Copper Alloy Discovery using Machine Learning

Supervised by Prof. Nick Birbilis

COMP4560 - Advanced Computing Project

Presentation by Abhinav Pandey

Outline

- Introduction
- ML Model Selection
  - For Tensile Strength Prediction
  - For Thermal Conductivity Prediction
- Smart Alloy Generation System (SAGS)
- Results
- Limitations and Future Work
- Alloy Generation Demo

Introduction

Copper alloys

- Very versatile
- Can have properties like high tensile strength, thermal conductivity
- More than 500 alloys already exist

Motivation for the project?

- Conventional development of new alloys –
  - depends on Expert judgement
  - depends on Trial and Error
  - Is time **consuming** and **expensive**

There is a need for a reliable "property-based" alloy composition recommendation system.

The Smart Alloy Generation System

Takes user input :

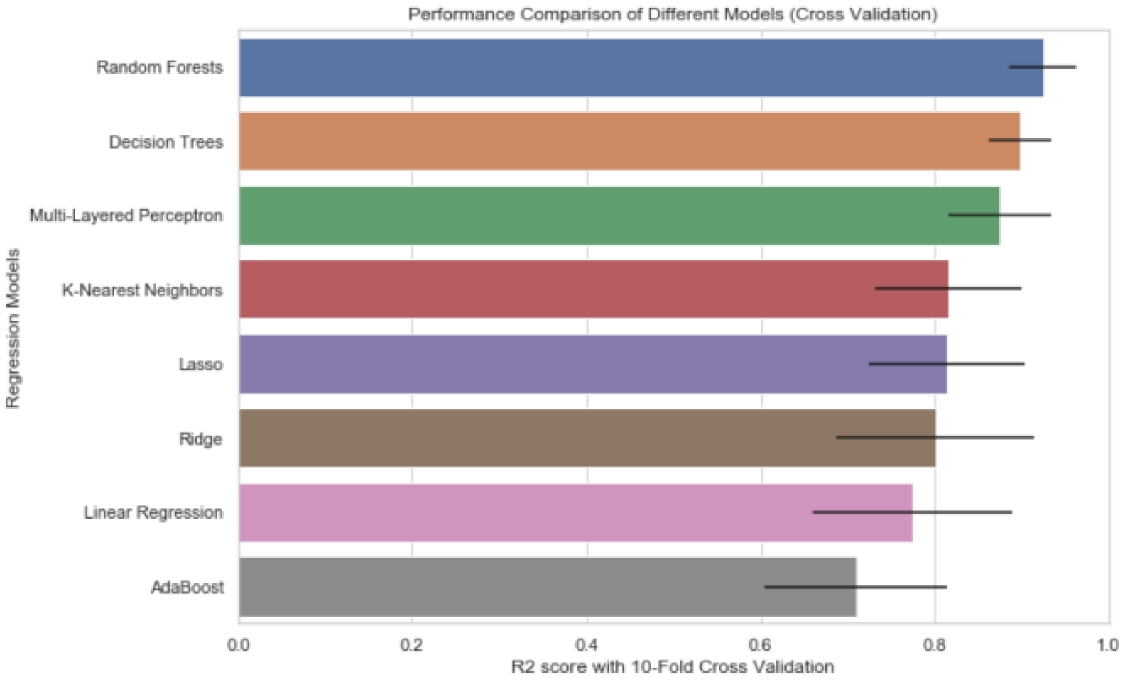
1. Alloy property (*Tensile Strength* or *Thermal Conductivity*)
2. Magnitude of selected property

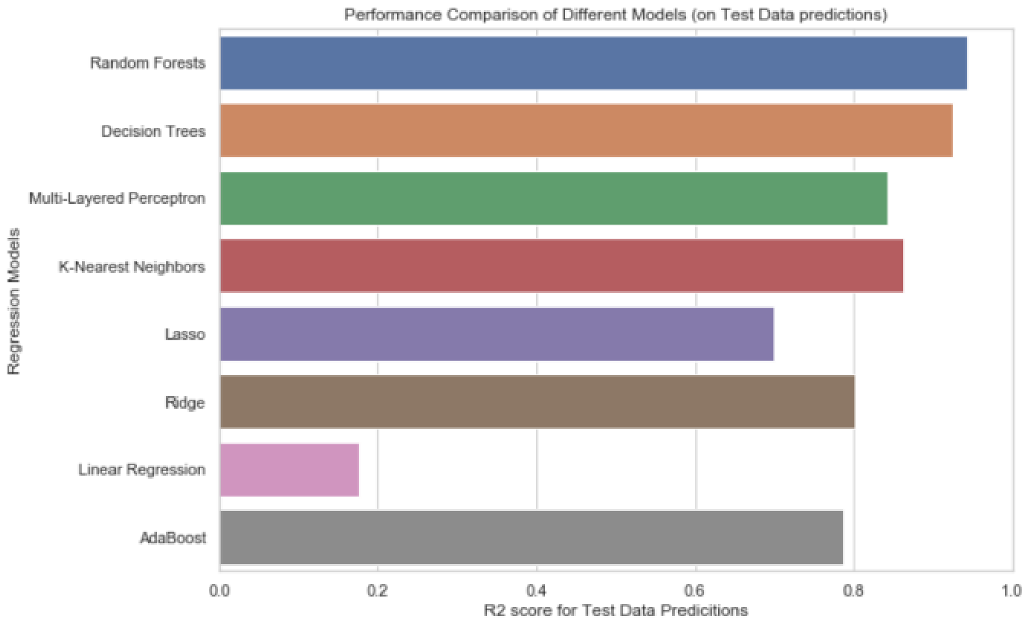
Returns :

1. Alloy compositions
2. Processing Conditions (for tensile strength based alloy recommendations)

How? Using Machine Learning!

Tensile Strength prediction model

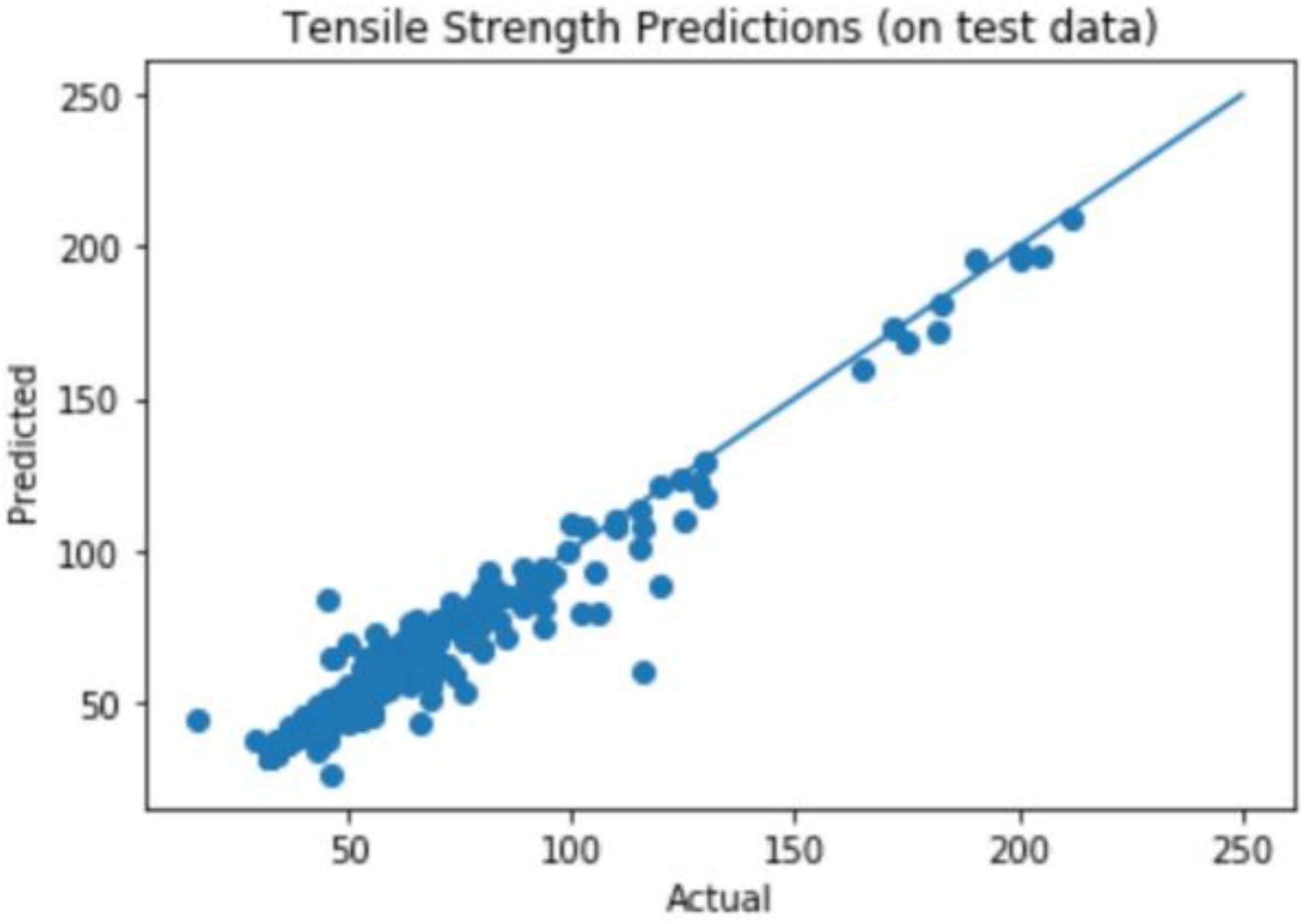




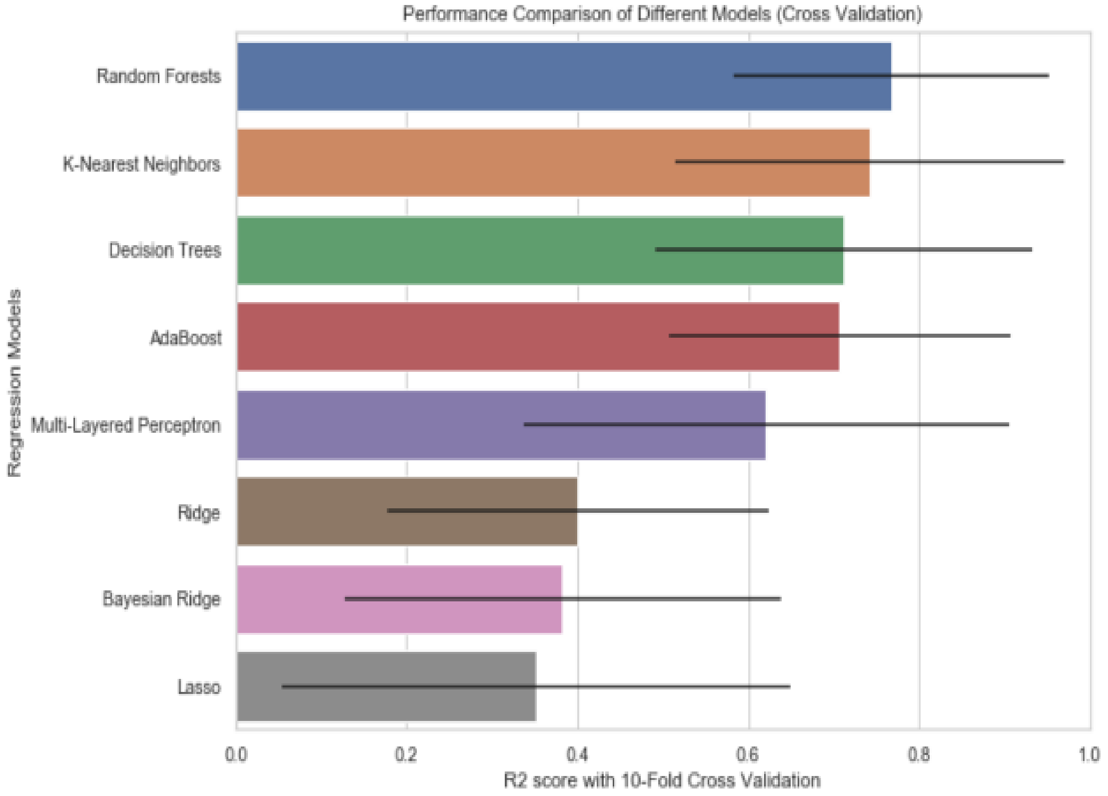
Prediction Quality
(Tensile Strength)

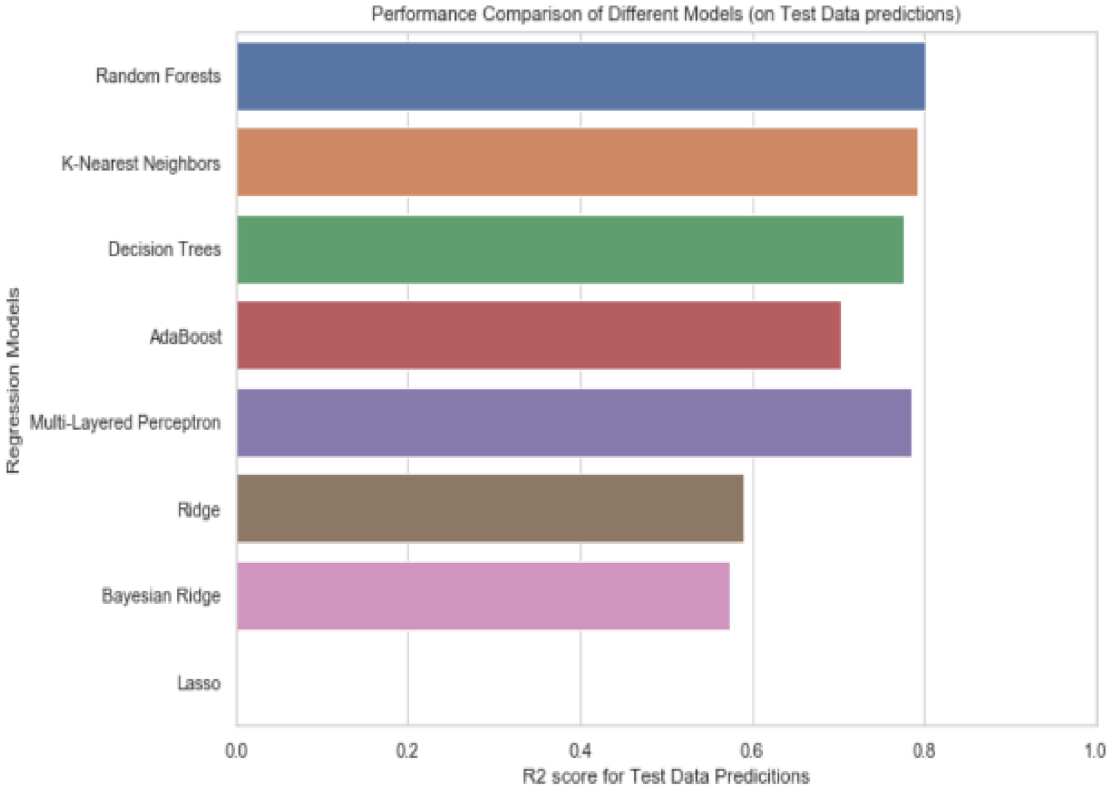
10-Fold Cross-Validation Performance = 92.55 %

Accuracy on Unseen Data = 93.85%

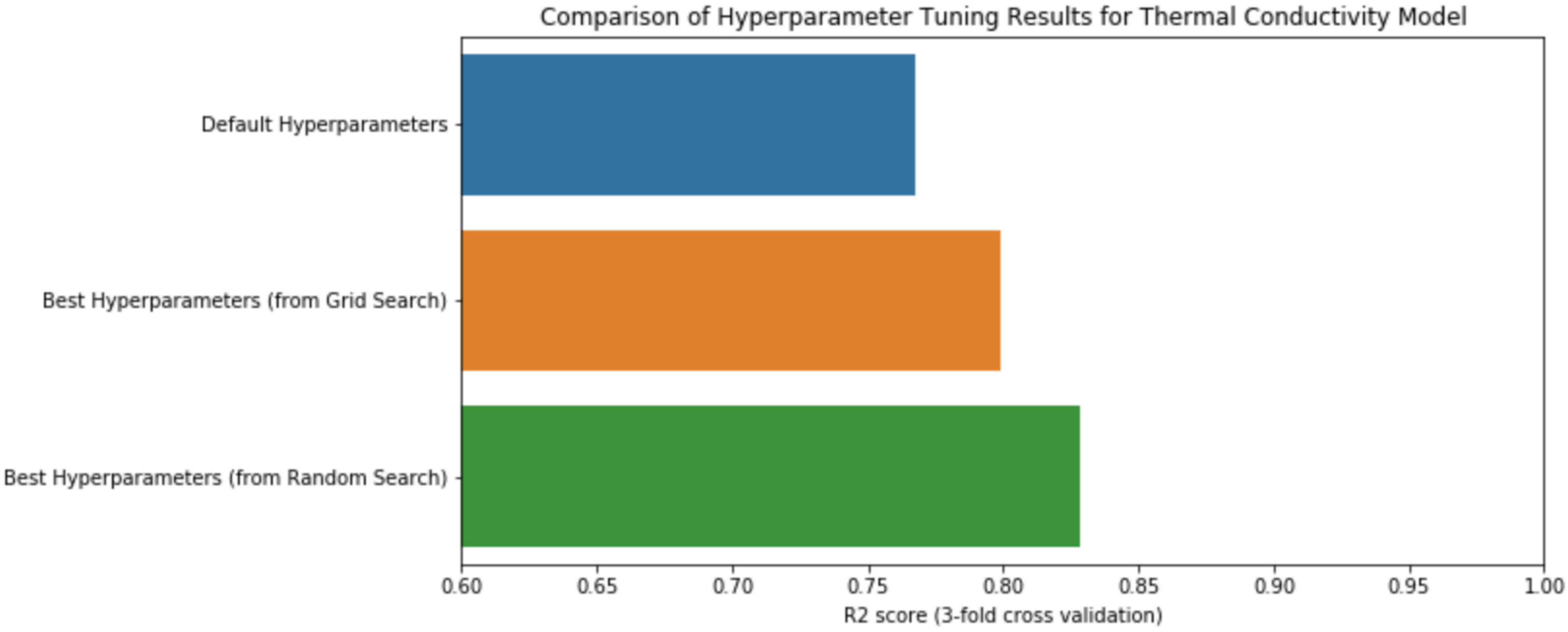


Thermal Conductivity prediction model





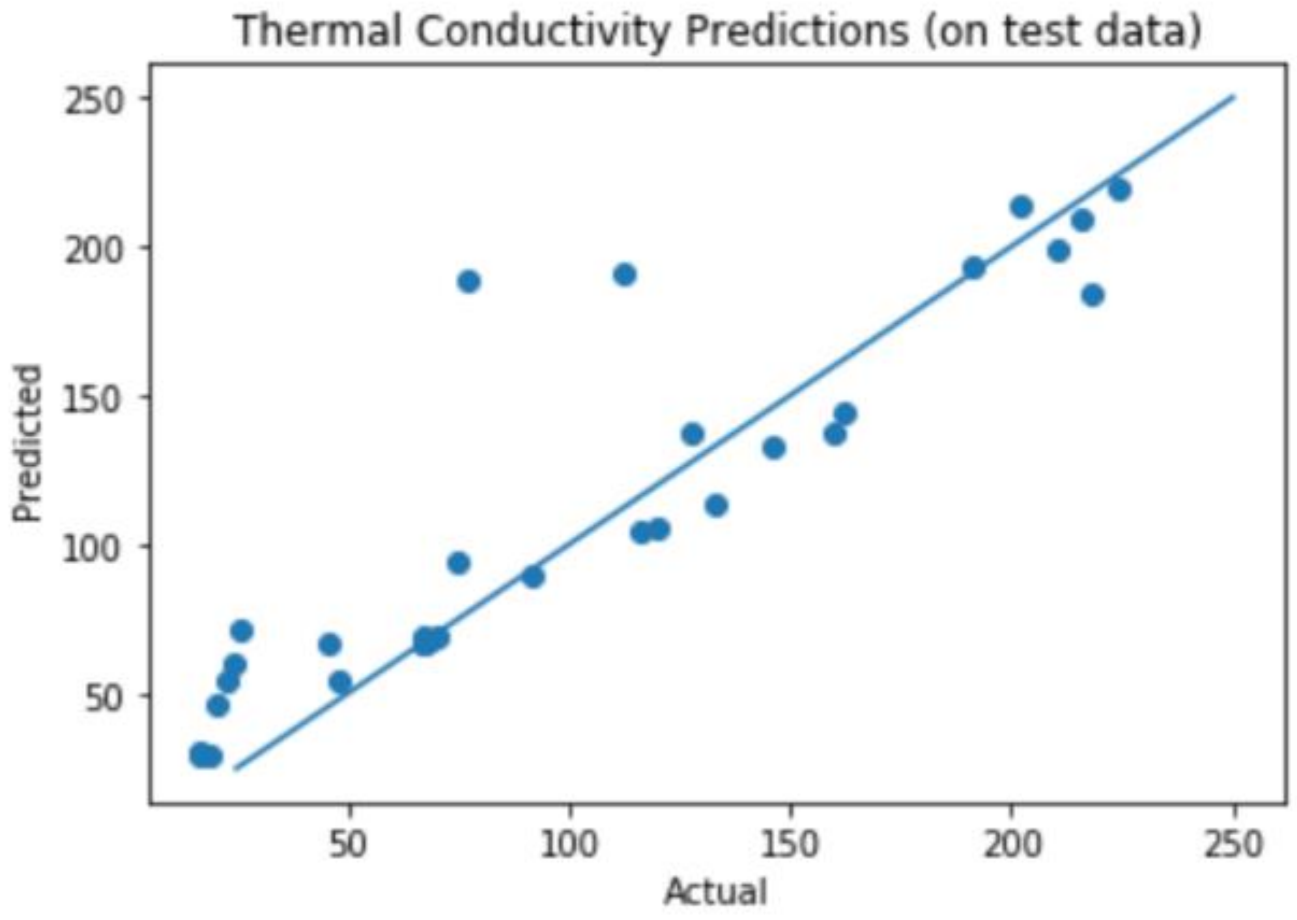
Hyperparameter Optimization



Prediction Quality
(Thermal Conductivity)

10-Fold Cross-Validation Performance = 82.26 %

Accuracy on Unseen Data = 83.17%



Smart Alloy Generation System Flowchart

START

Does our data already have an alloy with the desired value?

YES

Proceed to add that alloy to the results (indicating 100% confidence)

NO

Select top n alloys with property values closest to the desired value

GENERATE NEW DATA

Generate unique permutations of the selected samples

MAKE PREDICTIONS ON GENERATED DATA

Use the relevant model to make predictions of the relevant property values for the generated data.

RETURN BEST SAMPLES

Return the compositions of the alloys with the predicted values closest to the value specified

SAVE THE RECOMMENDATIONS IN A CSV FILE

Example of Promising Result

Inputs:

- Property = Tensile Strength
- Property Magnitude = 78.5

- Tensile Strength of Recommended alloy = 80

Confidence %	Form	Temper	Cu	Pb	Zn	Fe	P	Ni	Sn
100	wire	Precipitation Heat Treated or Spinodal Heat Treated and 1/2 Hard	97.55	0.6	0.05	0.05	0.2	1.5	0.05
100	strip	Extra Hard	88.5	0.05	10.96	0.03	0.06	0.8	0.7
92.5	products	Extra Hard	97.377	0.054	0.311	0.132	0.215	0.159	1.751
92.5	products	Extra Hard	96.594	0.051	0.051	0.051	0.203	1.017	2.034

C50580

Chemical Composition

	Element						
	Cu(1)	Pb	Sn	Zn	Fe	P	Ni
Min (%)			1.0		0.05	0.01	0.05
Max (%)	Rem	0.05	1.7	0.30	0.20	0.35	0.20

Limitations

- The system is most reliable when the specified value lies in the range of the training data values, for both physical properties.

  For instance, if we search for alloy compositions with tensile strength = 250 ksi, then the recommended alloys have an actual value of only 212 ksi.

- The recommended alloys can only have the elements which are present in the training data. Since, the training data does not contain alloys with Carbon (which have shown to result in high tensile strength alloys), the recommendations do not have Carbon based alloys.

- Due to the small size of the dataset for thermal conductivity it is hard to say if the datapoints are a good representative sample of all copper alloys (More alloy data needs to be added)

Questions?