MT-CGCNN: Integrating Crystal Graph Convolutional Neural Network with Multitask Learning for Material Property Prediction

Soumya Sanyal, Janakiraman Balachandran, Naganand Yadati, Abhishek Kumar, Padmini Rajagopalan, Suchismita Sanyal, Partha Talukdar

MOTIVATION

The motivation for this work was to develop accurate, transferable and computationally inexpensive machine learning models that can accelerate the discovery and development of new materials. Some of the major challenges:

- Limited availability of materials data as compared to other domains
- Lack of universal descriptor for different materials to explain its various properties

CONTRIBUTION

- Effective multi-tasking framework for material property prediction using crystal Graph Convolutional Networks
- Demonstrate the ability of our model to learn from fewer samples
- Empirically show superior predictive performance on metal/nonmetal classification task

MULTI-TASK LEARNING

Hard parameter sharing The architecture shares a common set of layers across all tasks and then some task-specific output layers are present for each individual task. The key motivation is to force the model to learn better representations that can be used to learn multiple related tasks at the same time.

Soft parameter sharing Here, there are independent models with own set of parameters for each of the tasks being learned. But then, the distance between the parameters are regularized to encourage learning of similar parameters for the different models.

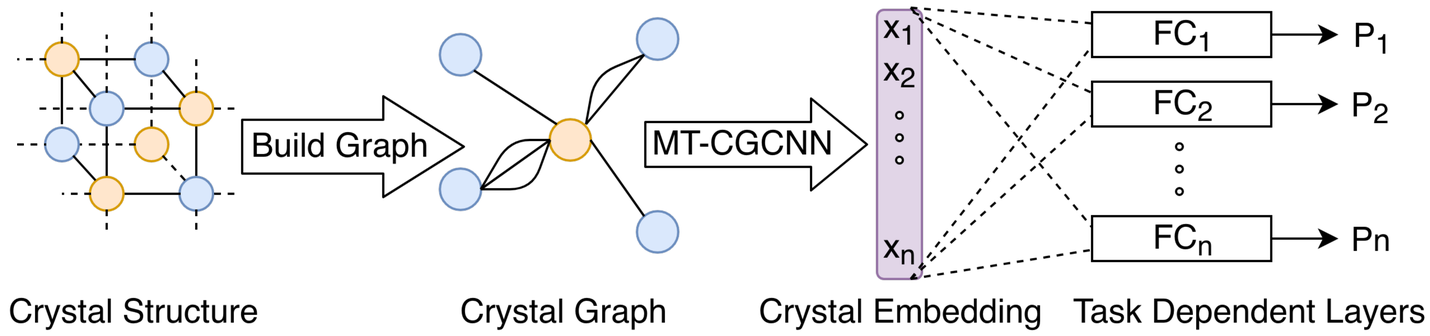
Benefits of MTL:

- The learned crystal representations are well generalized since its able to explain multiple properties/aspects of the crystal through a single representation
- Due to sharing of parameters, our model is parameter efficient and is able to train quicker than single task learning

FUTURE DIRECTIONS

In future, we plan to implement soft parameter sharing and include more material properties. Also, we plan to implement dynamic weighted loss formulation to reduce hyperparameter tuning efforts for training the model.

PROPOSED METHOD



The architecture of MT-CGCNN consists of three parts:

1. **Generating graph from given crystal structure:** Builds a graph from the Crystallographic Information File (CIF) where the nodes represent the atoms and edges represent the bonds.
2. **Graph Convolutional Network (GCN):** Learns atom embeddings using a crystal GCN formulation defined by Xie and Grossman[1].

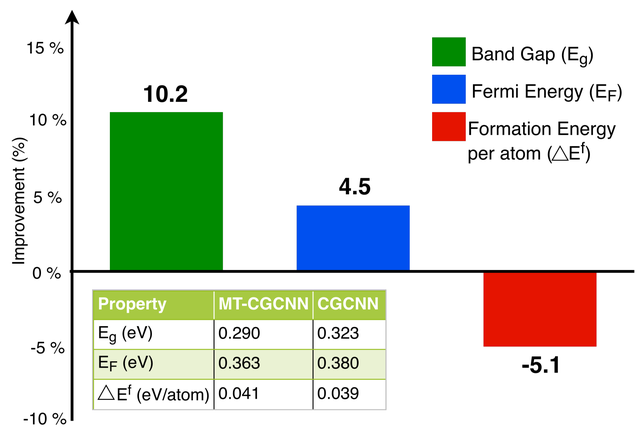
$$\boldsymbol{v}_i^{(t+1)} = \boldsymbol{v}_i^{(t)} + \sum_{j,k} \sigma(\boldsymbol{z}_{(i,j)_k}^{(t)} \boldsymbol{W}_c^{(t)} + \boldsymbol{b}_c^{(t)}) \odot g(\boldsymbol{z}_{(i,j)_k}^{(t)} \boldsymbol{W}_s^{(t)} + \boldsymbol{b}_s^{(t)})$$

   Pooling of the atom embeddings then give a crystal graph embedding.

3. **Fully-connected networks:** The crystal embedding is used by multiple fully-connected non-linear layers to predict various material properties in tandem. Weighted mean-squared error formulation is used as loss function for training the model.

RESULTS

Plot depicting percentage improvement that MT-CGCNN achieves over the CGCNN baseline for various material properties. The metric used is Mean Absolute Error. For Band Gap prediction, there's a **10% improvement** when jointly predicted with Formation Energy.



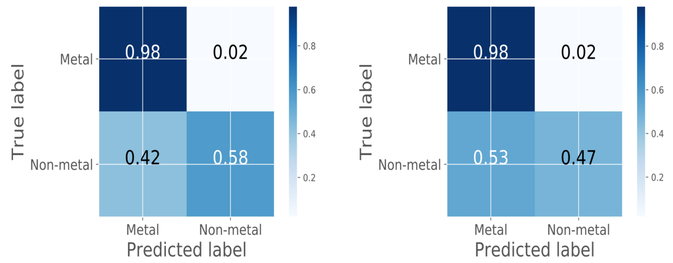
Property	MT-CGCNN	CGCNN
E_g (eV)	0.290	0.323
E_F (eV)	0.363	0.380
$\triangle E^f$ (eV/atom)	0.041	0.039

Table showing Band Gap prediction with reduced training data using CGCNN and MT-CGCNN. We observe comparable performance of MT-CGCNN even for **33% reduced training data**.

E_g prediction	30%	40%	50%	60%
CGCNN	0.385	0.356	0.332	**0.323**
MT-CGCNN	0.346	**0.326**	0.301	0.290

ERROR ANALYSIS

Confusion matrix for metal/nonmetal classification task. Band Gap(E_g) is used for the classification with a thresholding at 0.025eV ($=k_BT$ at room temperature). MT-CGCNN (left) performs better than the CGCNN baseline (right).



SOURCE CODE

https://github.com/soumyasanyal/mt-cgcnn/

Contact
soumyasanyal@iisc.ac.in
J.Balachandran@shell.com

REFERENCES

[1] Tian Xie and Jeffrey C. Grossman. Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties. *Phys. Rev. Lett.*, 120:145301, 2018.