Predicting the Critical Temperature of Superconductors

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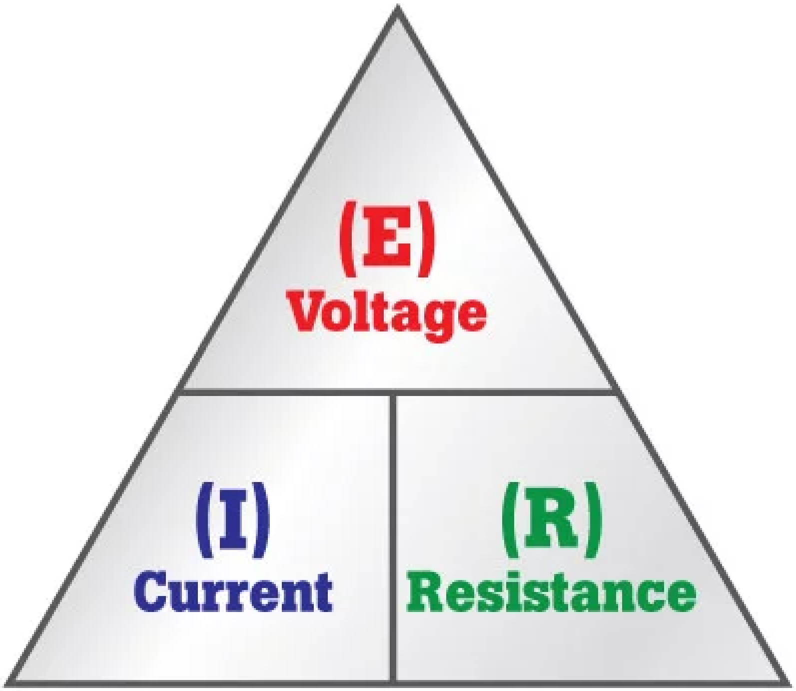
Objective

- Predict the critical temperature for 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, electronic current can be maintained without external voltage
- With zero resistance, an electronic current can be maintained indefinitely.

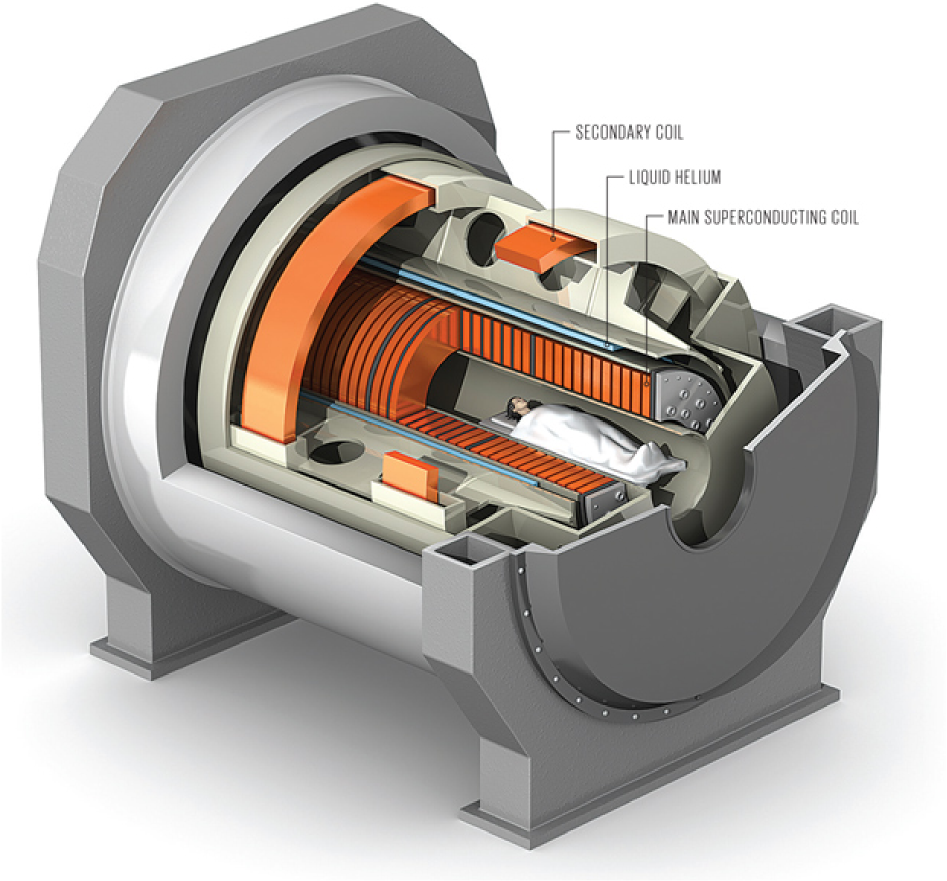


Source:https://www.fluke.com/en-us/learn/best-practices/measurement-basics/electricity/what-is-ohms-law

Applications for Superconductors

- Superconducting magnetic in Magnetic Resonance Imagining. (MRI)
- Superconducting coils in the Large Hadron Collider
- Superconductors could components in electronic powered systems [1]

MRI machine

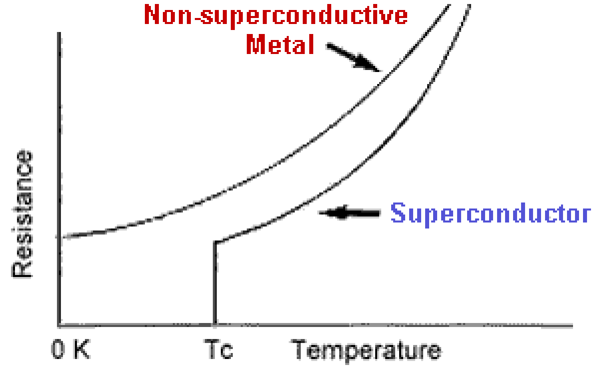


Source: https://phys.org/news/2013-10-world-powerful-mri-online.html

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

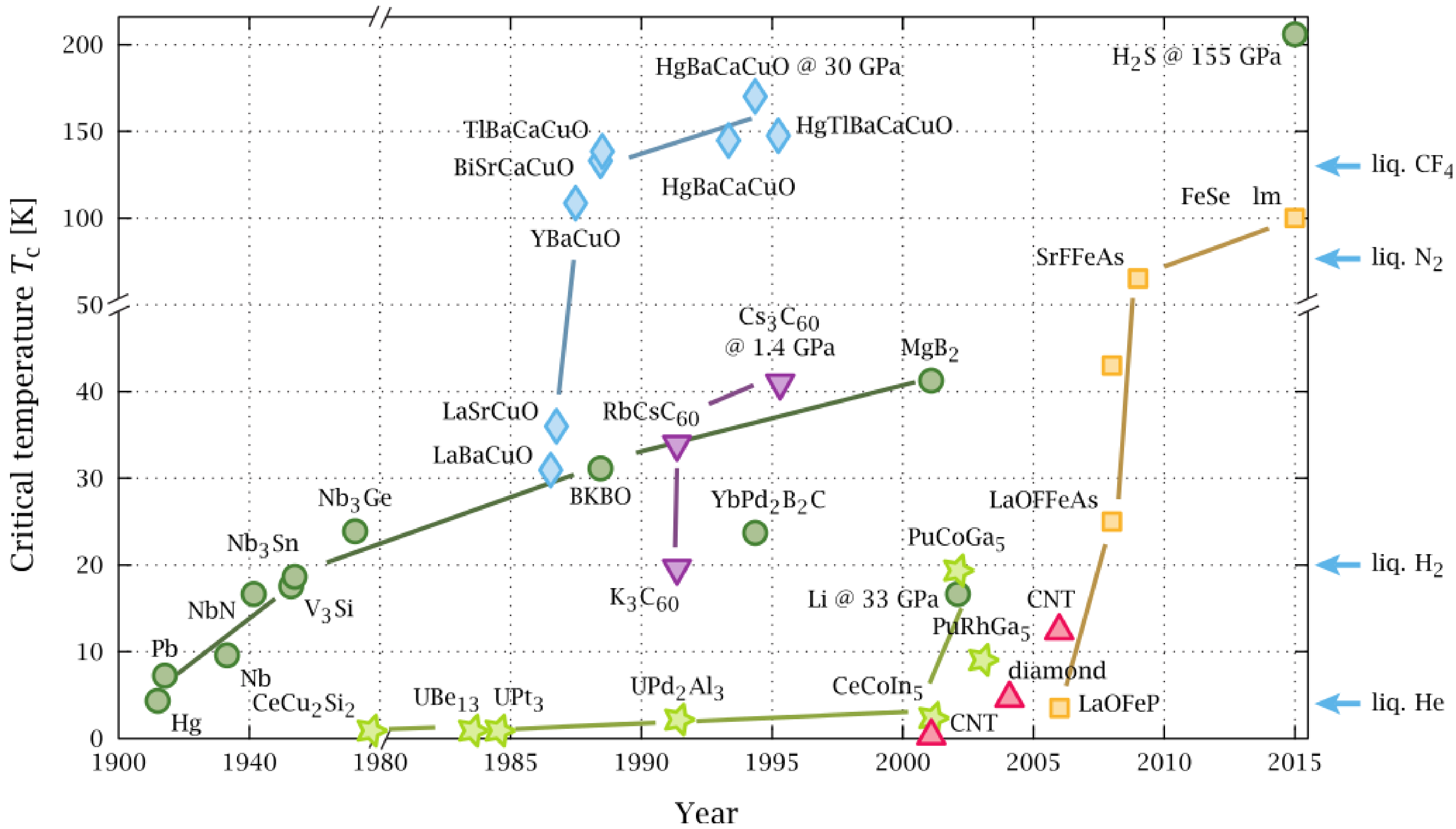
Critical Temperature

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



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

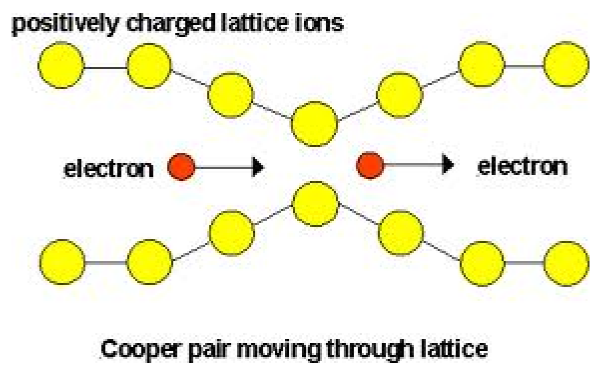
Critical Temperatures



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

Superconductor Theory

- There is not universal theory for superconductivity.[1]
  - In 1957, Bardeen, Cooper, Schrieffer (BCS) theory was proposed.[2]
    - Electrons are bound as Cooper Pairs.
    - Works well for low temperature superconductors (type I)
    - Not so well 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

Data

- With no universal theory to predict critical temperature, we have to derive them from regressions.
- Data set contains:
  - 21,263 superconductors
  - 80 attributes
    - 8 properties derived from the elemental components
    - 10 statistical values determined from the 8 properties
    - 8 X 10 = 80
  - A complete list of the ratios elements for each superconductor (Not used by the original analysis by Hamidieh)

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

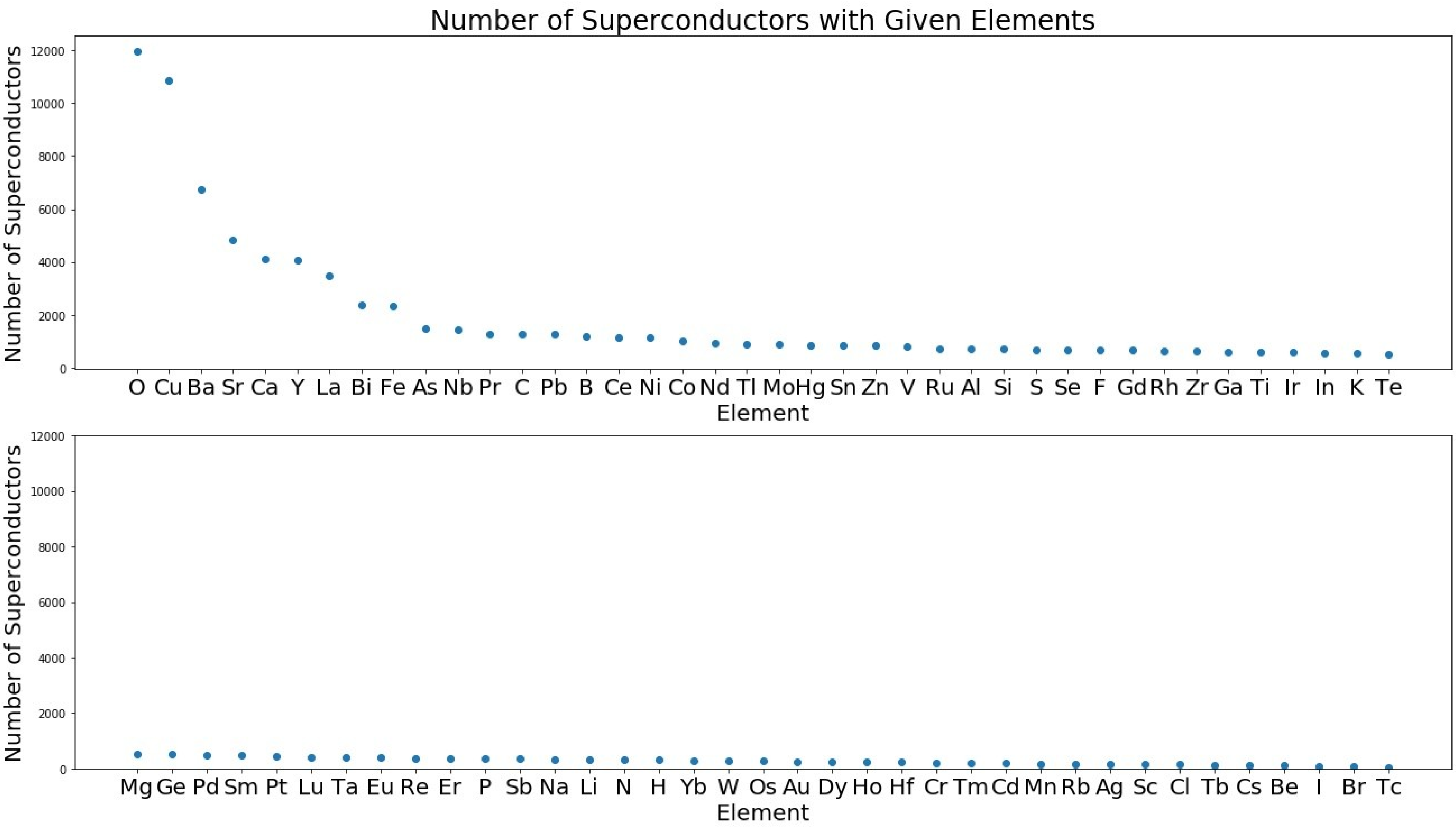
Attributes

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

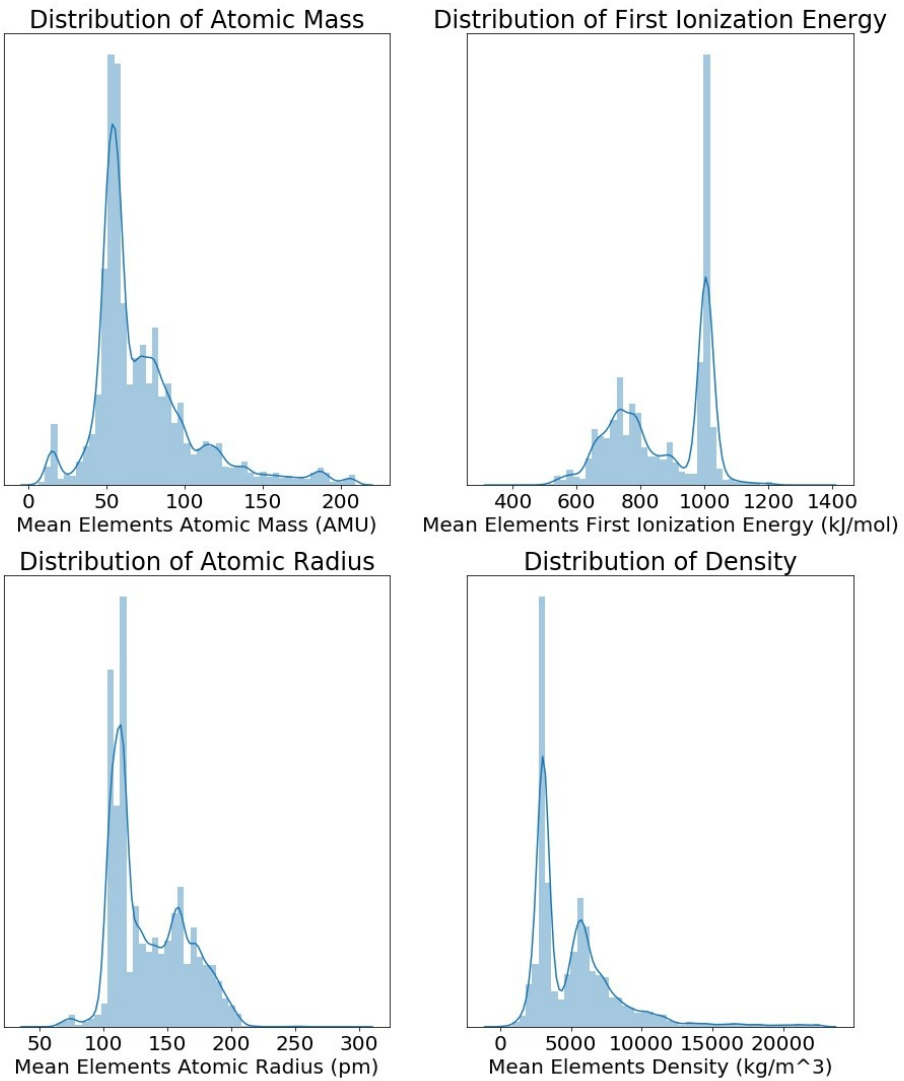


Element analysis

- There are 77 elements in the database.
- 60 elements appear in less than 5% of superconductors.
- Oxygen and Copper are the most common element
- 58.92% 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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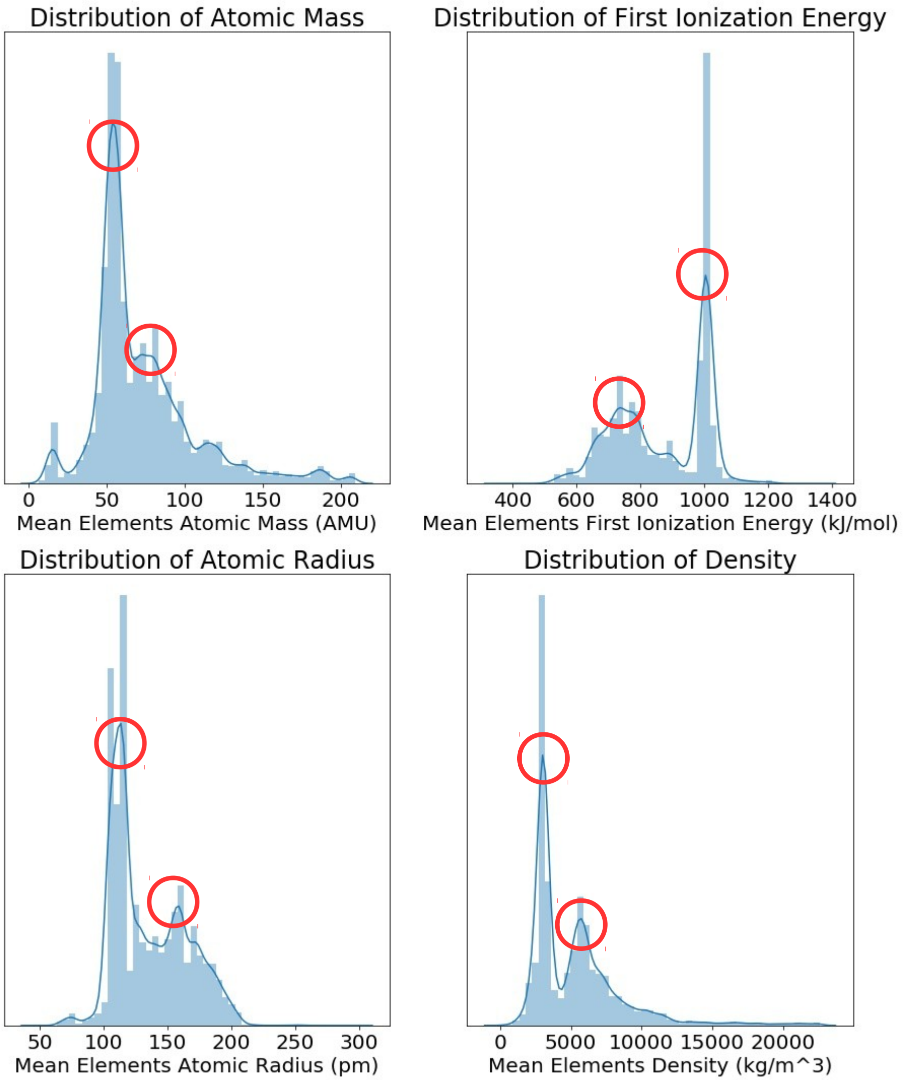

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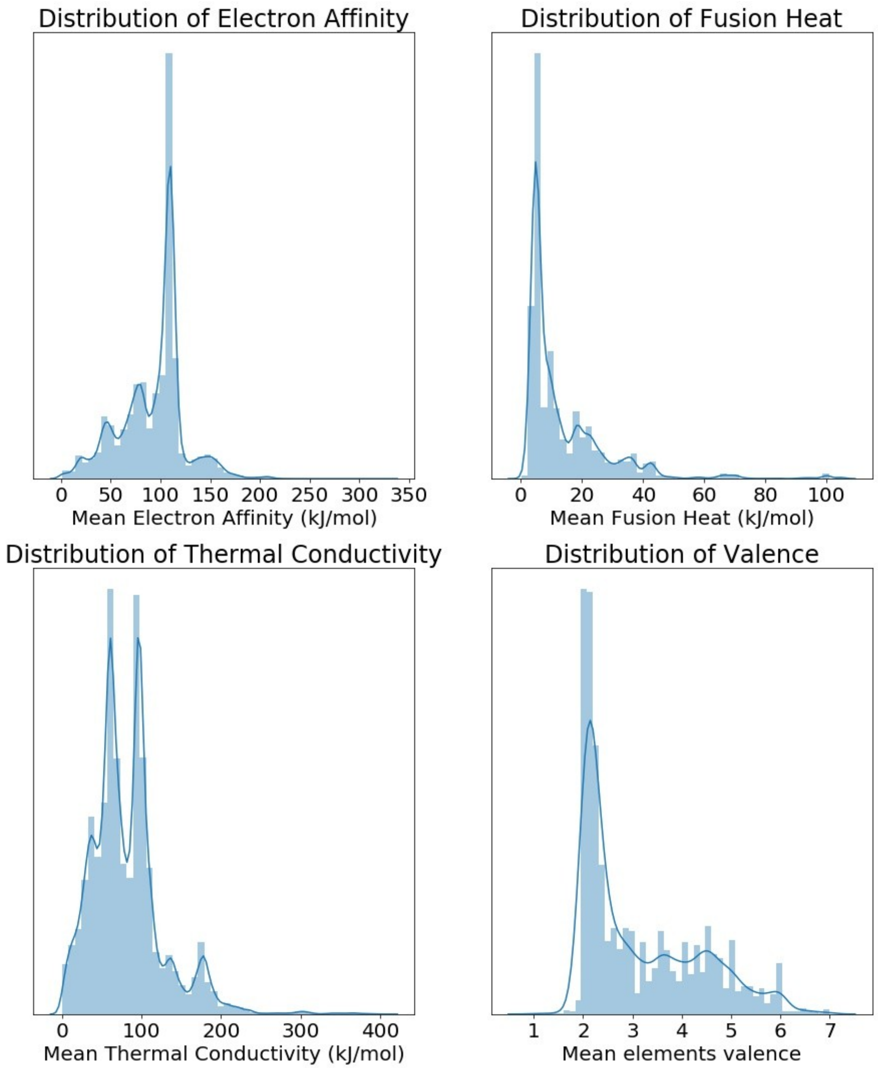

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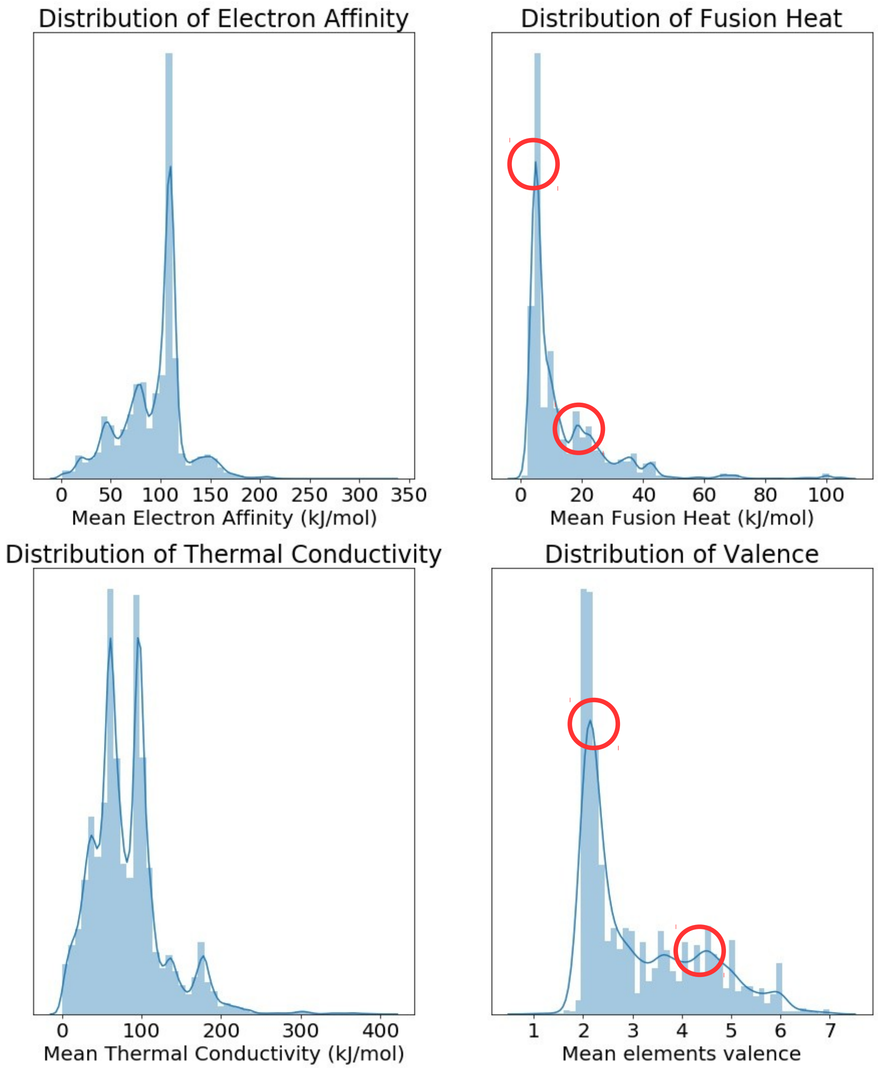
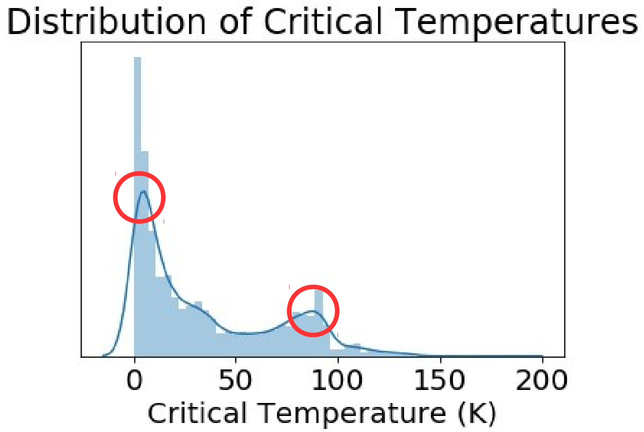
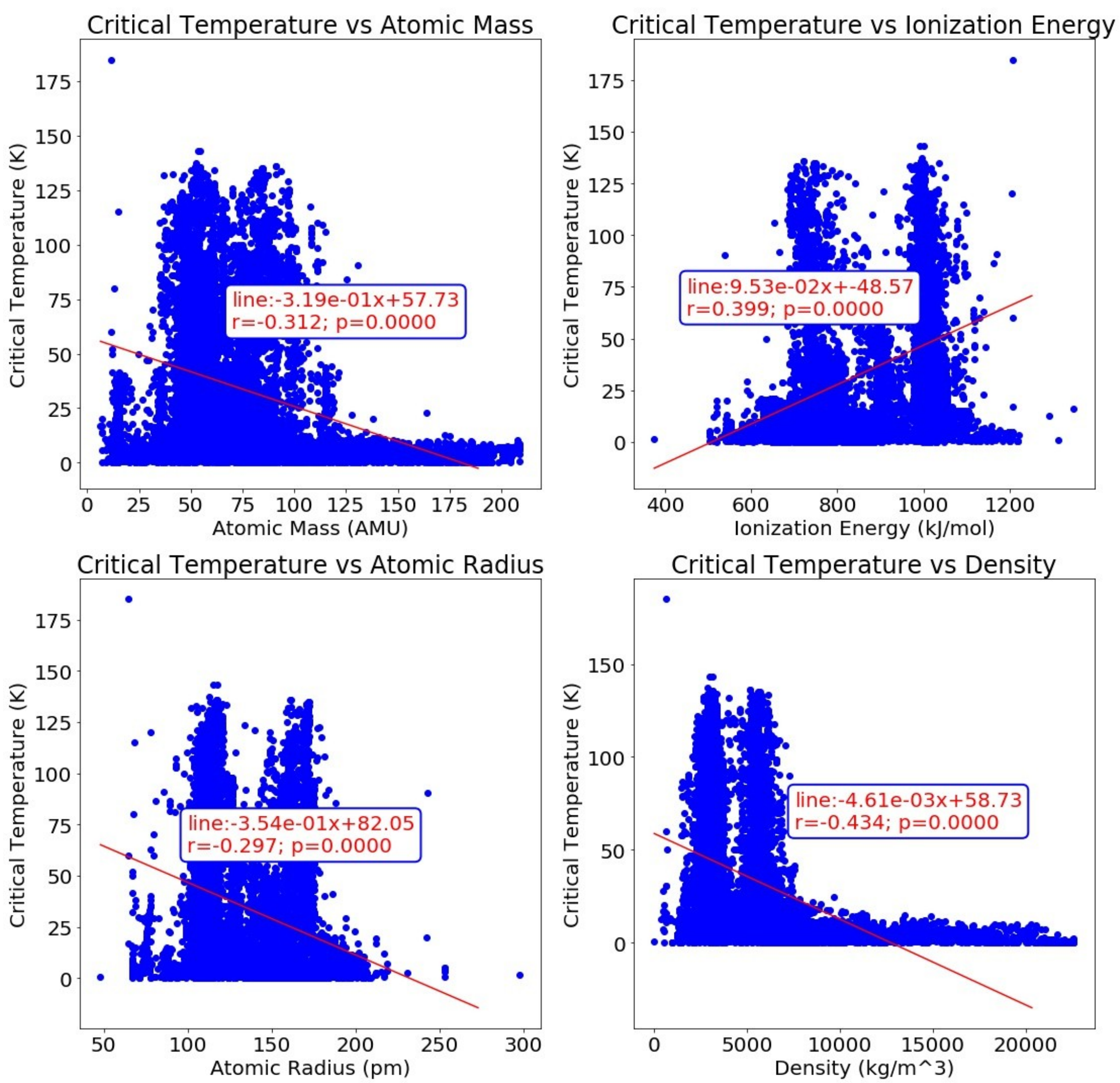


Critical temperature distribution

- The distributions suggest that there are two populations of superconductors in the data set.
- Possably type I and type II superconductors.
- Type I are significantly lower temperature then type II



Scatter Plots of the Weighted Mean



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