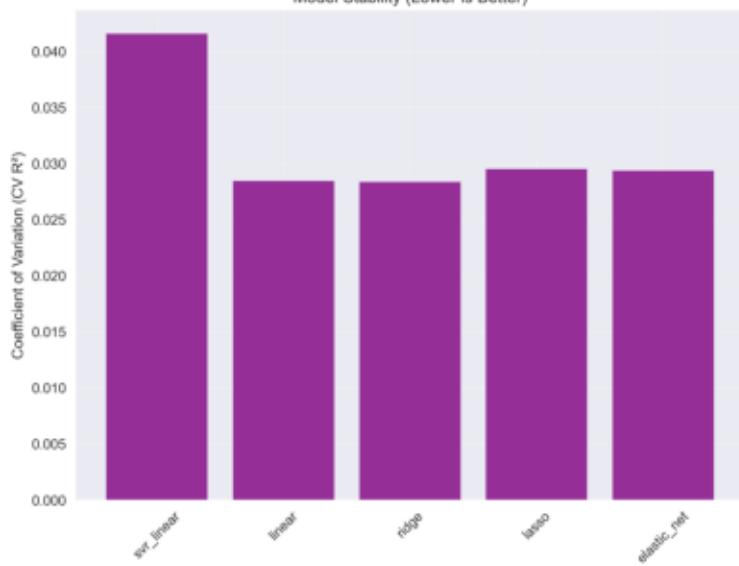
Model MAE Performance Comparison



Model RMSE Performance Comparison

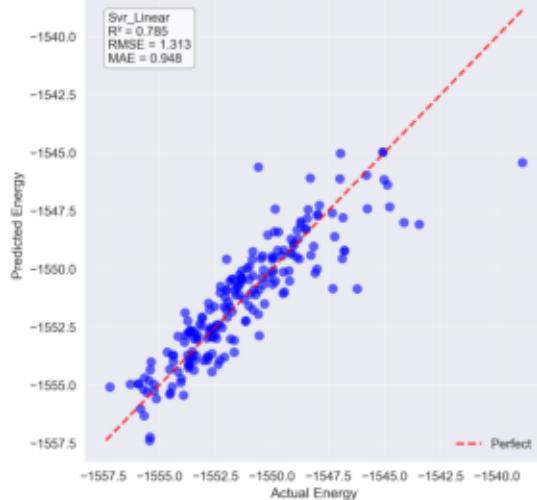


Model Stability (Lower is Better)

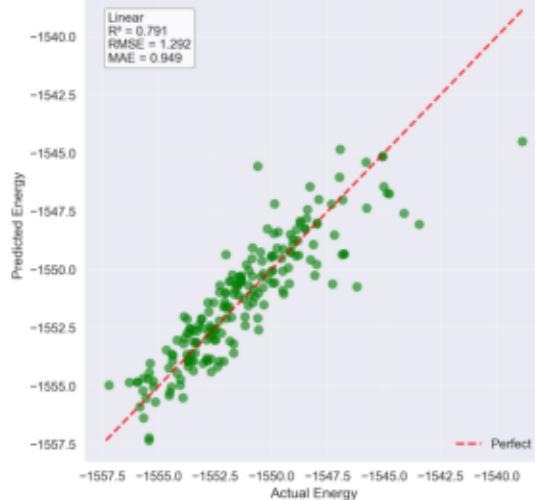


Combined Predictions Vs Actual

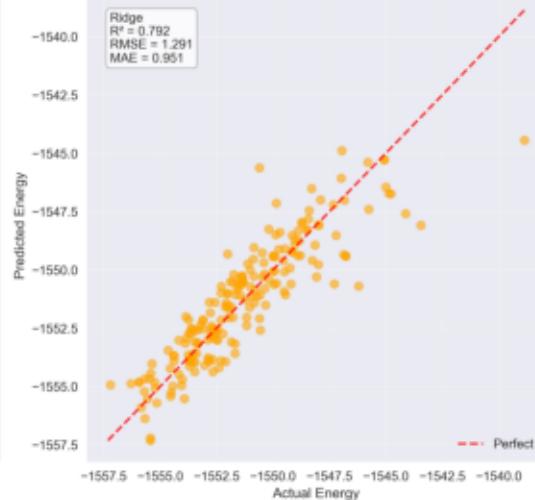
Svr_Linear Predictions



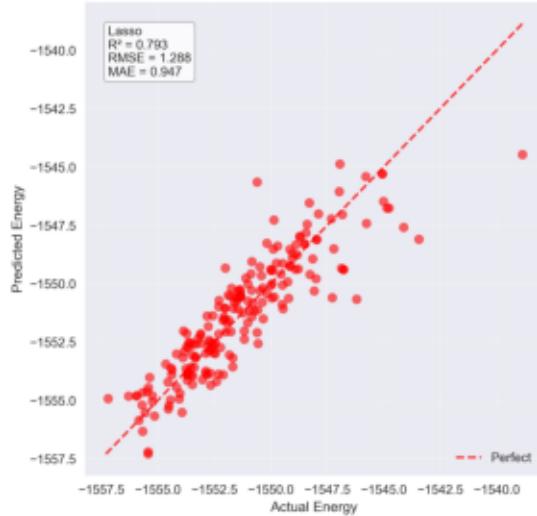
Linear Predictions



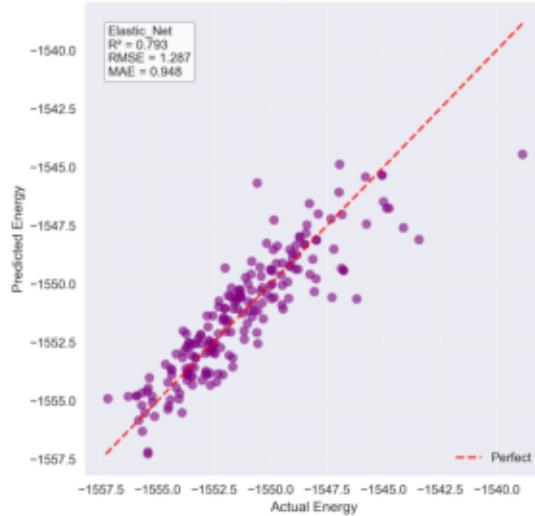
Ridge Predictions



Lasso Predictions

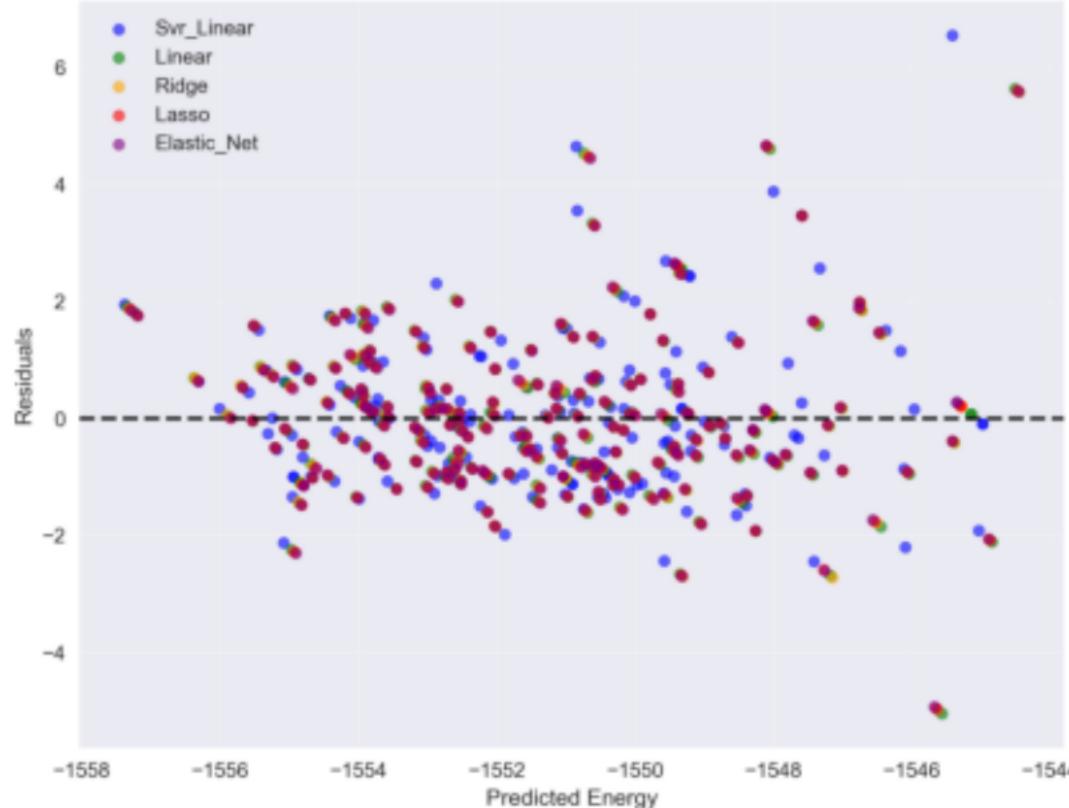


Elastic_Net Predictions

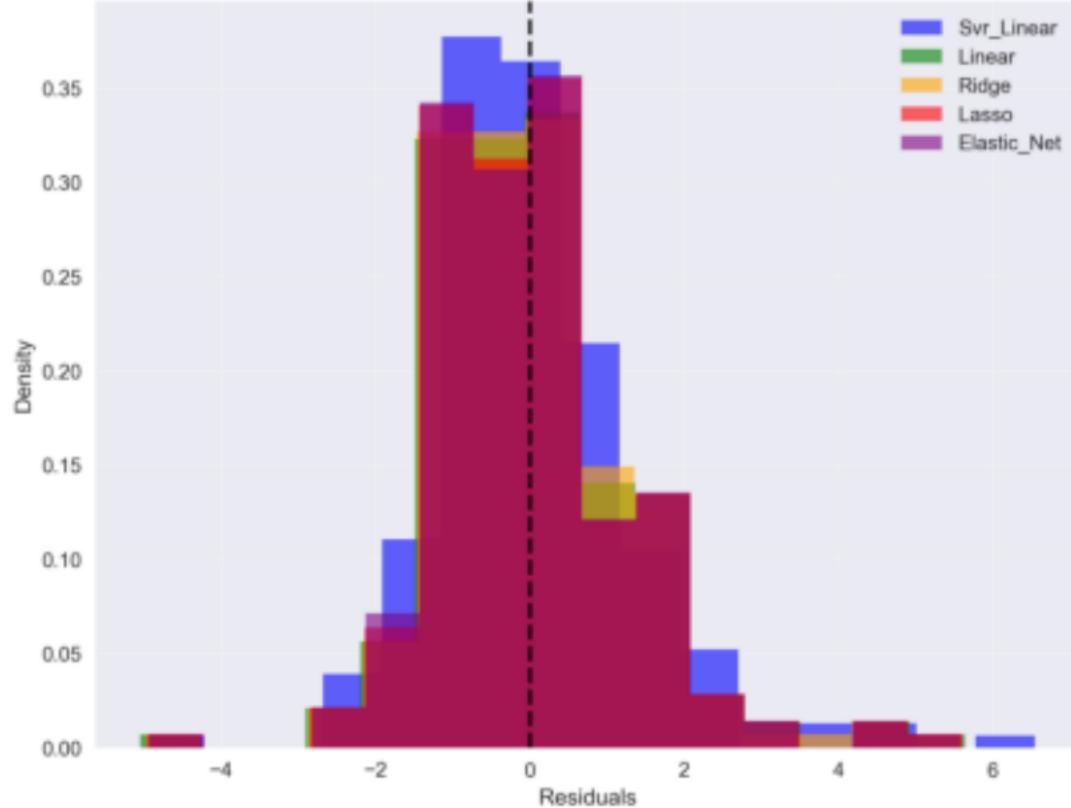


Combined Residual Analysis

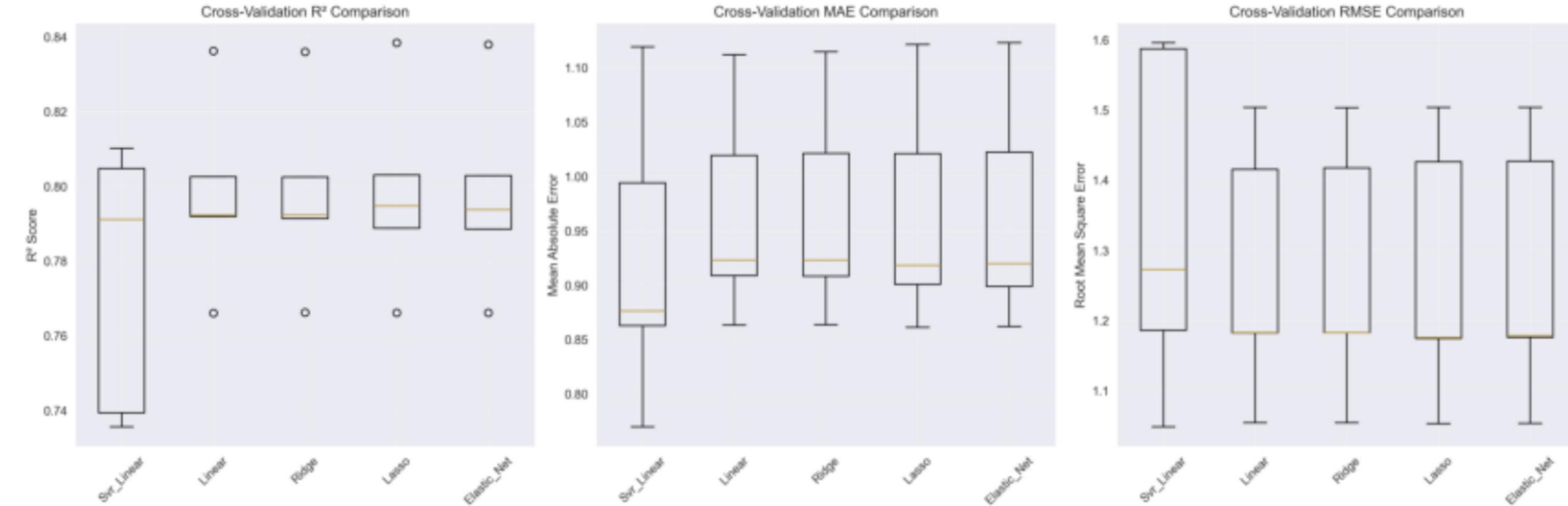
Combined Residuals vs Predicted



Combined Residuals Distribution

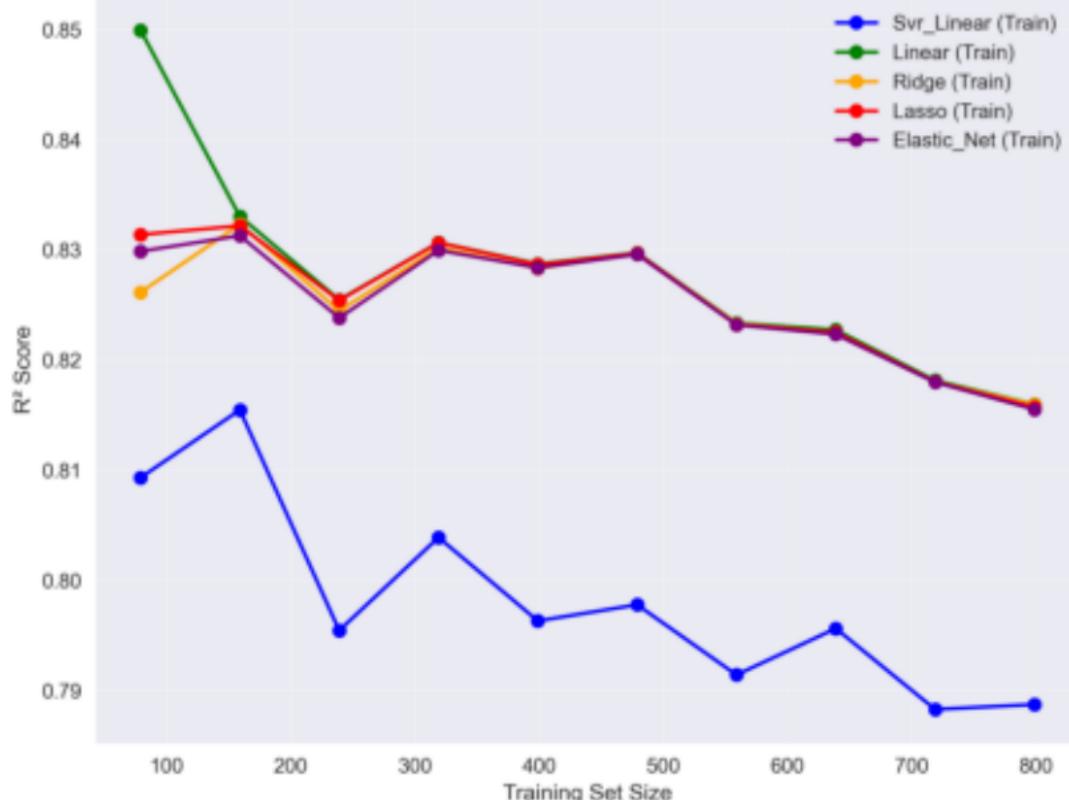


Combined Cv Comparison

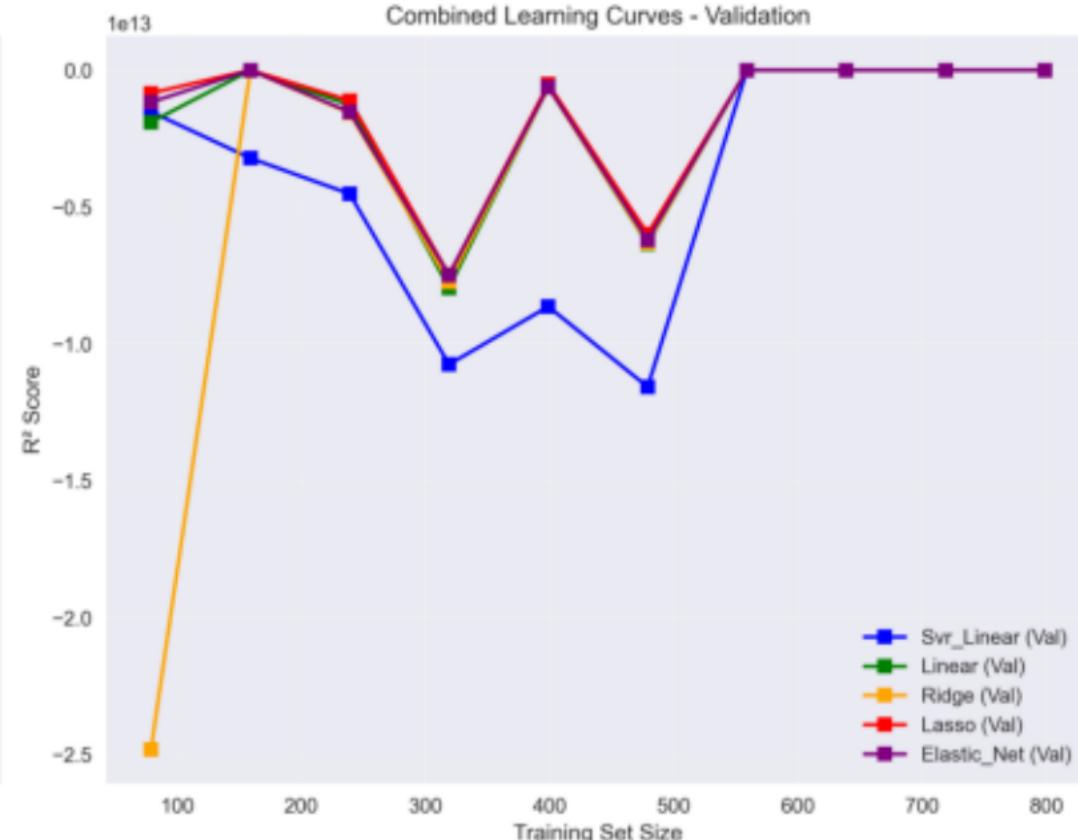


Combined Learning Curves

Combined Learning Curves - Training

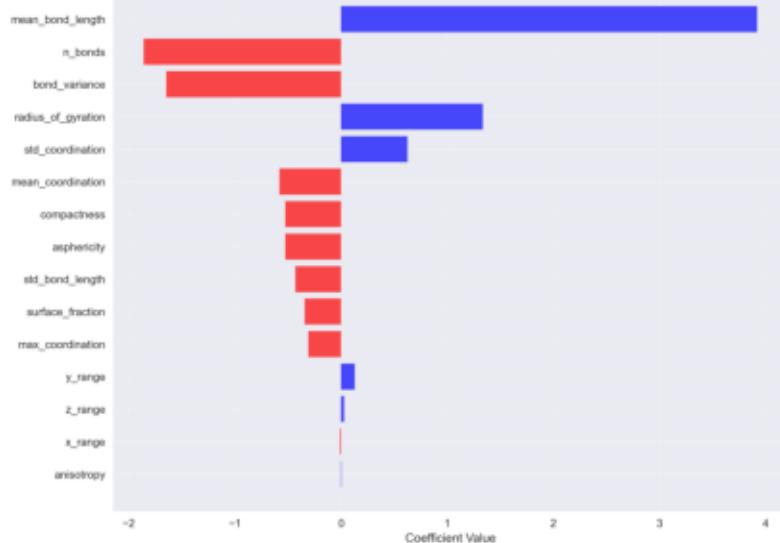


Combined Learning Curves - Validation

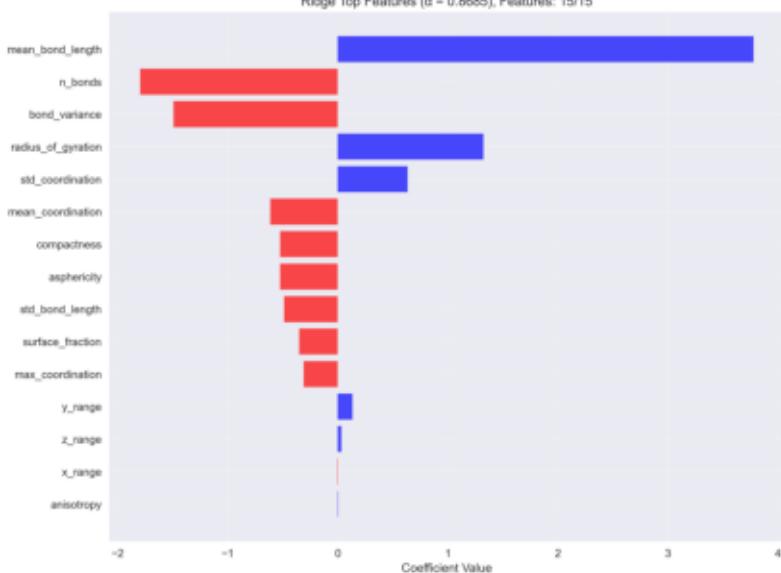


Feature Importance Comparison

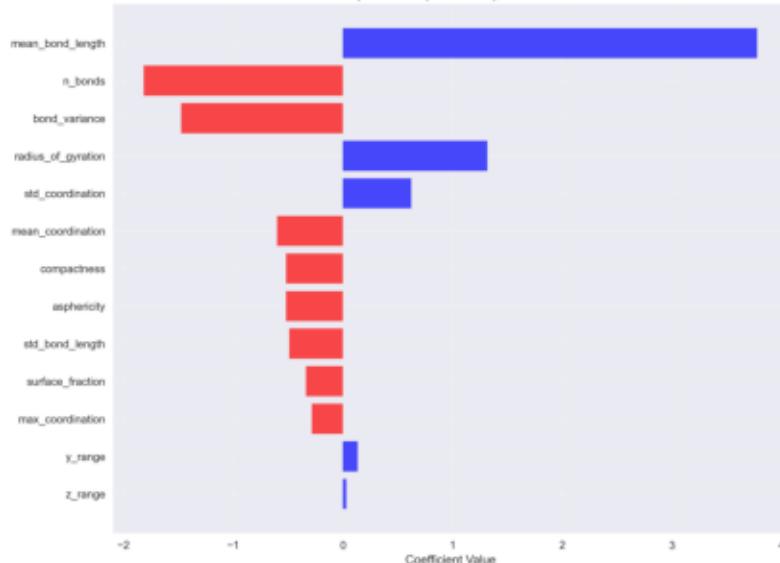
Linear Top Features



Ridge Top Features ($\alpha = 0.8685$), Features: 15/15



Lasso Top Features ($\alpha = 0.0037$), Features: 13/15



Elastic_Net Top Features ($\alpha = 0.0043$), Features: 13/15

