Predicting the Critical Temperature of Superconductors

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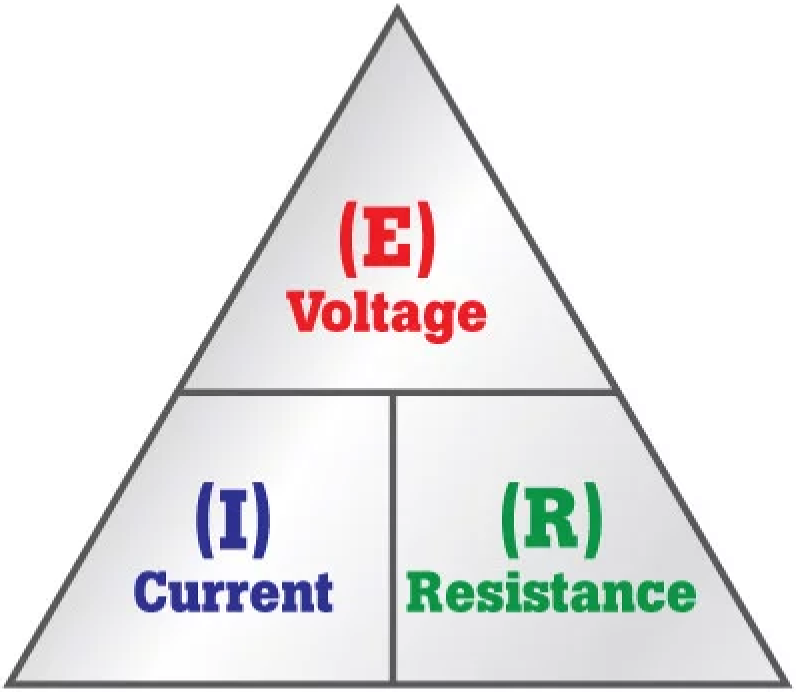
Objective

- Creating a predictive model for the critical temperature of superconductors.
- Data Source:
  - UCI Machine Learning Repository database of superconductors and extracted properties (http://archive.ics.uci.edu/ml/datasets/Superconductivty+Data)

What is a Superconductor?

- Superconductor are materials with zero resistance
- With zero resistance, an electronic current can be maintained
  - without external voltage
  - indefinitely

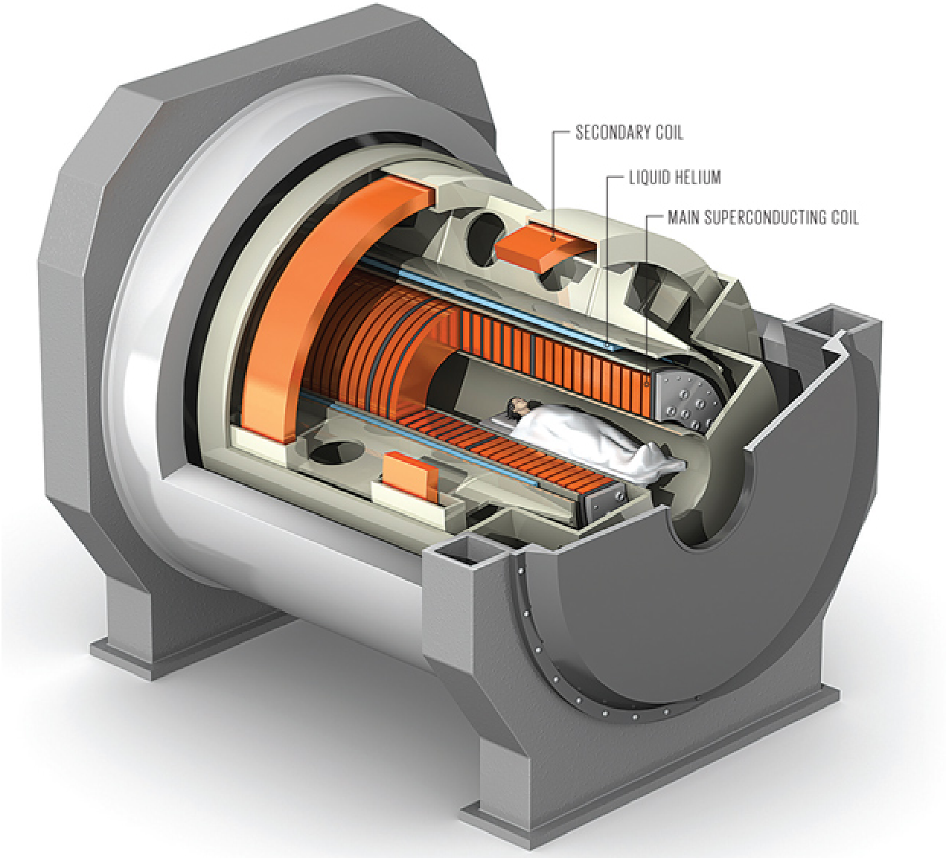


Source:https://www.fluke.com/en-us/learn/best-practices/measurement-basics/electricity/what-is-ohms-law

Applications for Superconductors

- Superconducting magnet in Magnetic Resonance Imaging (MRI)
- Superconducting coils in the Large Hadron Collider
- Superconductors could replace components in electronic powered systems [1]

MRI machine

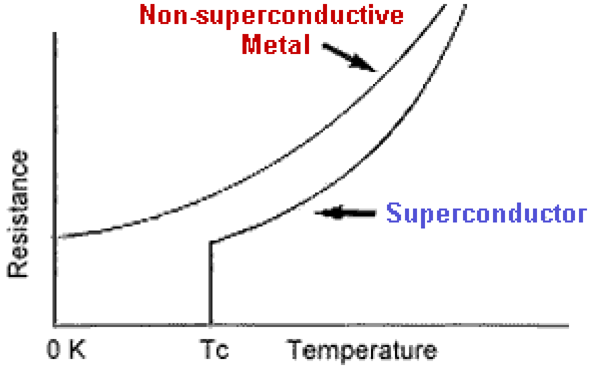


Source: https://phys.org/news/2013-10-world-powerful-mri-online.html

[1] W. V. Hassenzahl, et. al. *Proceedings of the IEEE*, **92 (**10),1655-1674, 2004

Critical Temperature

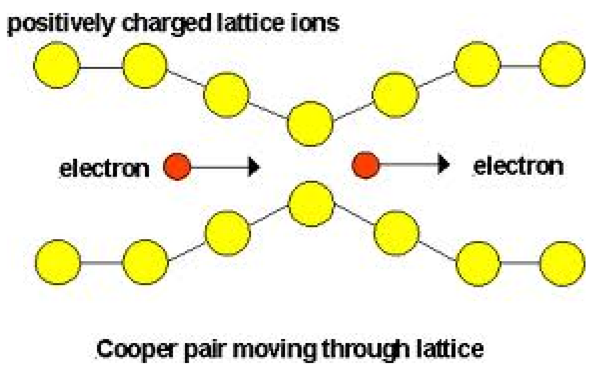
- Superconductivity can only be maintain below a certain temperature.
- This is called the critical temperature.
- Superconductors have to refrigerated in order to maintain superconductivity in, for example,
  - Liquid Helium (4 K)
  - Liquid Nitrogen (77 K)



Source: http://www.superconductors.org/tc_graph.gif

Superconductor Theory

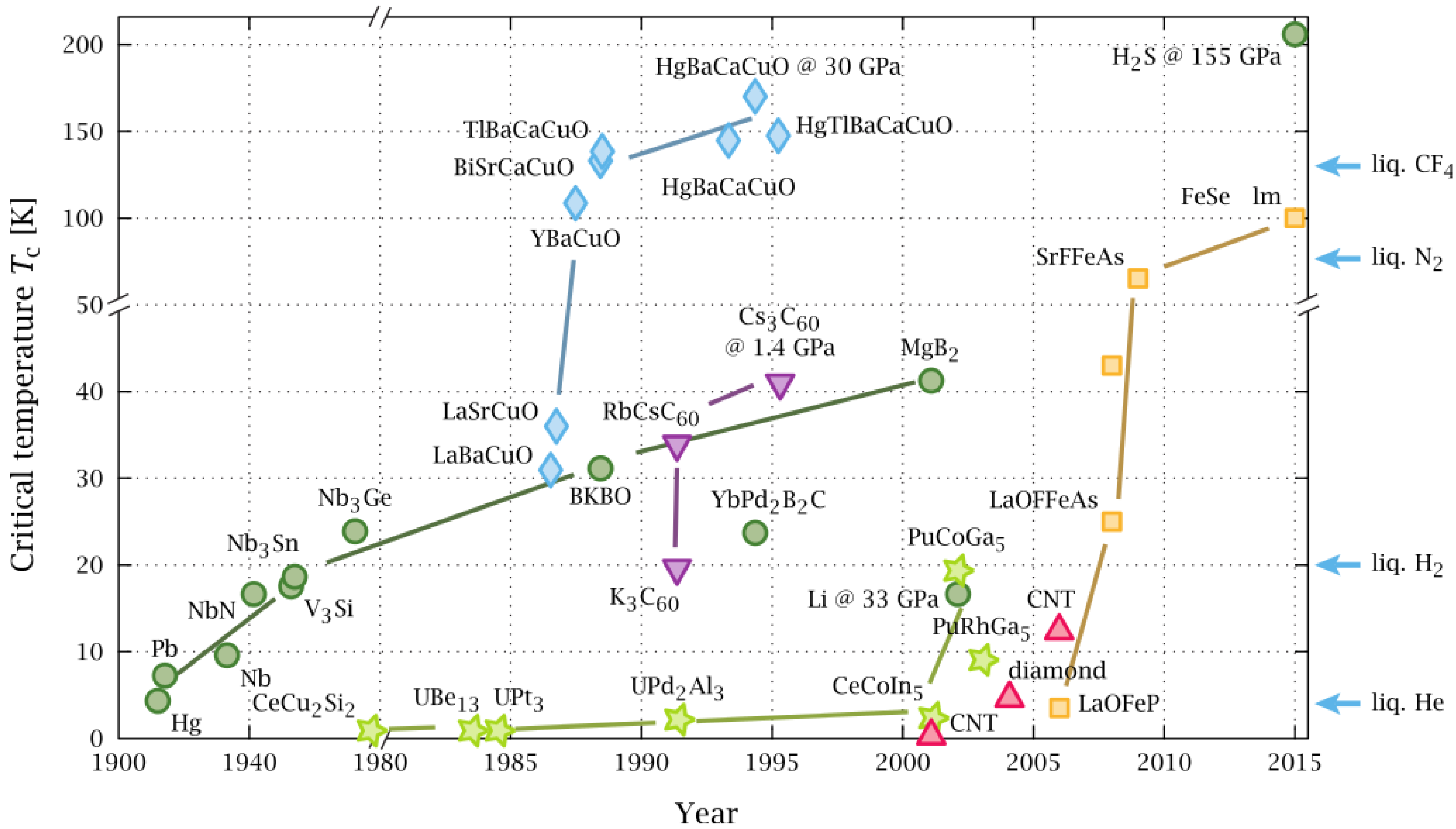
- There is no universal theory for superconductivity.[1]
  - In 1957, the Bardeen, Cooper, Schrieffer (BCS) theory was proposed.[2]
    - Electrons are bound as Cooper Pairs.
    - Works well for low temperature superconductors (type I)
    - Does not account for higher temperatures superconductors which were later discovered (type II)
  - Other theories include
    - Resonating-valence-bond theory[3]
    - Spin fluctuation theory [4]



Source:https://physics.stackexchange.com/questions/126742/do-all-the-electrons-form-cooper-pairs-at-absolute-zero

[1] A. Mann, *Nature*, **475**, (21), 280-282, 2011
[2] J. Bardeen, et al. *Phys. Rev.* **106** **(**5), 162–164, 1957
[3] P.W. Anderson, *Science*, **235** **(**4793), 1196–1198, 1987
[4] P. Monthoux, et al. *Phys. Rev. Lett.*, **67** **(**24), 3448–3451, 1991

Critical Temperatures



Source: https://en.wikipedia.org/wiki/Superconductivity

Data

- Data driven method to critical temperature.
- Data set contains:
  - 21,263 superconductors
  - 81 features
    - 8 properties derived from the elemental components
    - 10 statistical measurements determined from the 8 properties
    - 8 X 10 = 80
    - The final feature is the number of elements.

K. Hamidieh, *Computational Materials Science*, **154**, 346-354, 2018

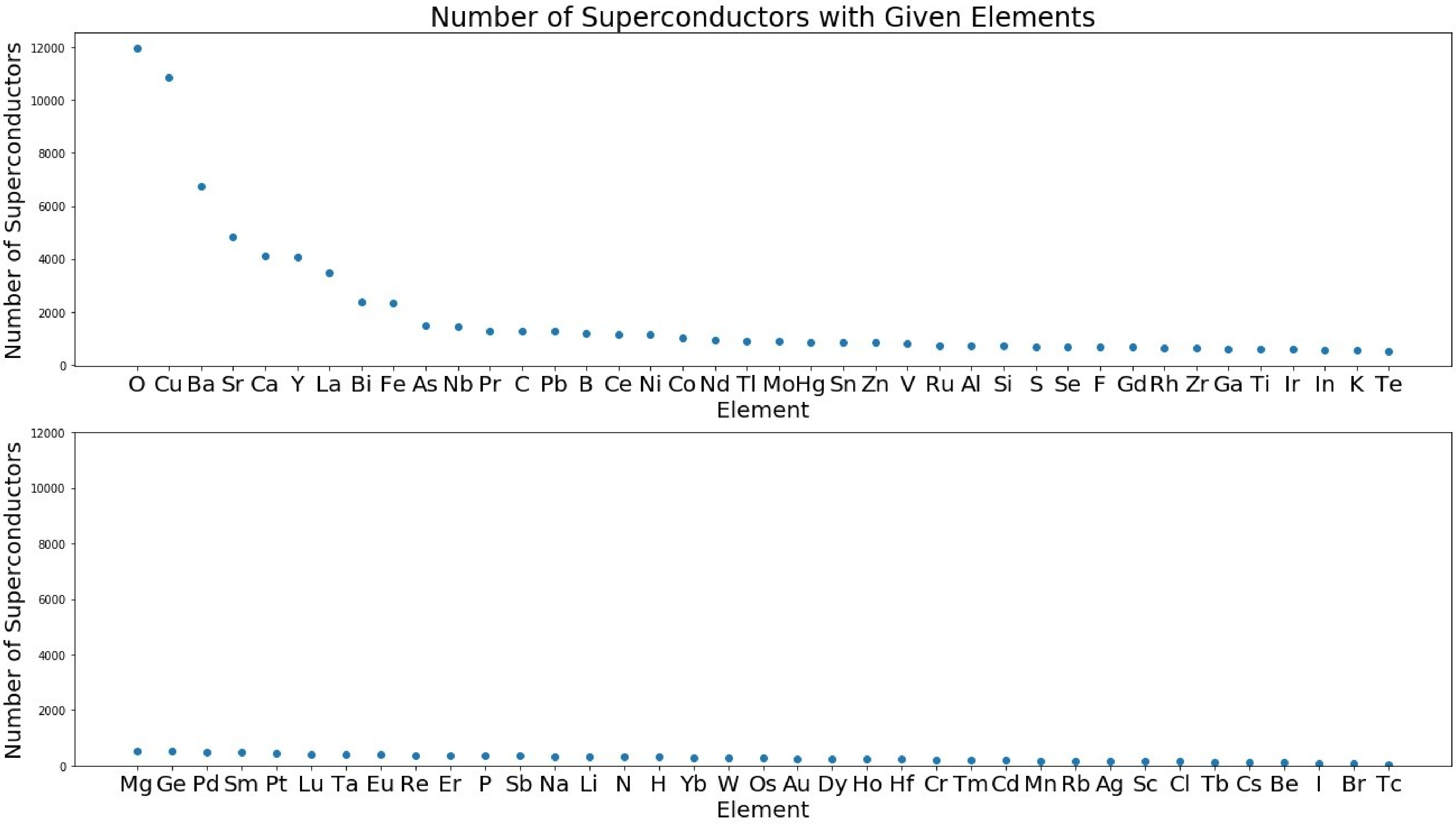
Features

Variable	Units	Description
Atomic Mass	atomic mass units (AMU)	total proton and neutron rest masses
First Ionization Energy	kilo-Joules per mole (kJ/mol)	energy required to remove a valence electron
Atomic Radius	picometer (pm)	calculated atomic radius
Density	kilograms per meters cubed (kg/m^3)	density at standard temperature and pressure
Electron Affinity	kilo-Joules per mole (kJ/mol)	energy required to add an electron to a neutral atom
Fusion Heat	kilo-Joules per mole (kJ/mol)	energy to change from solid to liquid without temperature change
Thermal Conductivity	watts per meter-Kelvin (W/(m $\times$ K))	thermal conductivity coefficient κ
Valence	no units	typical number of chemical bonds formed by the element

Feature & Description	Formula
Mean	$= \mu = (t_1 + t_2)/2$
Weighted mean	$= \nu = (p_1 t_1) + (p_2 t_2)$
Geometric mean	$= (t_1 t_2)^{1/2}$
Weighted geometric mean	$= (t_1)^{p_1} (t_2)^{p_2}$
Entropy	$= -w_1 \ln(w_1) - w_2 \ln(w_2)$
Weighted entropy	$= -A \ln(A) - B \ln(B)$
Range	$= t_1 - t_2 \ (t_1 > t_2)$
Weighted range	$= p_1 t_1 - p_2 t_2$
Standard deviation	$= [(1/2)((t_1 - \mu)^2 + (t_2 - \mu)^2)]^{1/2}$
Weighted standard deviation	$= [p_1 (t_1 - \nu)^2 + p_2 (t_2 - \nu)^2)]^{1/2}$

K. Hamidieh, *Computational Materials Science*, **154**, 346-354, 2018

Element analysis

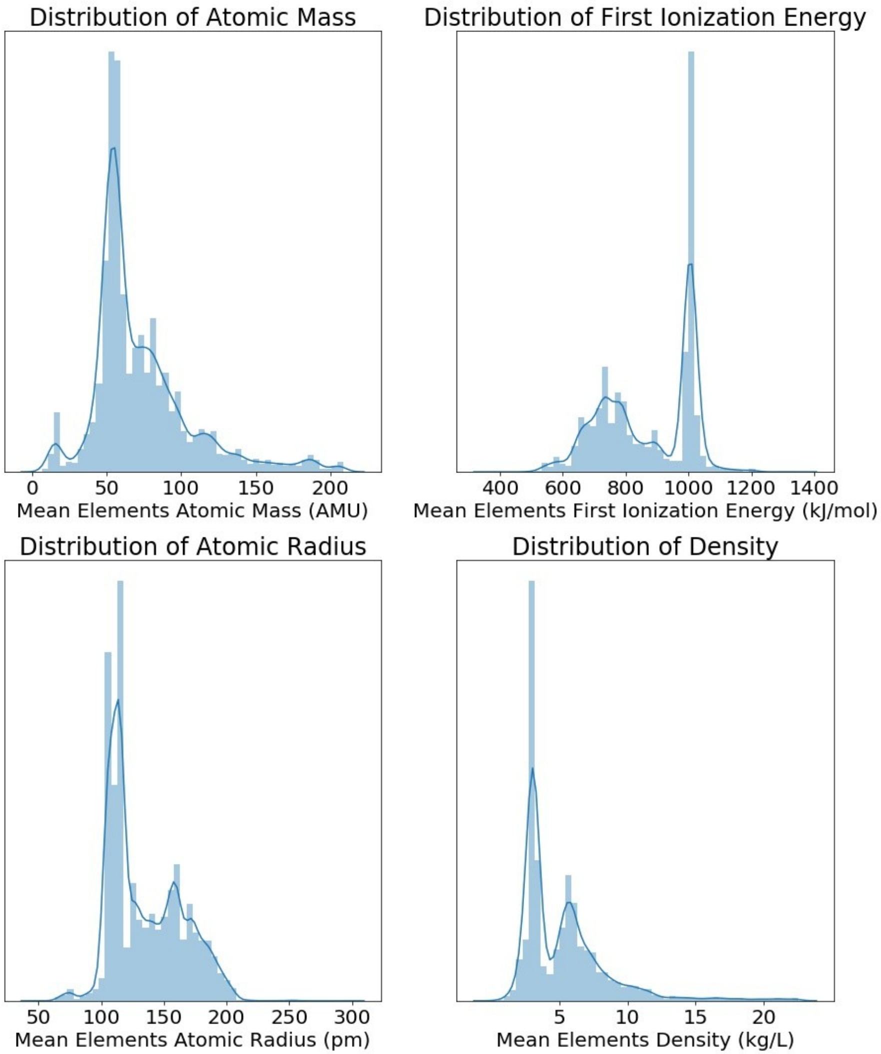


Element analysis

- There are 77 elements in the data set.
- 60 elements appear in less than 5% of superconductors.
- Oxygen and copper are the most common element
- 59% of superconductors have oxygen or copper.
- It would be interesting to see how well a model does using only elements.

Superconductors with Element		
	Percent	Number
Oxygen	56.27%	11964
Copper	50.97%	10838
Barium	31.75%	6751
Strontium	22.82%	4852
Calcium	19.34%	4112
Yttrium	19.16%	4075
Lanthanum	16.29%	3463
Bismuth	11.24%	2389
Iron	11.00%	2339
Arsenic	7.06%	1502

Property Distribution of the Weighted Mean



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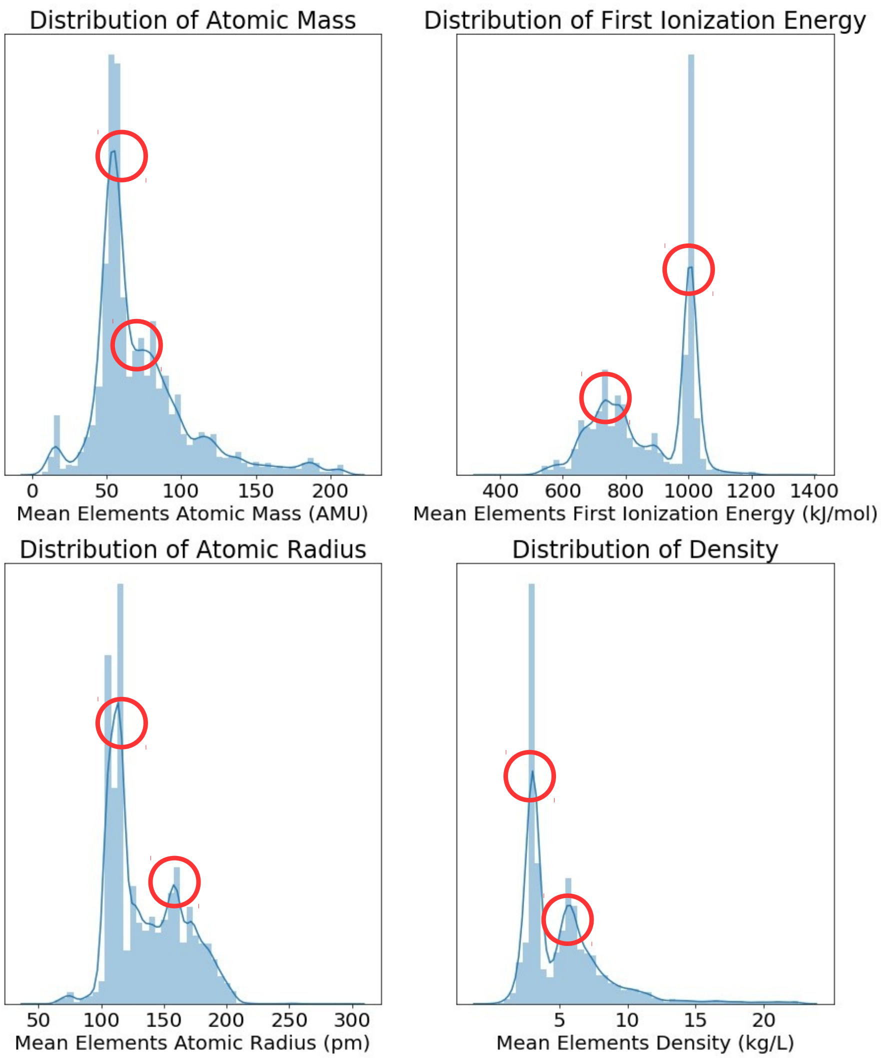

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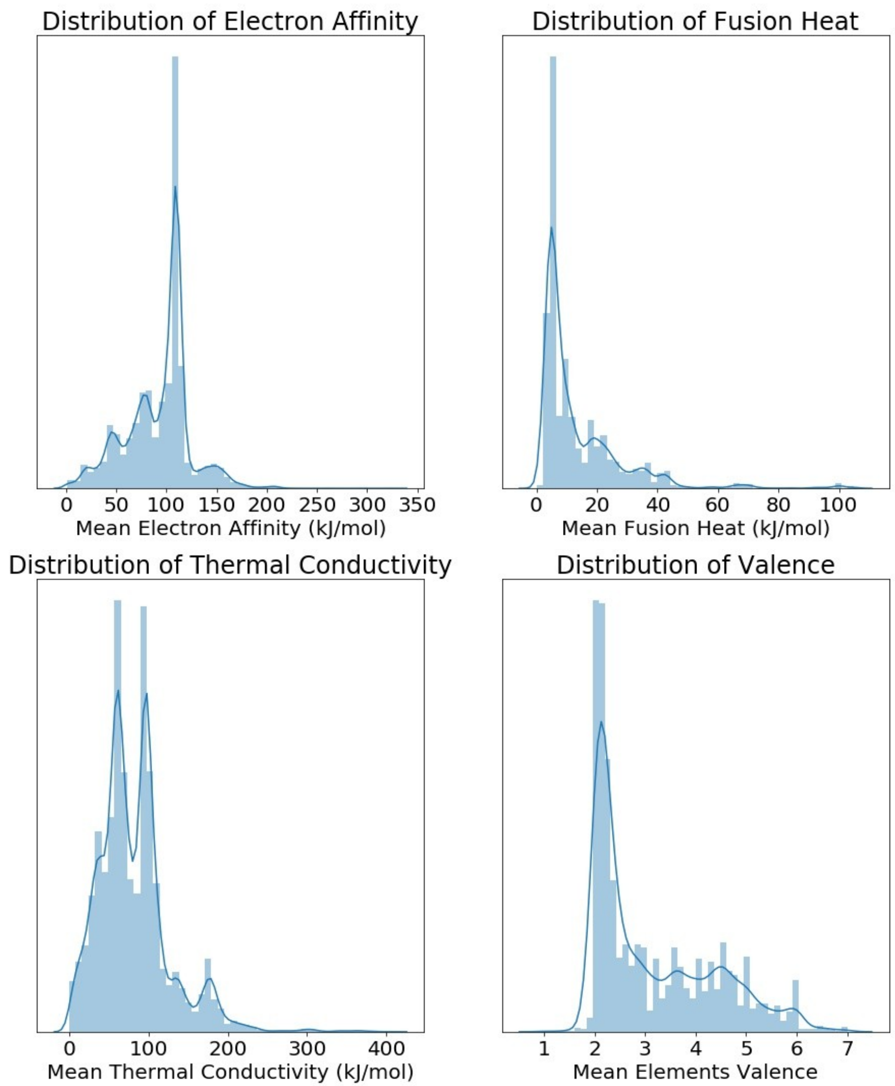

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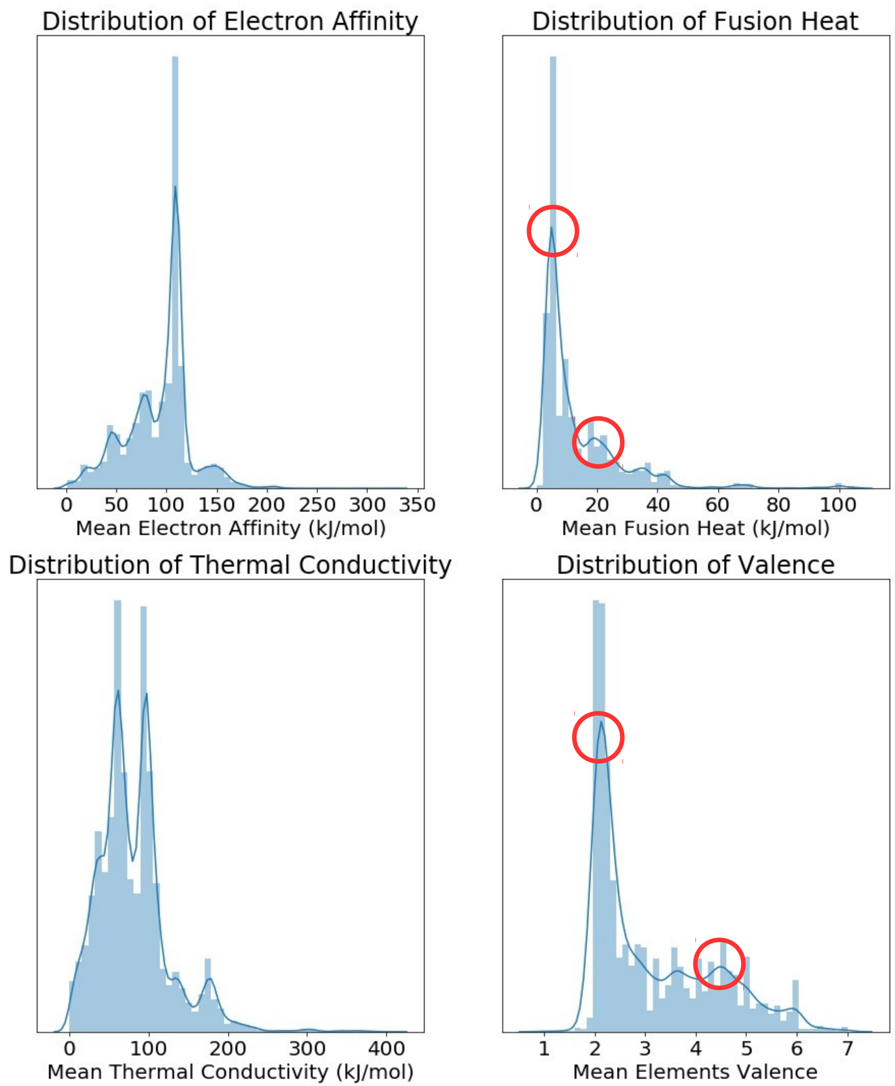
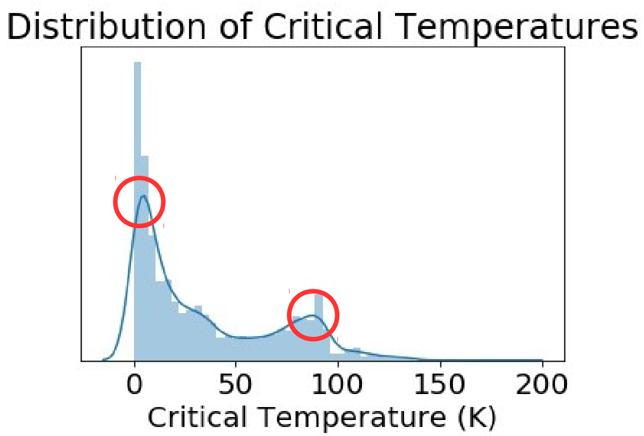


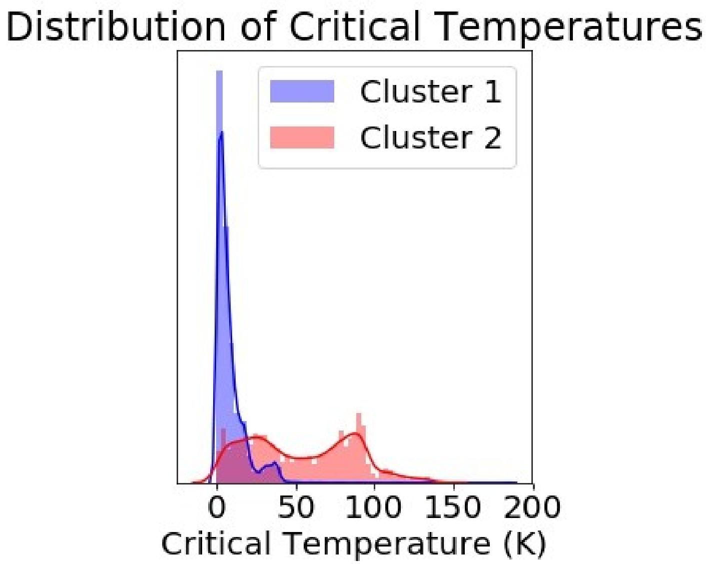
Critical temperature distribution

- The distributions suggest that there are two populations of superconductors in the data set.
  - Possibly type I and type II superconductors.
- Type I are typically has a lower temperature than type II.
- After clustering, there were too many type II superconductors in the lower temperature cluster
  - Populations in bimodal distribution not based on type

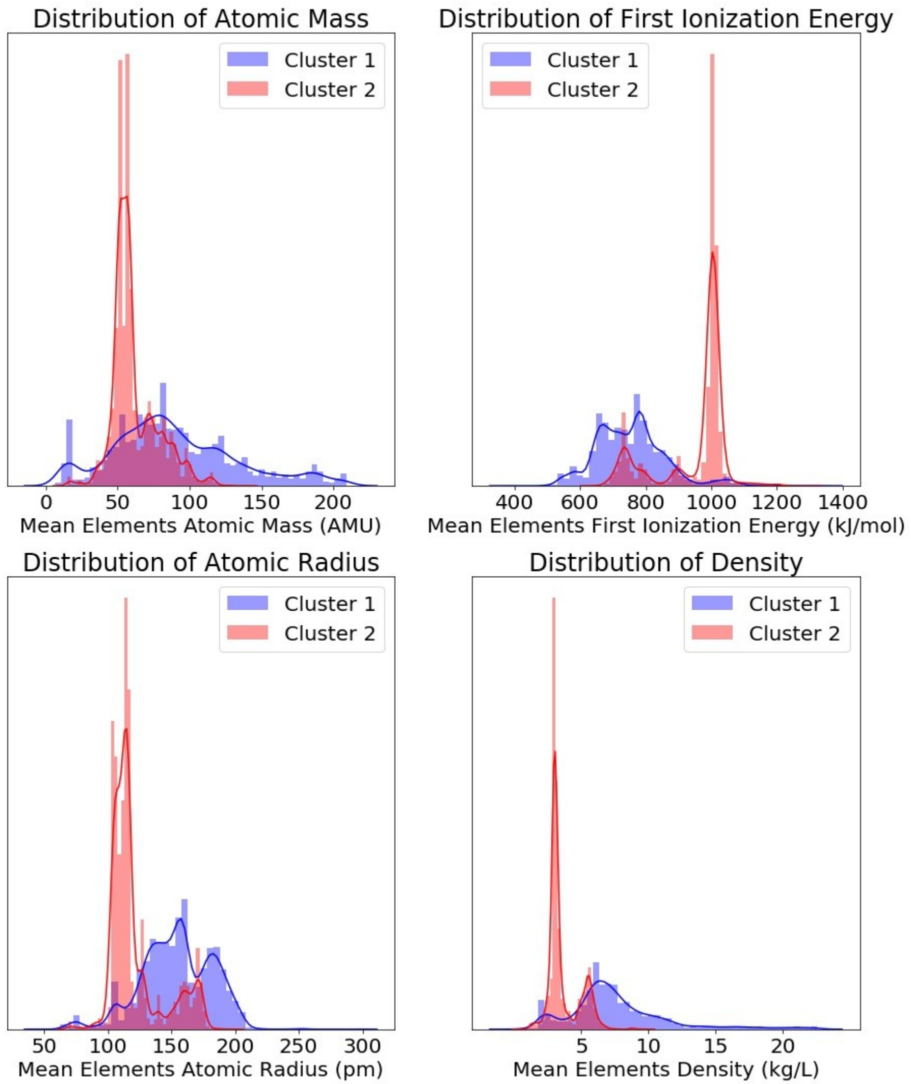


K-means Clustering

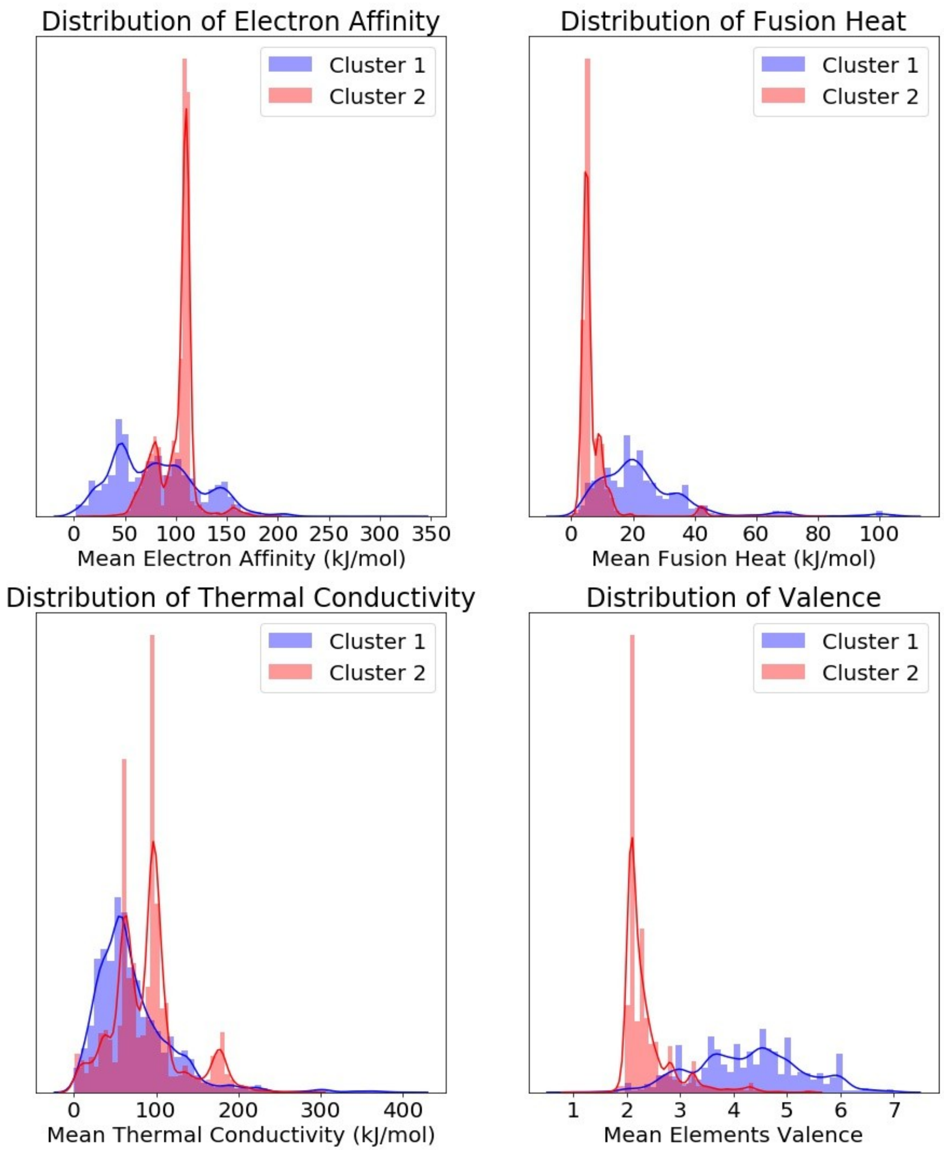
- Superconductors were clustered into two distinct clusters.
  - Cluster 1: 8792 superconductors
  - Cluster 2: 12471 superconductors
- Is there is any predictive value to clustering?



K-means Clustering

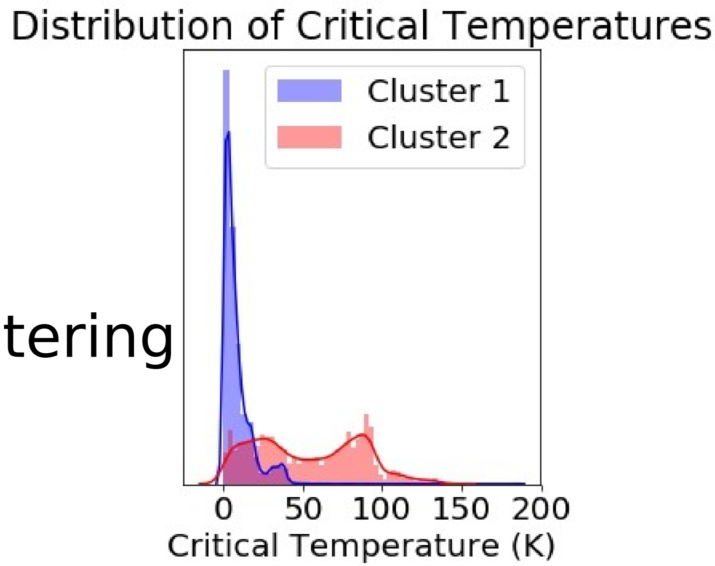


K-means Clustering



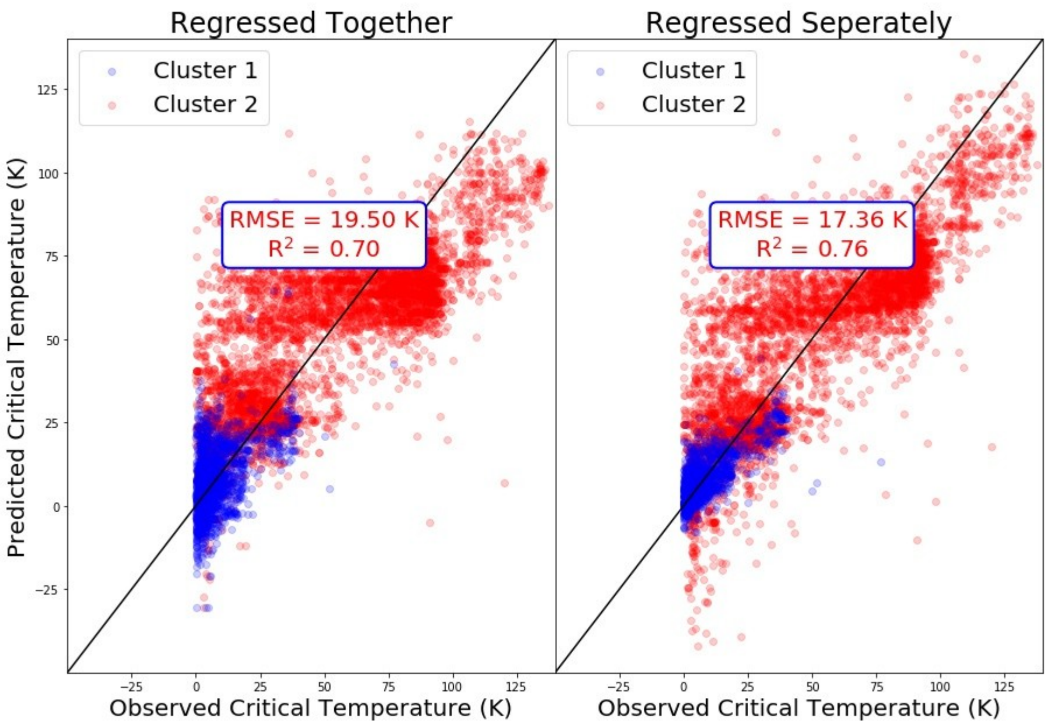
Data Separating

- 7000 data points obtained from each cluster for training data set
  - Same number of data points per cluster to avoid an unbalanced model
- Two strategies were used for each machine learning method.
  - Clusters were modeled together
  - Clusters were modeled separately
  - Allows us to see the effects of clustering
- Two methods were used for modeling:
  - Linear Regression
  - Gradient Boosting



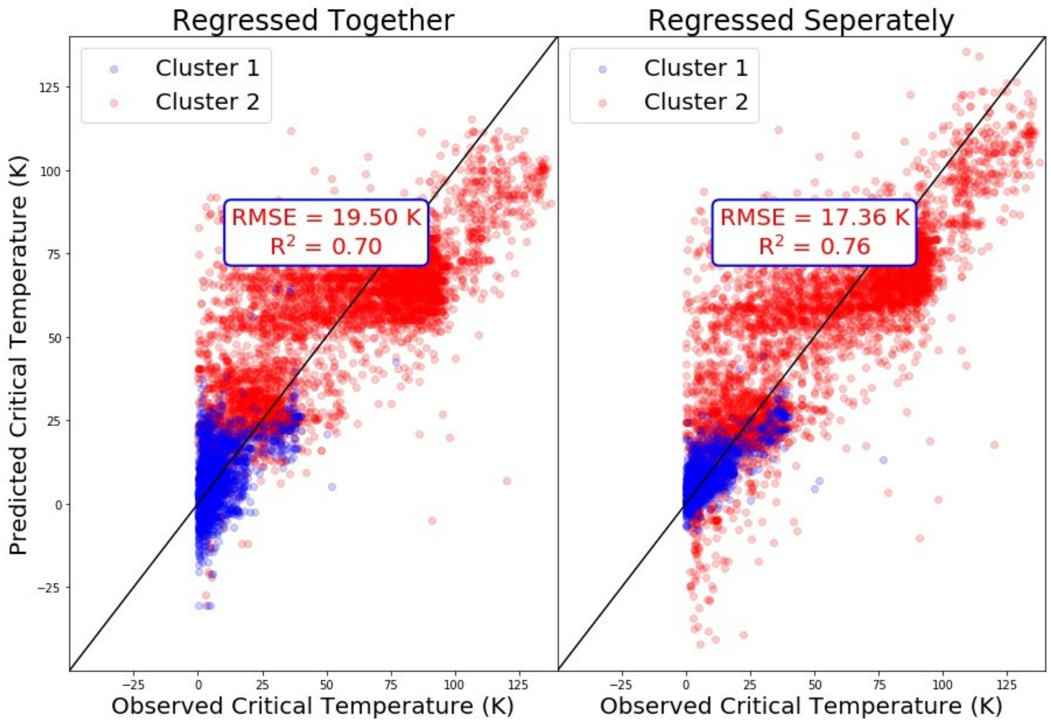
Linear Regression

- Performed using scikit-learn python libraries
- Features are standardized by
    - Centering by the mean.
    - Then dividing by the standard deviation



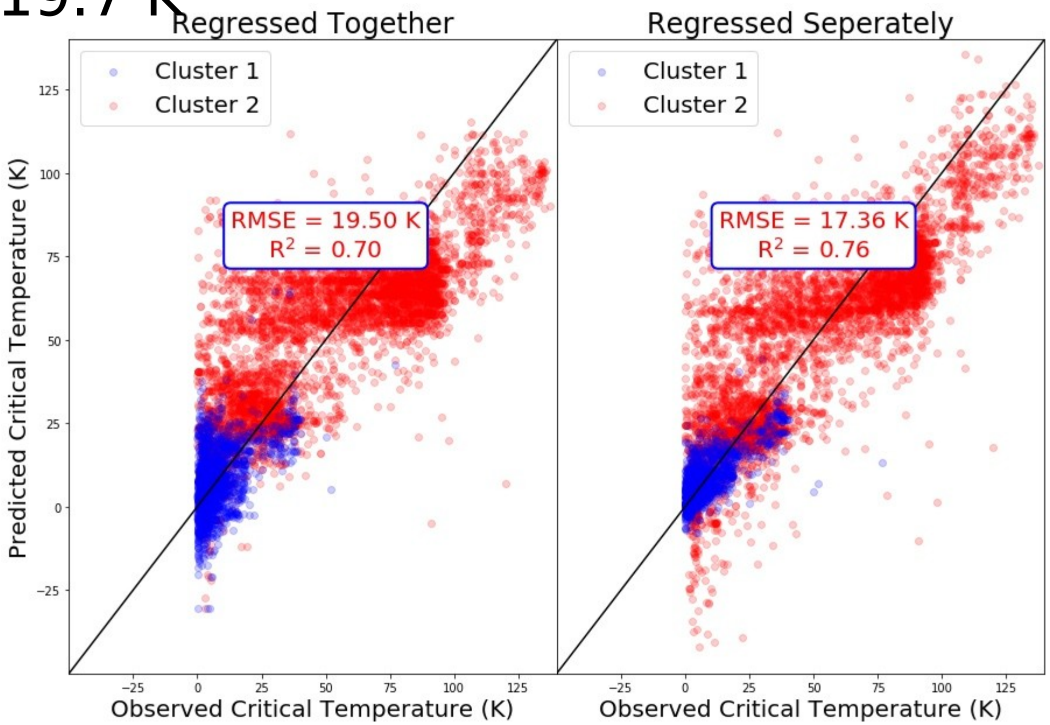
Modeling Cluster with Linear Regressions

- Modeling cluster separately reduced RMSE and R^2
  - Modeled clusters Together: RMSE: 19.5 K
    R^2: 0.70
  - Modeled clusters separately: RMSE: 17.4 K
    R^2: 0.76



Modeling Cluster with Linear Regressions

- Cluster 1 error is significantly decreased by modeling clusters separately
  - RMSE :9.6 K to 6.0 K
  - R^2: -0.21 to 0.53
- Cluster 2 error decrease was less significant:
  - RMSE: 21.8 K to 19.7 K
  - R^2: 0.58 to 0.65



Gradient Boosting

- Performed using XGBoost python library
- 4-fold cross validation was performed using scikit-learn python library
- XGBoost’s scikit-learn API was slow so custom API were created.
  - This API was 5 times faster than the scikit-learn API build-in to XGBoost.
- Features were standardized
  - centered at the mean
  - Divided by standard deviation.
- Tuned hyperparameters.

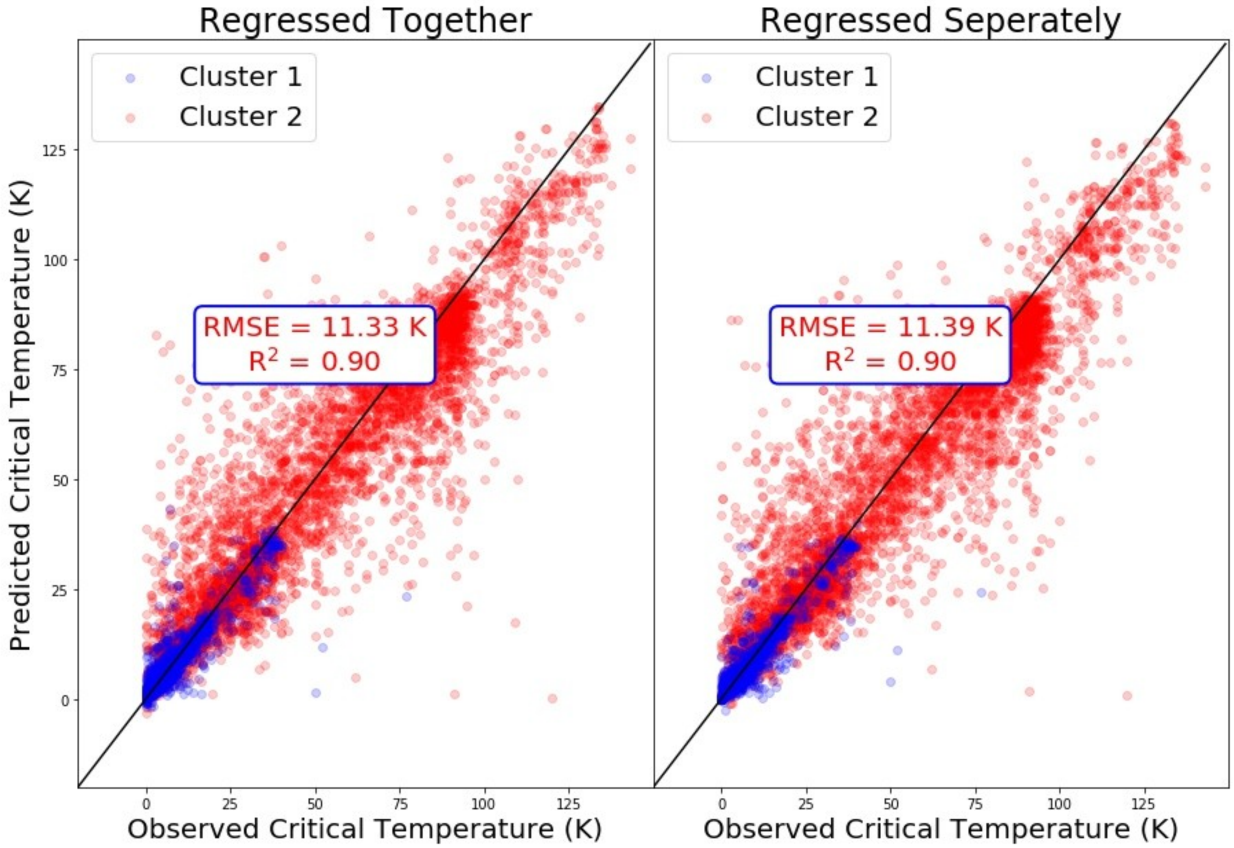
Tuning Hyperparameters

- Tuned hyperparameters with a random search of 200 possible combinations.

Parameters	Both Clusters	Cluster 1	Cluster 2	Values searched
n_estimators	230	130	139	1,2,3…699
min_child_weight	18	3	13	1,2,3…20
max_depth	17	18	12	1,2,3…20
learning_rate	0.40	0.28	0.34	0.01,0.02,0.03…1.00
subsample	1.00	0.75	1.00	0.50,0.75,1.00
solcample_bytrue	1.00	0.75	1.00	0.50,0.75,1.00

Gradient Boosting Results

- Gradient boosting performed significantly better than linear regressions
- Modeling clusters separately had no effect on accuracy



Important Features

Both Cluster		Cluster 1		Cluster 2	
Feature	Fraction Gain	Feature	Fraction Gain	Feature	Fraction Gain
Range thermal conductivity	0.594	Weighted mean atomic mass	0.253	Weighted mean thermal conductivity	0.460
Weighted geometric mean thermal conductivity	0.131	Range first ionization energy	0.114	Weighted mean valence	0.072
Standard deviation atomic mass	0.020	Weighted mean valence	0.054	Standard deviation atomic mass	0.062
Weighted mean valence	0.018	Weight geometric mean electron affinity	0.035	Weighted geometric mean valence	0.055
Weighted geometric mean valence	0.017	Mean first ionization energy	0.033	Weighted standard deviation electron affinity	0.036
Weighted standard deviation electron affinity	0.014	Weighted standard deviation thermal conductivity	0.026	Range atomic radius	0.014
Weighted range atomic mass	0.013	Mean density	0.024	Weighted entropy thermal conductivity	0.013

Conclusion

- We successfully created models that predict the critical temperature of superconductors using features derived from the properties of the elements in the superconductors.
- Best model: RMSE: 11.33 K and R^2: 0.90
- Gradient boosting was more accurate than linear regression.
- Modeling the clustering separately improved accuracy for linear regression but not gradient boosting.
  - Separating by clustering may add flexibility to the linear regression model while gradient boosting (being non-linear) was sufficiently flexible.

Special Thanks

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