Superconductivity

Predicting the Critical Temperature of a Superconductor

## presented by

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1. Introduction

This study evaluated features that were extracted from materials to predict the critical temperature of a superconductor. These predictions aren’t for determining whether something is a superconductor but rather what the critical temperature is for superconductors. Features extracted include thermal conductivity, atomic radius, atomic mass, electron affinity, and valence. The dataset is very impressive with having tens of thousands of rows of data.

1. Prediction Accuracy

The model used an XGBoost regression. The top characteristics that influenced the accuracy of predicting critical temperature were listed above. Additional features were present but didn’t have as much of a significant impact. A base model was constructed and with minimal data and feature engineering, a root mean squared error was about 9.3 Kelvin. Then, using GridSearchCV, a handful of hyperparameters were brute force tuned to improve the models performance. This new model did demonstrate an improvement of a root mean squared error of 8.86 Kelvin. The predictions compared to the actuals for each model are shown here:

|  |  |
| --- | --- |
| First Model | Enhanced Model |
| A graph of a graph with red and blue lines  AI-generated content may be incorrect. | A graph with red and blue lines  AI-generated content may be incorrect. |
|  |  |

Although the two models don’t appear to be that different, the problem is that more than half of the data has a superconducting temperature less than 80 Kelvin. Meaning, with the better model an error of more than 10% can occur on more than half of the materials. The small improvement from the first model to the second model, albeit small, is impactful proportionally speaking.

Since the second model was a search of autotuning hyperparameters, it took significantly longer to run than the base model.

1. Python Notebooks

Below are Github Gist links to the notebooks we used during this case study:

1. Implications

The critical temperature of superconductors can be comfortably predicted using the second model established. Further tuning of the hyperparameters could yield an even better predictions. Something also to take note of with the data, some materials were only sampled once while others were sampled numerous times. Repeated sampling and measurement of these singular materials would increase the confidence in predicting its critical temperature.