

Utilizing Neural Networks to Design High-Entropy Functional Alloys

Emi Sohi, Mechanical Engineering
Mentor: Houlong Zhuang
Ira A. Fulton School of Engineering



Abstract

This research presents an innovative approach that integrates Graph Neural Networks (GNNs) and Feedforward Neural Networks (FNNs) with Density Functional Theory (DFT) and classical molecular dynamics simulations for the data-driven design of high-entropy alloys (HEAs) with superior thermoelectric properties. Leveraging a diverse dataset of HEAs and the power of machine learning, this integrated framework expedites materials design by predicting key thermoelectric properties, offering a promising pathway for the development of sustainable thermoelectric technologies and underlining the potential of data-driven approaches in materials science.

Goals

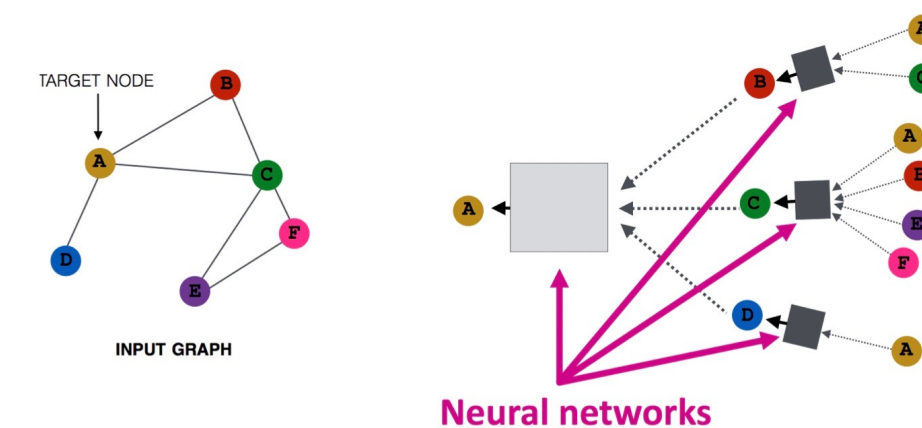
Train a GNN to predict thermoelectric properties, such as the Seebeck coefficient, electrical conductivity, and thermal conductivity. This involves using labeled data to teach the GNN how to relate the material's atomic structure to its thermoelectric behavior.

- Assign nodes in the graph to represent individual atoms or molecules within the material.
- Assign edges in the graph to represent the interactions or connections between atoms
- Generate network graphs using a network visualization library.

Current Progress

Leveraging Density Functional Theory (DFT) datasets, machine learning (ML) techniques are employed to develop Atomic Interaction Models (AIMs). These AIMs serve as efficient alternatives to labor-intensive first-principles thermodynamics simulations, enabling simulations at previously unattainable length and time scales.

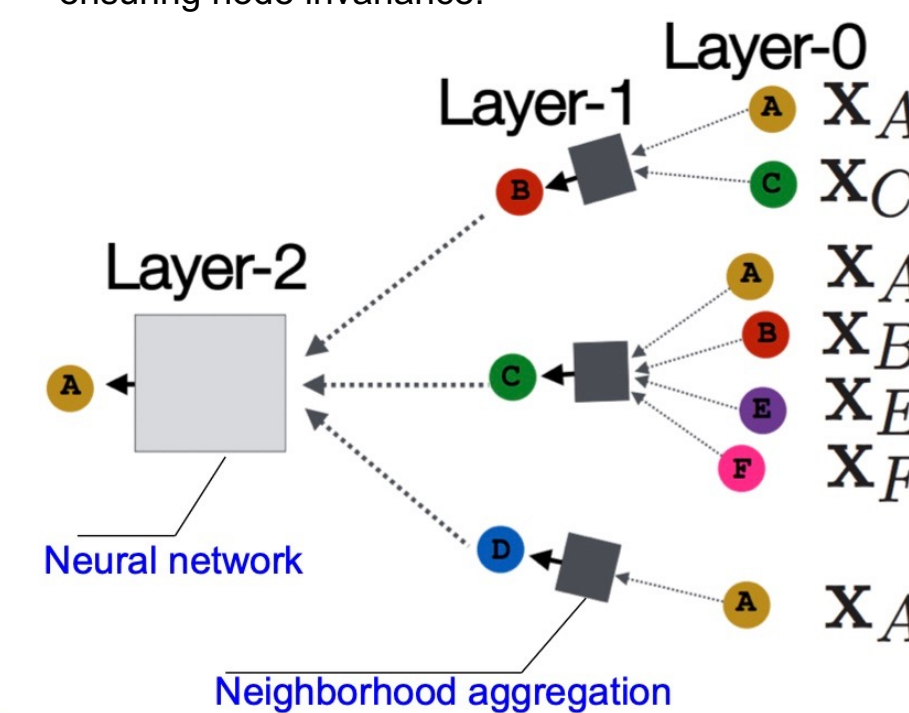
Figure 2. This figure shows how Nodes aggregate information from their neighbors using neural networks



Reference: The graph neural network model. McGill University. (n.d.). https://cs.mcgill.ca/~wh/comp766/files/chapter4_draft_mar29.pdf

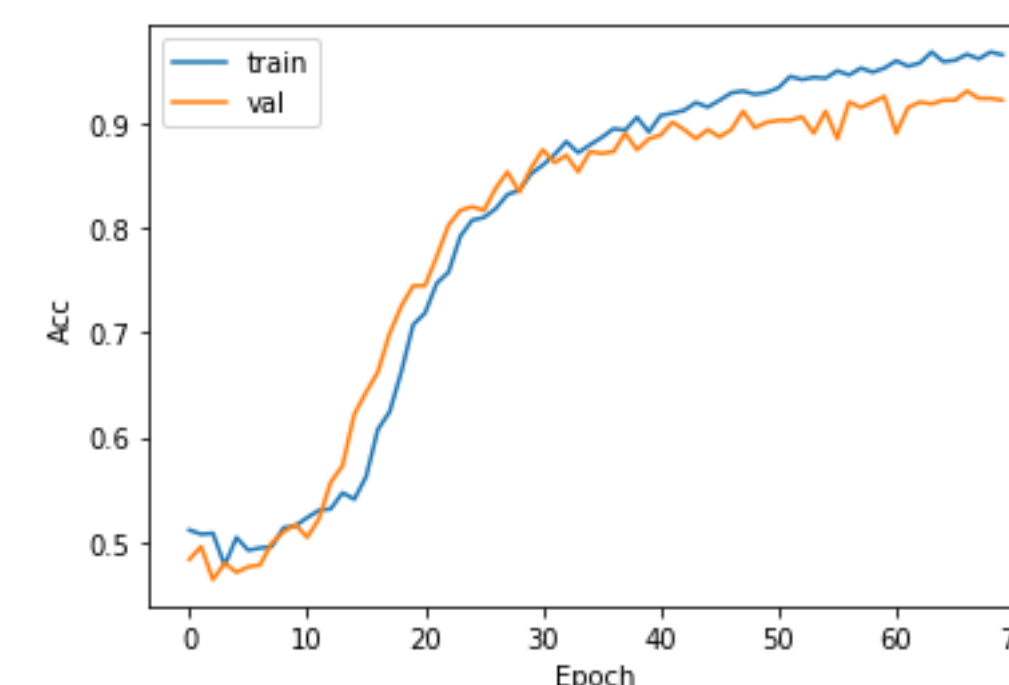
ML models have demonstrated excellent performance in predicting the bulk properties of HEAs, such as phase formations and mechanical properties.

Figure 1. This figure shows the system for aggregating information from neighbors and ensuring node invariance.

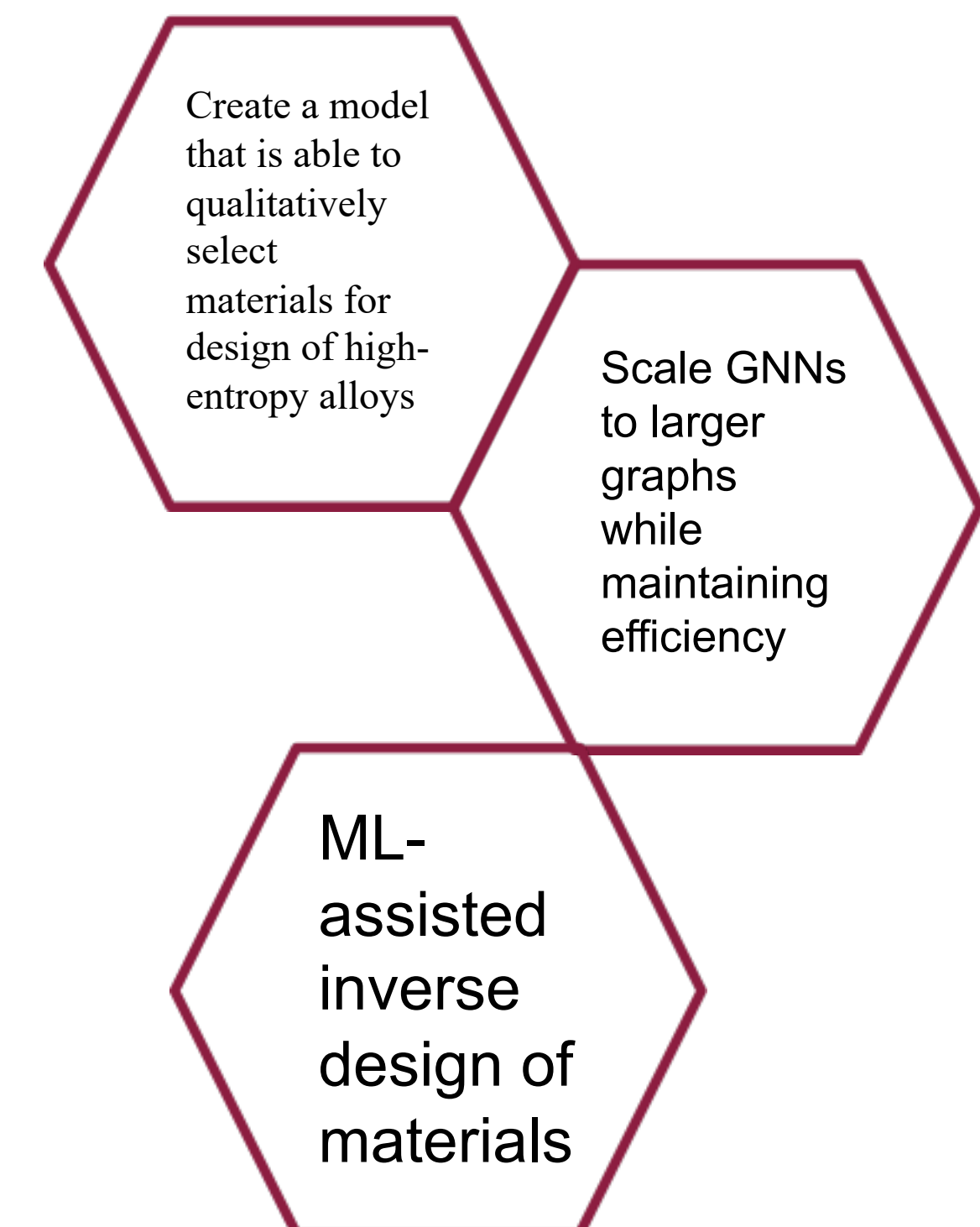


Reference: Stanford. (n.d.). Graph Neural Networks. <https://snap-stanford.github.io/cs224w-notes/machine-learning-with-networks/graph-neural-networks>

Figure 3. This figure shows the accuracy of the model for the training and validation data over epochs. After 70 epochs, the accuracy is above 90%



Future Work



References

- Finn, P. A., Asker, C., Wan, K., Bilotti, E., Fenwick, O., & Nielsen, C. B. (2021, June 4). *Thermoelectric materials: Current status and future challenges*. *Frontiers*. Retrieved March 14, 2023, from <https://www.frontiersin.org/articles/10.3389/femat.2021.677845/full>
- Li, X., Zhang, J., & Pei, Z. (2022, September 15). *Machine learning for high-entropy alloys: Progress, challenges and opportunities*. *Progress in Materials Science*. <https://www.sciencedirect.com/science/article/pii/S0079642522000998>