Motivation

- 2D layered materials have emerged as an important subdiscipline in nanotechnology.
- The few 2D materials studied so far have shown extraordinary electrical, mechanical, thermal, and optical properties that can be utilized in fabricating next-generation transistors, sensors, and energy devices.
- The band gap (Eg) of a material plays a critical role in determining its properties. 2D materials have significantly different band gaps compared to their 3D bulk counterparts.
- Computational/experimental methods enable fast predictions.

Problem Definition

Use deep learning techniques to predict the band gaps of 2D materials from the properties of their 3D bulk counterparts.

Data and Features

- MLP and Linear Regression Models: The dataset contains 694 samples (chemical compounds) of 2D materials with their PBE-calculated band gap values ranging from 1.0 to 6.9 eV.
- Baseline Model for Transfer Learning: This dataset contains 6105 samples of 3D bulk materials. The input features include the samples’ bulk properties such as bulk band gap, density, crystal system, etc.
- Pre-processing: For both the models, only the most stable compounds for the given composition were used.

Models and Cost Functions

<table>
<thead>
<tr>
<th>Models</th>
<th>Cost Function</th>
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<tbody>
<tr>
<td>Linear Regression</td>
<td>$\text{Cost} = \frac{1}{2} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$</td>
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<tr>
<td>Multilayer Perceptron (MLP)</td>
<td>$\text{Cost} = \frac{1}{2} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$</td>
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Analysis

Model Comparison with Standard

- No comparison standard for 2D material band gaps in literature, band gap prediction has only been done for 3D materials.
- Previous neural networks that predicted 3D material band gaps have had Mean Square Error (MSE) ranging from 0.5 - 8 units.
- All three models for the 2D dataset had lower error than the 3D prediction models — may indicate that 2D band gaps are easier to predict.

Results

- Frozen for new model
- Retrained in new model

Model Analysis

- All three models obtained their lowest MSE when optimized with the Adaptive Moment Estimation (Adam) algorithm.
- Both the MLP and the model used for transfer learning were trained with mini-batches of size 32 (resulting in the spikes in the loss curve).
- Initially, the model used for transfer learning overfit the data (high training set MSE, high validation set MSE). To address this, we reduced the number of neurons in each layer.
- MSE of the model used for transfer learning was higher than the MSE of the standard MLP - this may be due to the higher MSE of the MLP for the 3D dataset, since its larger size causes overfitting.

Future Work

- Utilize a database that specifies the band gap type (direct/indirect) to better understand the properties of each material.
- Train a Convolutional Neural Network (CNN) on a database of the band structure images to get better predictions.
- Use one-hot vector encoding that uses a vector of length that equals the total number of elements present in the dataset, so the neural network can learn about each element individually.

References