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Prediction study on critical temperature (C) of different atomic numbers superconductors (both gaseous/solid elements) using machine learning techniques

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Abstract

Superconductors has been comprehensively studied as huge research effort taking into consideration of actuality that its invention ruins a theme of passionate discuss once its discovery completed. The standard behind this paper is the study about explaining as well as scrutinizing how different regression methods are used for predicting the superconducting critical temperature Tc from Superconductors database collected from Kaggle dataset source. Mainly, regression models such as linear Regressor, decision tree Regressor, Lasso Lars Regressor, Bayesian Ridge Regressor, XGB Regressor, and Huber Regressor have been studied to forecast critical temperature in superconductor materials.

Introduction

The Superconductors materials such as metals, organic materials, and ceramics as well as deeply intoxicate which conduct electricity with no resistance. The superconductivity materials can carry electrons without any resistance and therefore heat, energy or any other sounds is not emitted. This superconductivity takes place at particular materials critical temperature which is named as Tc. As temperature value decreases, the superconducting materials resistance slowly decreases until it reaches critical temperature. At this specific point, resistance drowsed, over and over again to zero as mentioned in the Fig. 1.

Currently most materials accomplish an enormously very least energy state by means of high pressures, low temperatures so as to attain superconductivity. In general, Superconductivity is probably more expensive, and incompetent cooling processes meanwhile superconductors which are very well-organized, competent at higher temperatures are in progress during investigation.

The superconductivity materials materialized from resistant state. The superconducting transition temperature makes improvement in superconducting materials mainly oxide metals [14] as well as conferred the localization performance in proximity background to Ferro-electricity. Superconductors reveal the distinctive features in addition with capability of conducting current. For scenario: many banish magnetic fields while conversions into superconducting state which may be because of Meissner effect[12] discovered by Meissner (in the year 1920) in which the superconducting materials placed the electric current near the surface at T_c, as a result, terminating the fields within the specified material itself.

A motionless magnet on a superconductor exhibits these consequences: as the superconductor cools via its critical temperature, the exclusion of magnetic flux from the conductor makes the magnet to increase above the material (Fig. 2).

The superconductor principles can be demonstrated as follows:

i) Ohm's law: Voltage is directly proportional to current and resistance. Lack of resistance in a current- carrying superconductor can be exemplified by Ohm's law.

$V = IR$ Where V is Voltage; I refer to current, R- Resistance.

ii) Superconductor materials carry current with no voltage i.e R = 0.

iii) Superconductivity does not contain power loss, given that power is defined as $P = I^2 R$

Since, R = 0 in any superconducting material and also power loss is zero.

The main scopes of this study are as follows:

a. First and foremost thing is extracting features of superconductors material data together with critical temperature.

b. Secondly, seven types of regression model is used for all superconductivity material data has to be calculated based on certain properties like atomic mass, mean entropy, range density, thermal conductivity.

The main objective of this current work is to forecast the critical temperature based on features extracted both in training and testing dataset using statistical analysis of machine learning algorithms especially regression models. The model performance as well as predicting critical temperature can be done via testing phase.

Section snippets

Related study

[1] Approached Bayesian Neural network for predicting critical temperature in Superconductors materials. The dataset is collected from the website http://www.victoria.ac.nz/robinson/hts-wiredatabase that permits to download both graphical images data and also essential data files. Based on case study, this paper exhibit the effectiveness of all related data which designed the system as well as comparing correlation between low temperature and performance.

Logan ward et al. [3] envisage varied…

Proposed work

Now, the purpose is to predict the critical temperature based on extraction of features in the dataset. Make predictions using the data in test.csv and unique_m_test.csv for finding the performance of the model by calculating the critical temperature as well as chemical formula for superconductor materials such as hydrogen (H), Helium (He), Lithium (Li), Beryllium (Be), Lead (Le), Zinc (Zn), etc.…

Conclusion

Superconductivity is one of the most important discoveries in the field of modern physics. The main usage of superconductors is the ability to carry massive amount of power with no loss underneath critical temperature, therefore superconductors can rescue more amount of energy. Error prediction in regression model is evaluated through R^2 score, Mean Squared Error, Root Mean Squared Error for predicting critical temperature. Several regression models namely Decision tree, XGB Regressor, Lasso…

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.…

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2022, Chemical Physics Letters

> *Citation Excerpt :*
>
> …The piezoelectric coefficient or piezoelectric modulus, usually written d33, measures the volume change when a piezoelectric material is subject to an electric field or the polarization on the application of a stress. There have been a variety of machine learning models developed for materials property predictions such as formation energy, band gaps [4,5], fermi energy [6], hardness [7], Poisson's ratios, elastic (shear/bulk moduli) [6,8,9], superconductor transition temperature [10–14], ion conductivity [15–18], flexoelectricity [19,20,2] and etc. These ML models can be categorized into three main categories in terms of the input information: composition descriptors based models, structure information based models, and hybrids.…

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Random Forest Regressor based superconductivity materials investigation for critical temperature prediction

2022, Materials Today: Proceedings

> *Citation Excerpt :*

> …There are few other characteristic properties such as resistance, impurity of materials, pressures, stress, and temperature, effects of isotopes [13], and magnetic fields that uniquely distinguish superconductors from other materials. Revathy et.al [1] proposed several regression models in predicting the critical temperature of superconducting materials with the dataset and delivered the comparisons of accuracies for each model. The work extended by performing exploratory data analysis with the dataset and by using them to predict the critical temperature.…

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First Principles and Machine Learning Identify Key Pairing Strength Factors of Cuprate Superconductors

2023, arXiv

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