

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:

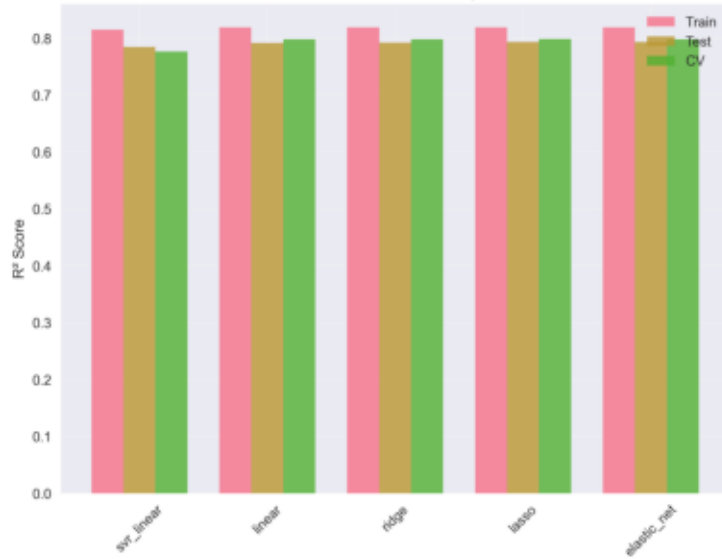
- Training samples: 799
- Test samples: 200
- Total features: 15
- SOAP features: 0

Best Model: Elastic Net

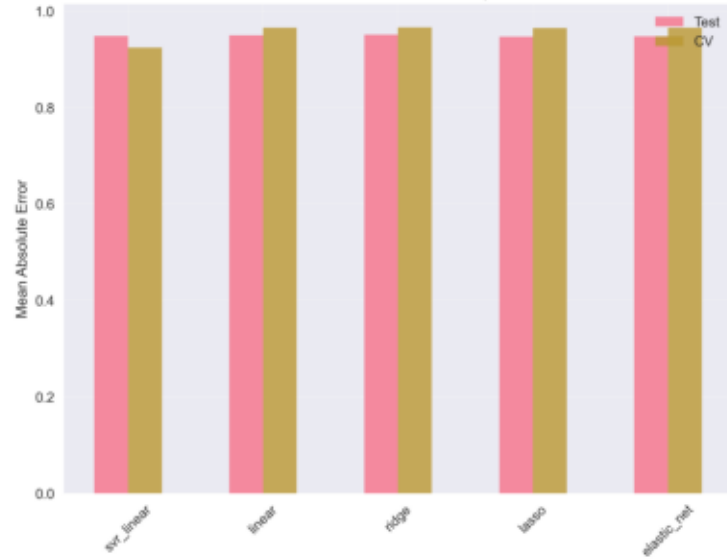
Best Test R^2 : 0.7930

Combined Model Comparison

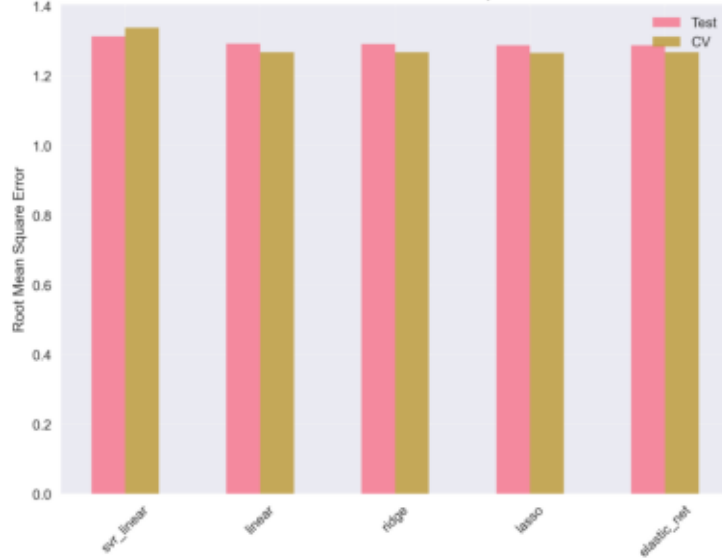
Model R² Performance Comparison



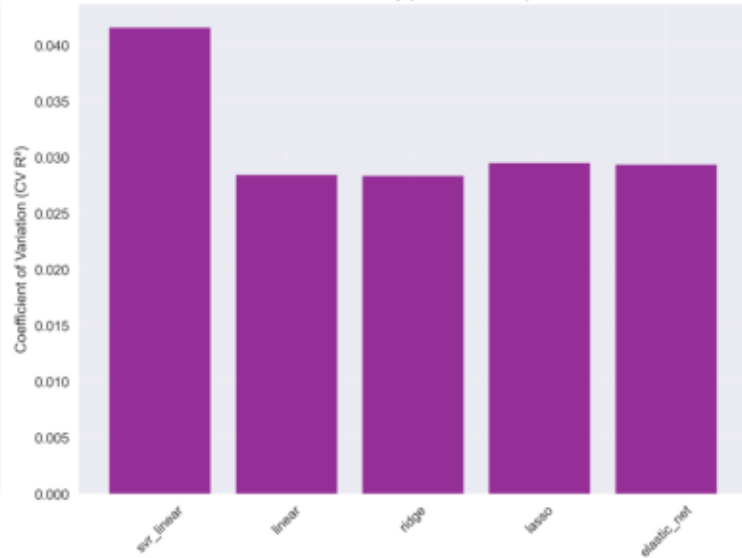
Model MAE Performance Comparison



Model RMSE Performance Comparison

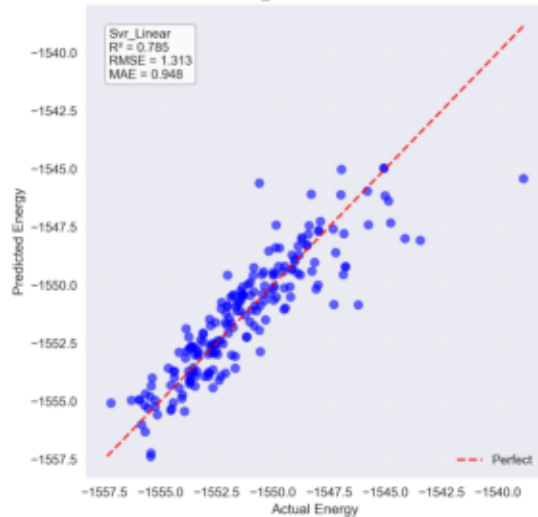


Model Stability (Lower is Better)

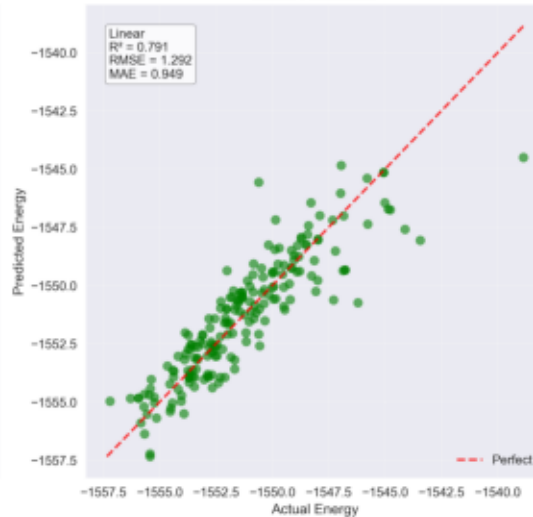


Combined Predictions Vs Actual

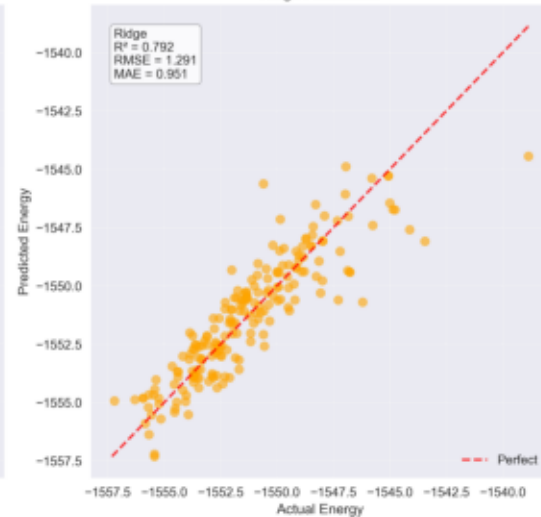
Svr_Linear Predictions



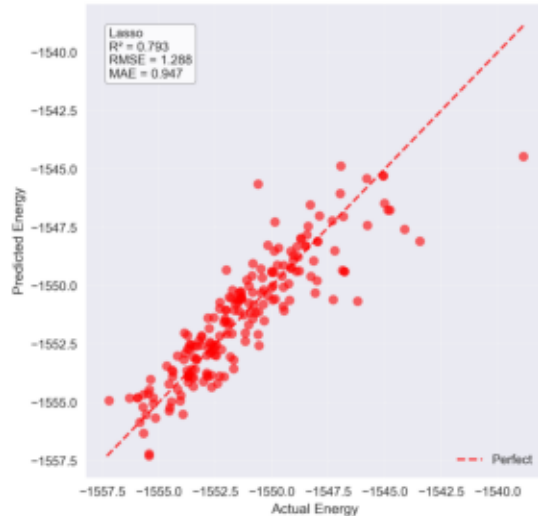
Linear Predictions



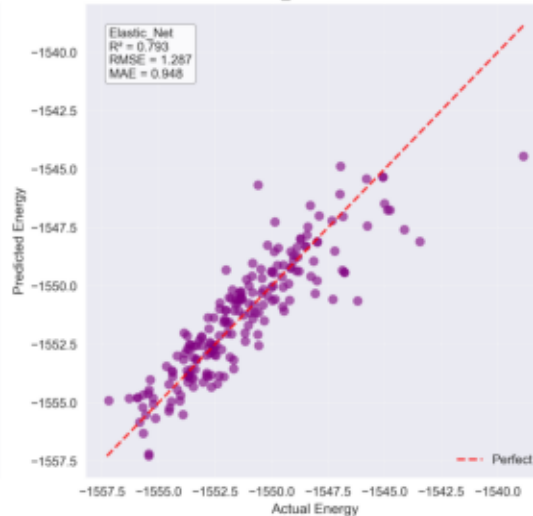
Ridge Predictions



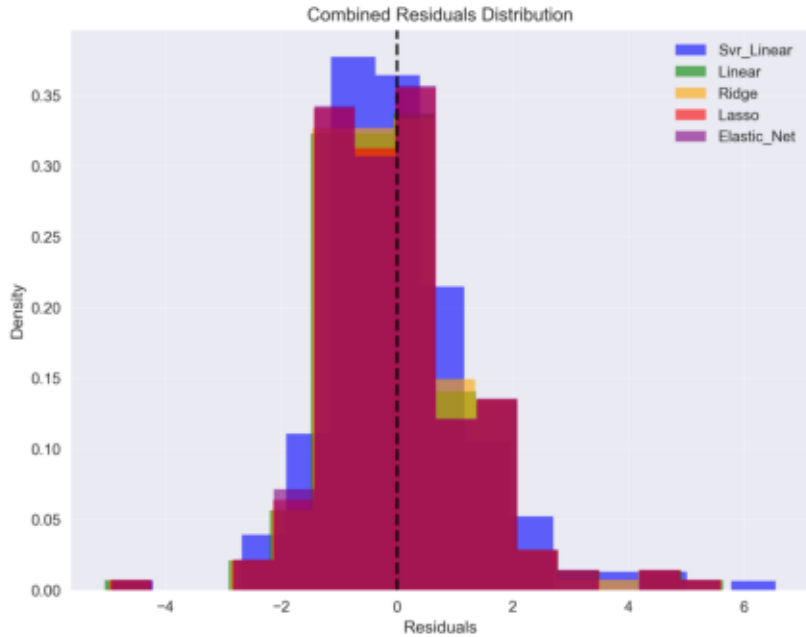
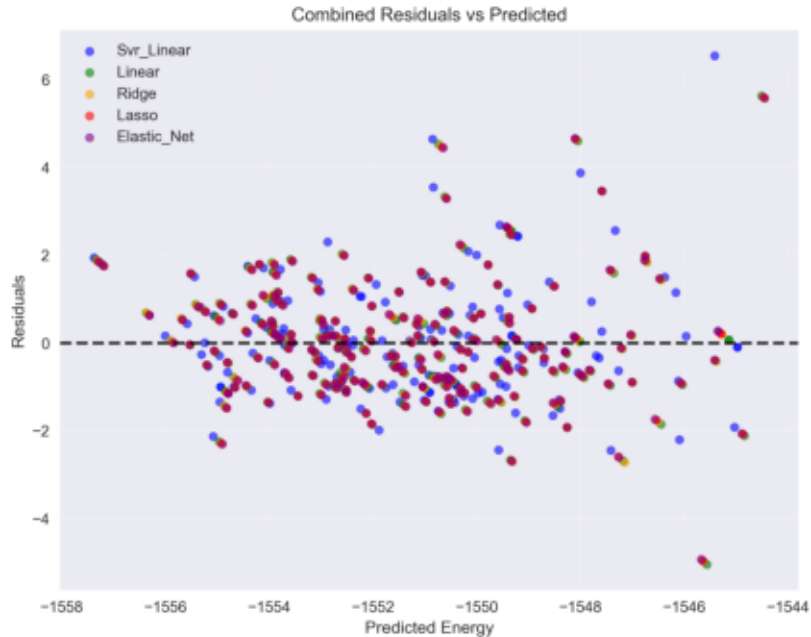
Lasso Predictions



Elastic_Net Predictions

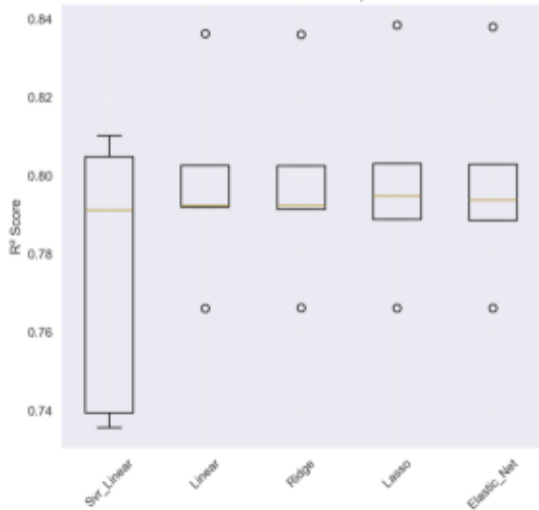


Combined Residual Analysis

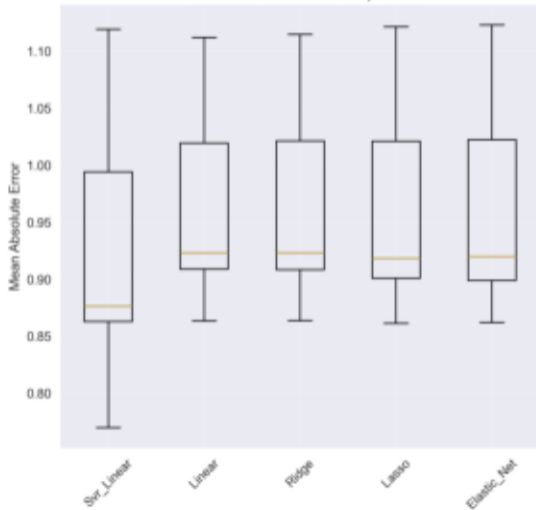


Combined Cv Comparison

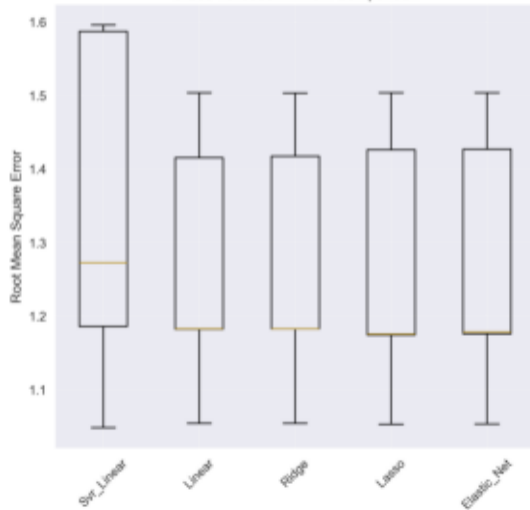
Cross-Validation R^2 Comparison



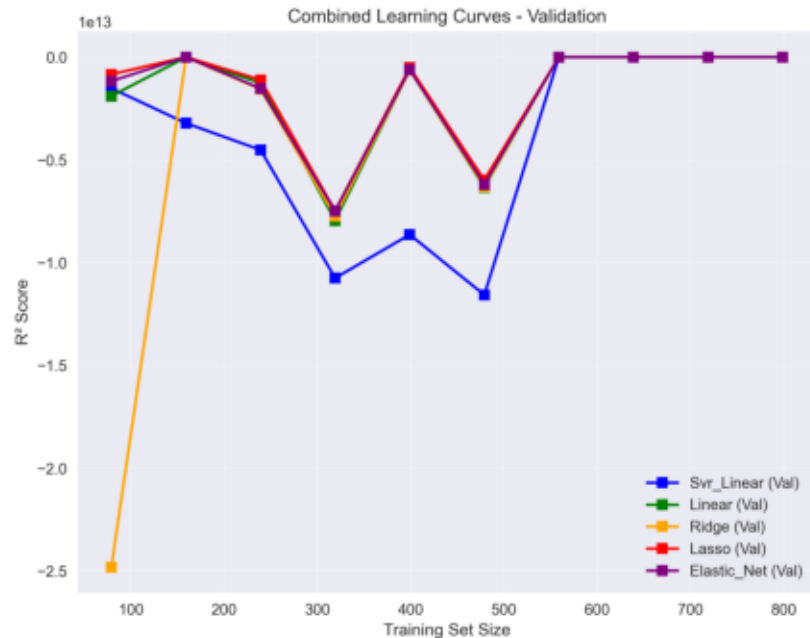
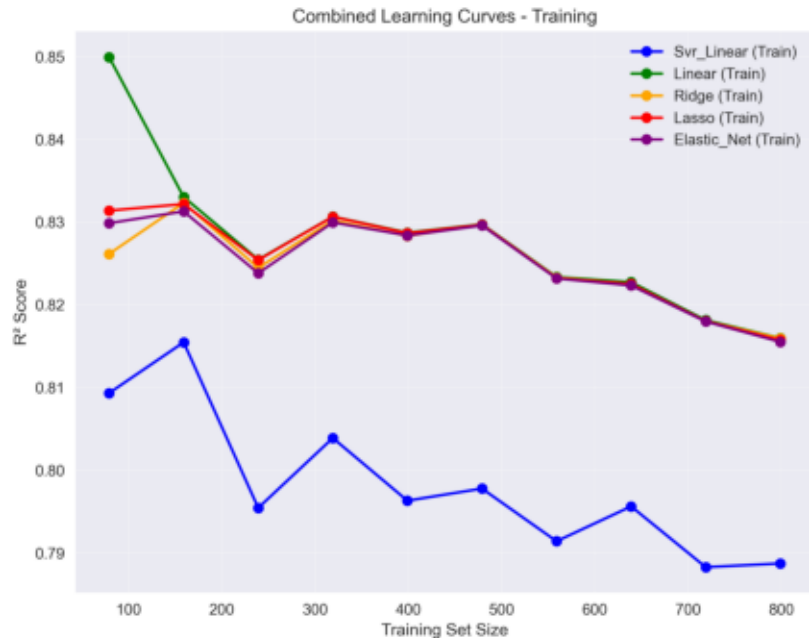
Cross-Validation MAE Comparison



Cross-Validation RMSE Comparison



Combined Learning Curves



Feature Importance Comparison

