ML for predicting band gap for dielectric materials.
A Presentation.

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Outline

Introduction

- ”Transition Metal Dichalcogenides” $\rightarrow$ Transition metals and chalcogens S, Se and Te.
- Trigonal TMDCs $\rightarrow$a=b$\neq$ *c* and $\alpha = \beta = 90^\circ, \gamma = 120^\circ$.
- Density-functional-theory based computational methods have been applied in various compounds to study their different types of properties, which are computationally expensive.[1]

[1] M. W. Lufaso and P. M. Woodward, Acta Crystallographica Section B: Structural Science 57, 725 (2001).

Literature Review

- P. C. Klipstein et al [2] (1986) studied the electronic properties of $HfTe_2$. They found that semimetallic behaviour arises from a small overlap of the tellurium p valence band and the hafnium d conduction band and estimate a band overlap of about 0.3 eV. Measurements of the conductivity and Hall coefficient show an increase in the band overlap and carrier concentration with pressure.
- S. Mangelsen et al reported an experimental and theoretical study on the layered transition-metal dichalcogenide (TMDC) HfTe2 that shows a large MR of 1350 % at T=2 K and Î¼0H=9T in the absence of Dirac or Weyl points. Moreover, the structure and electrical resistivity under pressure reveal a unique structural transition. These results clearly distinguish HfTe2 from TMDCs like MoTe2 or WTe2 which both exhibit larger MR and are viewed as Weyl semimetals.

Literature review

- Hazi Mohamad et al investigated the electronic and thermoelectric properties of (5, 0) single-wall M (M=Hf, Zr) X2(X=S, Se, Te) nanotubes by using first-principles calculations. They found that tubes, possess indirect bandgap varying between 1.12 and 0.075 eV and it was found that band gap was reduced upon increasing the chalcogen atomic size.
- David Hodul et al studied nature of the conductivity in hafnium ditelluride by study of the systems $HfSe_{2-x}Te_x$ (0 â¤ x â¤ 2) and HfTe2-x (0.05 ¡ x ¡0.6). Found resistivity and susceptibility indicated a nonmetal-to-metal transition at x â 0.1 in $HfSe_{2-x}Te_x$
- M.L. Adam et al studied phonon-mediated superconductivity and charge density wave in charge doped 1T-HfTe2. They found Electron doping induced superconductivity and a (2 Ã 2) charge density wave (CDW) instability. On hole doping superconductivity was induced and a phase transition to a metallic state.

Literature

- et al El Youbi (2020):They studied the dosed semi-metalic $HfTe2$ found the broadening of band gap and found the evidence of bulklike features.

Hyperparameter Tunning.

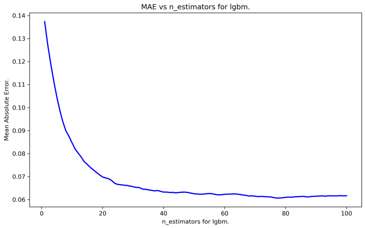
Models Studied

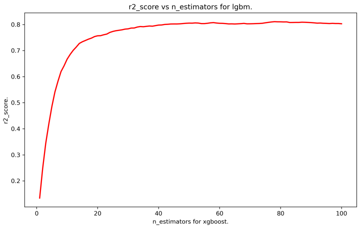
- Stochastic Gradient Boost (SGD)
- LightBGM
- XGBoost
- Random Forest
- ANN

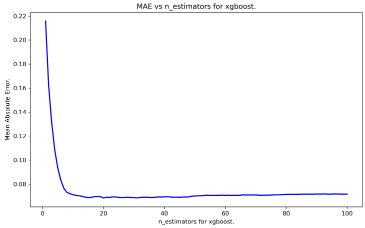
Parameters	Initiazation Value	Search space
n_estimators	100	[100, 200, 300]
max_depth	6	[6, 8, 10]
learning_rate	0.1	[0.1, 0.01]
objective	-	[regression]

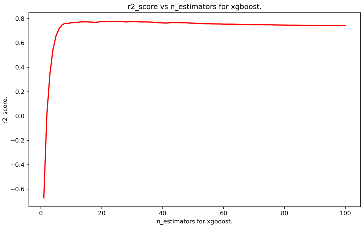
Table: Parameter Tunning.

Convergence Test.







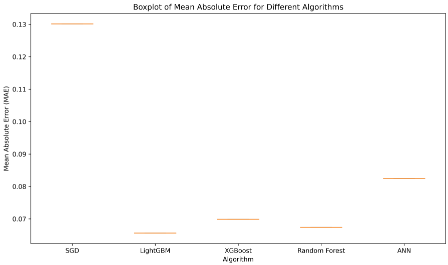


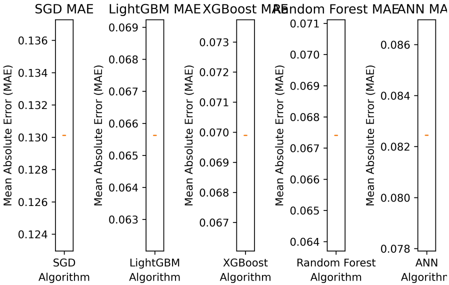
MAE for different Models.

Model	MAE
SGD	0.13012001665237308
LightGBM	0.06562523607532515
XGBoost	0.06989724752397243
Random Forest	0.06740825811781315
ANN	0.08244139381243276

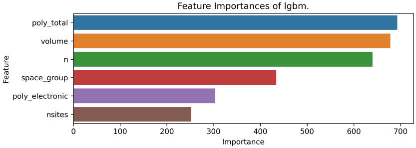
Table: Ground State Energies.

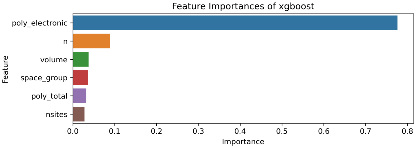
Comparision of diferrent models

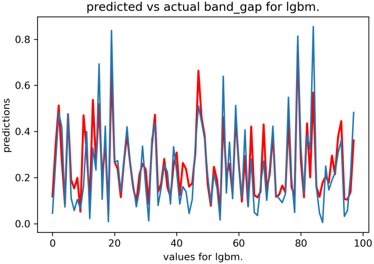


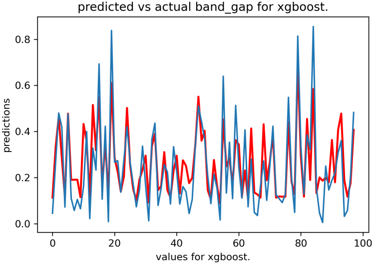


Feature importance and predictions.

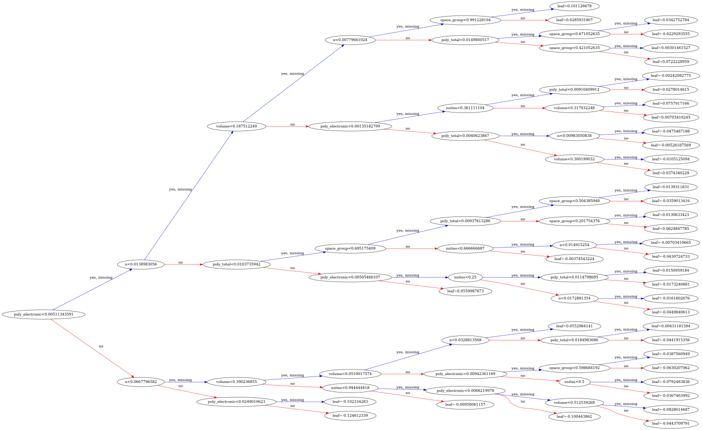








Visual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space_group<0.695175409
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volume<0.0510017574
nsites<0.944444418
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References

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19 S. Ravichandiran, Hands-On Deep Learning Algorithms with Python: Master deep learning algorithms with extensive math by implementing them using TensorFlow (Packt Publishing Ltd, 2019).

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thank.png