DEVELOP MULTI-MODAL TRANSFORMERS TO PREDICT DENSITY OF STATES FOR CRYSTALLINE STRUCTURES

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1 PROJECT OVERVIEW

The density of states (DOS) provides critical insight into the distribution of electron states across energy levels within solid materials, influencing various properties such as conductivity, thermal behavior, and optical characteristics. However, accurately determining the DOS distribution poses challenges, particularly in complex crystal structures or materials with strong electron-electron interactions. Conventionally, addressing these challenges involves a combination of high-energy resolution experimental techniques and precise theoretical modeling.

Theoretical models, such as density functional theory (DFT), traditionally compute DOS by analyzing the electronic band structure of materials. However, this approach is resource intensive, time consuming, and costly. Machine learning (ML) offers an alternative route that bypasses the need for extensive experimentation or domain expertise. For example, Chandrasekaran et al. utilized neural networks to predict DOS by mapping the atomic environment around each grid point to the corresponding electron density and the local density of states.

Recently, Namkyeong et al. introduced a multimodal transformer to integrate information from both the structure of the crystalline material and its energy levels, thus predicting DOS. In this project, our aim is to replicate the specific results of the authors' paper, particularly focusing on the multimodal transformer, prompt tuning, and positional encoding. Additionally, we also aim to access the impact of different atomic embeddings on the Transformer's performance.

2 DATASET

For this project, we will use two datasets utilized in the aforementioned publication. The first data set consists of DOS phonons previously used in previous work and the authors of the publication we consider developed a data set consisting of DOS electronic for crystalline materials. In their work, the authors also evaluate model performance metrics on 2 variants of the Electron DOS dataset, in-distribution and out-of-distribution. For the in-distribution setting, they randomly split the dataset into a train/valid/test of 80/10/10% and for the out-of-distribution setting, the dataset is split based on the structure of the crystals.

3 METHODS & POTENTIAL EXTENSIONS

We propose reproducing the DOSTransformer model, which is a multi-modal transformer that considers both the atoms and energy levels of the crystalline material and employs a multi-head cross-attention mechanism to model their relationships. Atom embeddings are generated by a Graph Neural Network (GNN) based on the connectivity and features of neighboring atoms. The energy levels are embedded as one-hot vectors and concatenated with atom embeddings. We also plan to evaluate our DOSTransformer against several baseline models such as Multi-Layer Perceptron, Graph Neural Networks, and E3NN- Euclidean network for encoding material representation for two scenarios: Phonon DOS and Electron DOS. We shall consider MSE, MAE and R^2 as performance metrics. Finally, we shall also perform hyperparameter tuning of our DOSTransformer model using Weights

and Biases. Kindly, note that we plan to stay consistent with the author's implementation of different base-line architectures. We shall use PyTorch to code all of these architectures.

We plan to extend the study above by using the Variational Auto Encoder (VAE) to learn the latent space of the crystal structures and use those as the atomic embeddings. This will elucidate the impact of atomic embeddings towards the density of states prediction. Moreover, upon availability of sufficient time, we also plan to test the DOSTransformer performance trained on a different set of embeddings obtained using Contrastive Learning as described in a recent article by Kong et. al.

4 REFERENCES

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