Modeling Critical Temperatures of Superconductors

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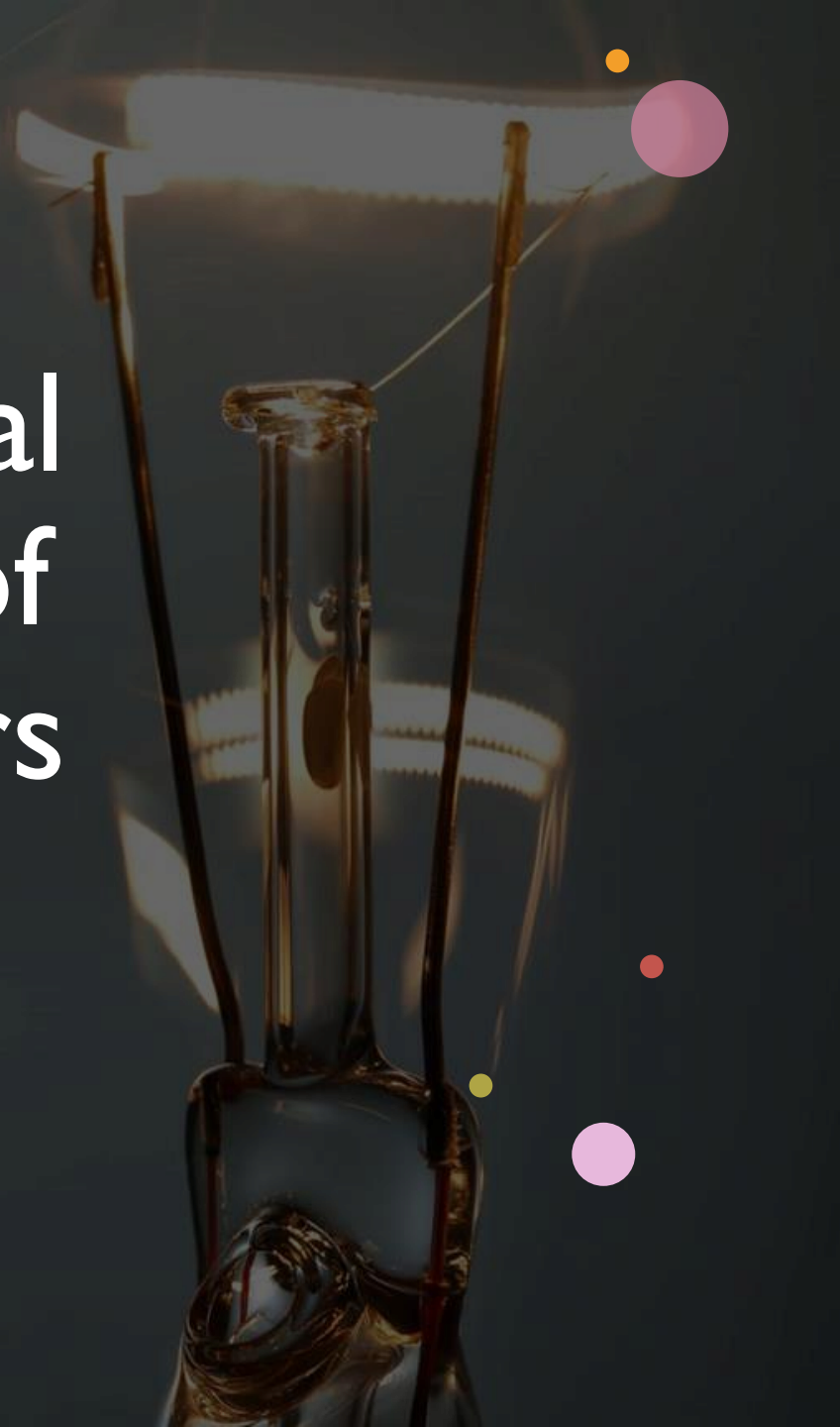
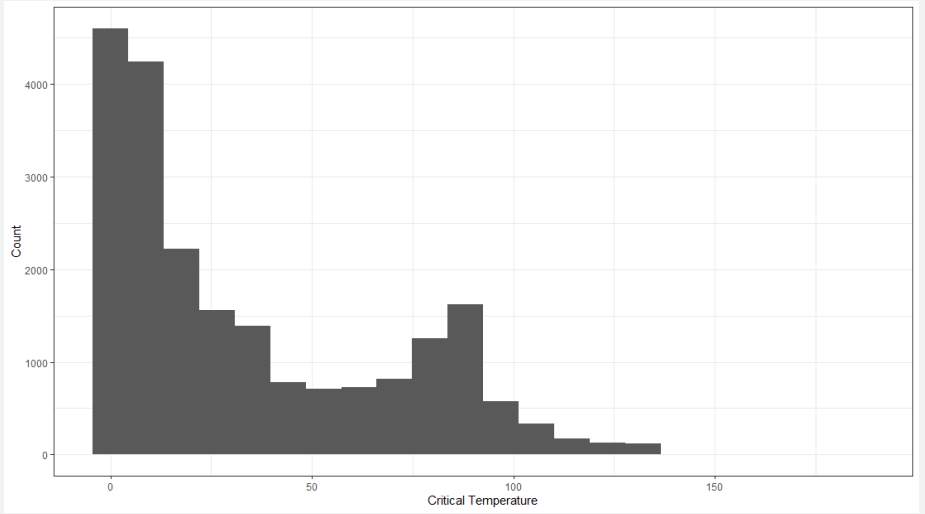
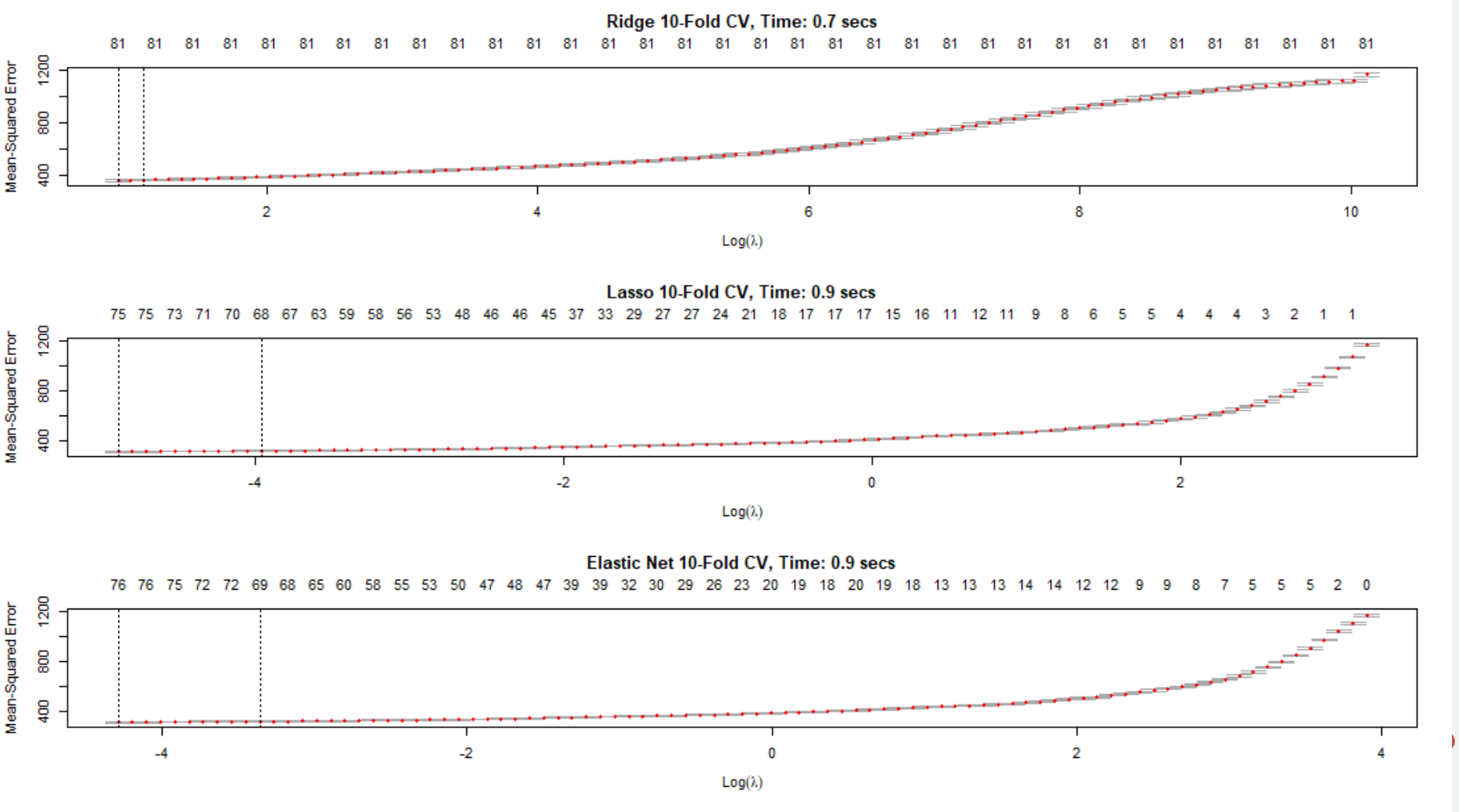


Background

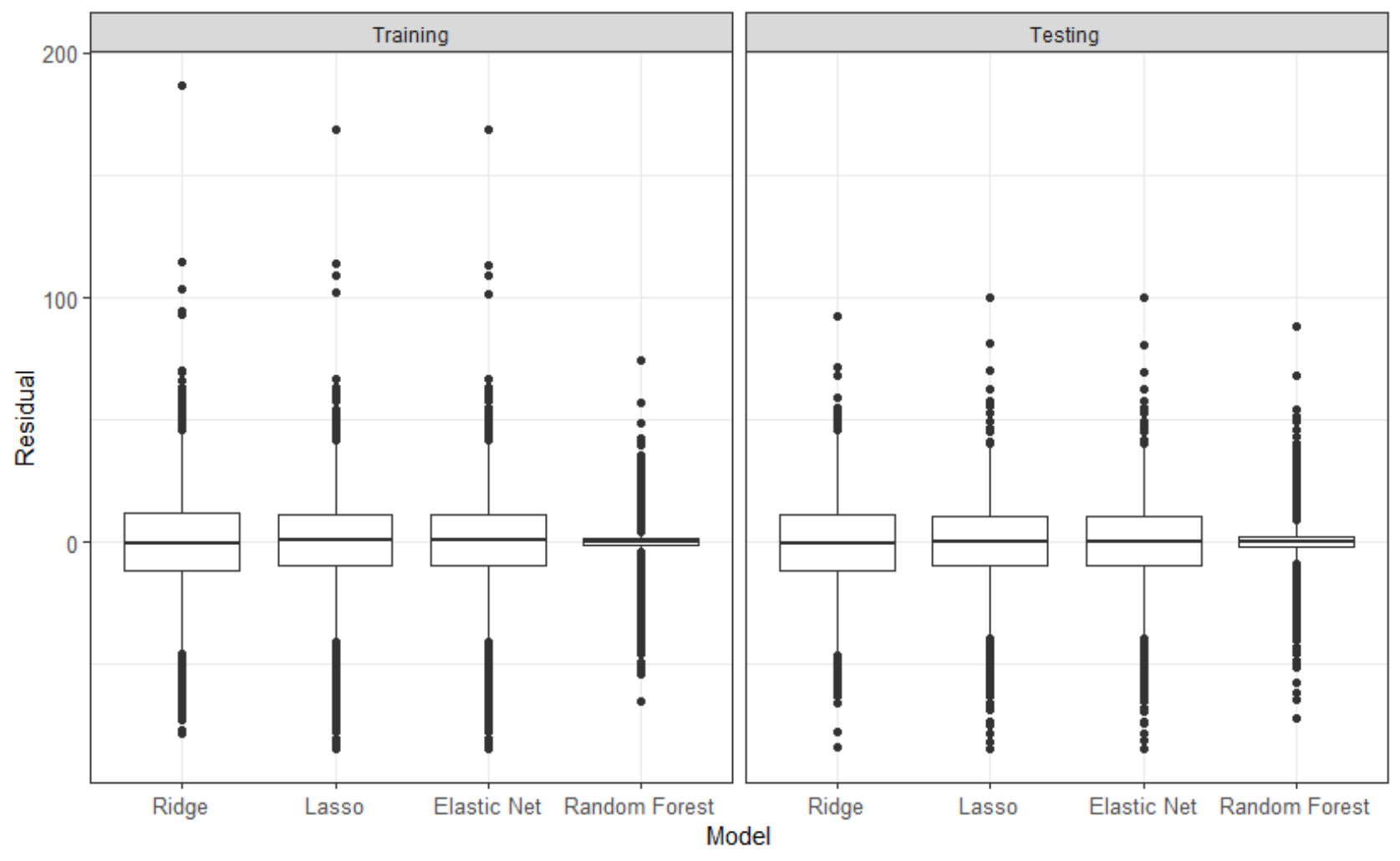
- 21263 different superconductors
- 81 features
  - Number of unique elements
  - Atomic mass
  - Atomic radius
- Response variable: superconductor's critical temperature
- Zero electrical resistance if cooled to critical temperature
- Most critical temperatures are very low
- Used in MRI machines, maglev trains, particle accelerators



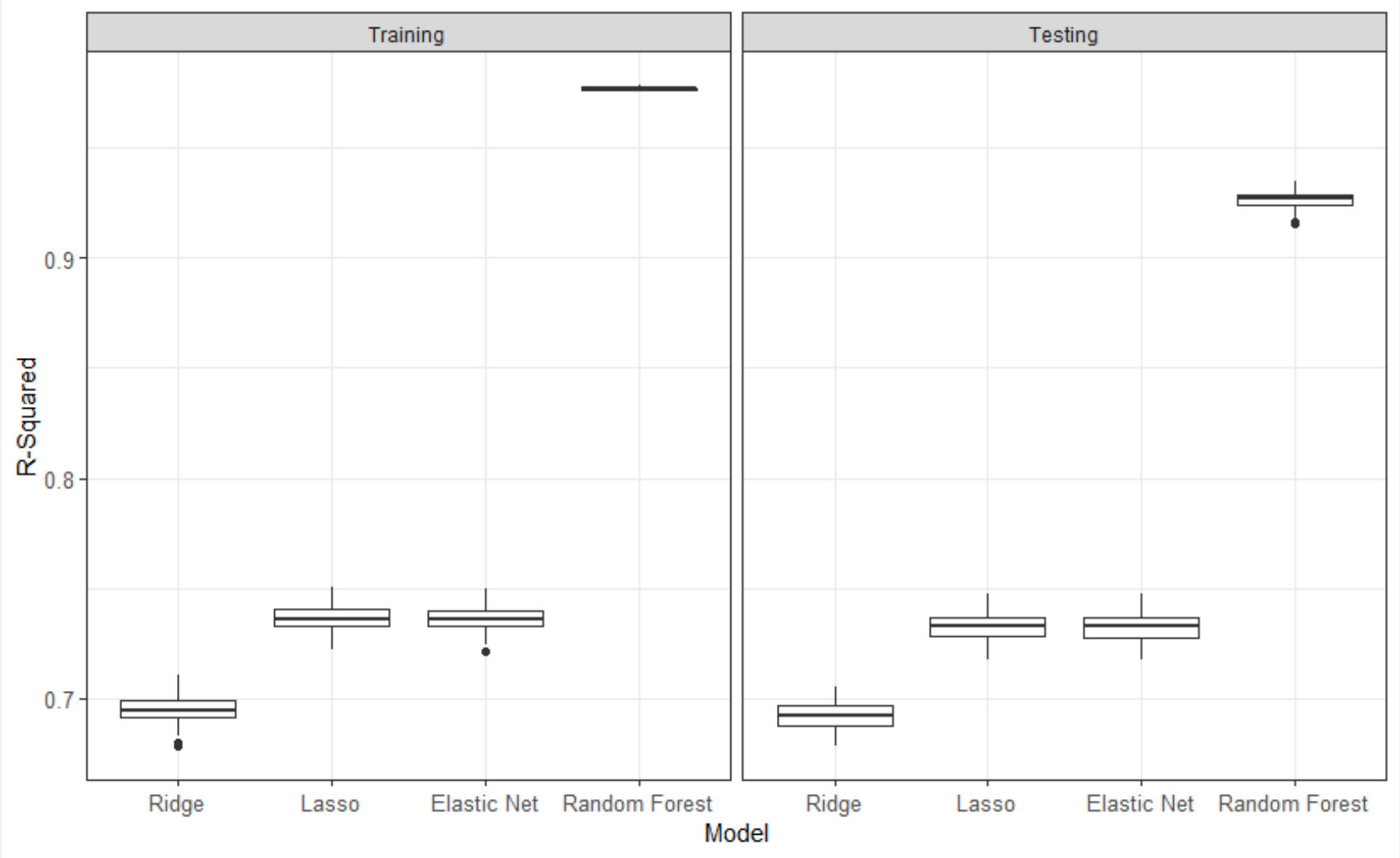
Cross Validation Curves



Residuals


Training
Testing
200
100
0
Residual
Ridge
Lasso
Elastic Net
Random Forest
Ridge
Lasso
Elastic Net
Random Forest
Model

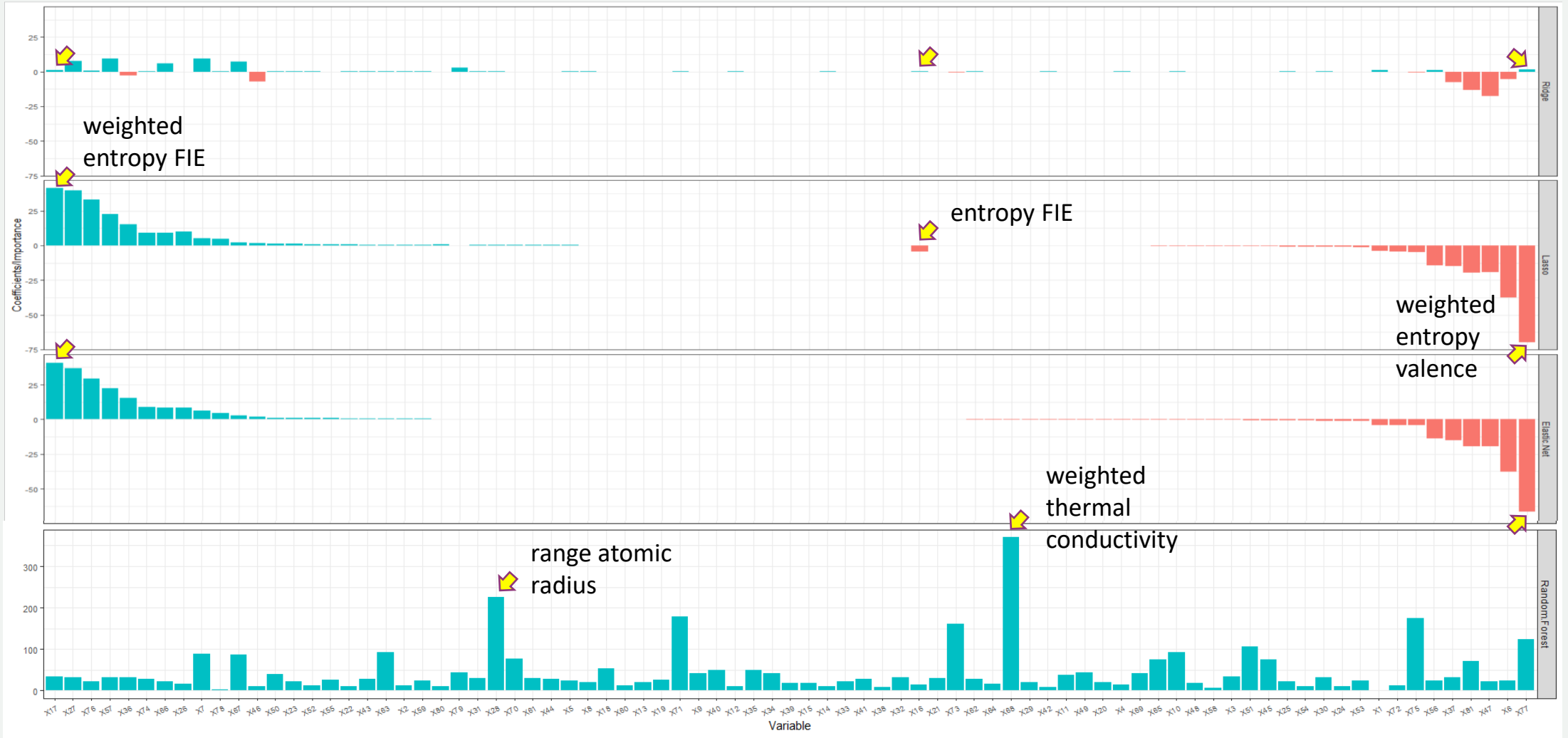
R-Squared


Training
Testing
R-Squared
0.9
0.8
0.7
Ridge
Lasso
Elastic Net
Random Forest
Ridge
Lasso
Elastic Net
Random Forest
Model

Intervals and Runtime

Model	90% Test R^2 Interval	Runtime on Entire Dataset
Ridge	0.68-0.70	1.4 secs
Lasso	0.72-0.74	1.3 secs
Elastic Net	0.72-0.74	1.2 secs
Random Forest	0.92-0.93	840 secs

Beta Coefficients and Importance



Conclusion

- Decision tree model performs much better than regression in predicting critical temps
- Huge tradeoff in time vs accuracy between tree-based and regression models
- Tradeoff not an issue once a model is developed
- These models cannot predict if a material is a superconductor

Questions?

https://github.com/allenwuny/superconductor_temp