UCLA

Predicting and Interpreting Energy Barriers of Metallic Glasses with Graph Neural Networks

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Motivation : AI for Material Science Research

- Metallic Glasses (MGs): Enjoy the advantages of plastics, metals, and ceramics.
- Scientists would like to explore material properties of MGs: ***Glass Transition, Plasticity, etc.***
    - What is the glass transition point?
    - How much force will cause plasticity?
- These properties are complicated and are hard to study directly.
- One approach is to study the **energy barrier** as an intermediate step, which is highly correlated with the material properties.

Background on Material Science

- Energy Barriers: Measure the average energy difference between the atom’s stable state and the transition state.

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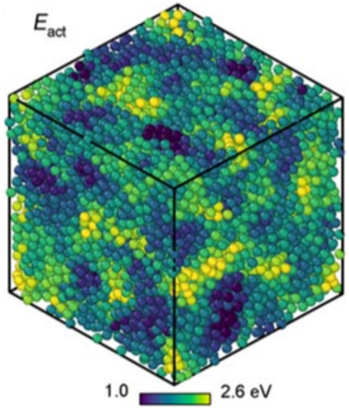
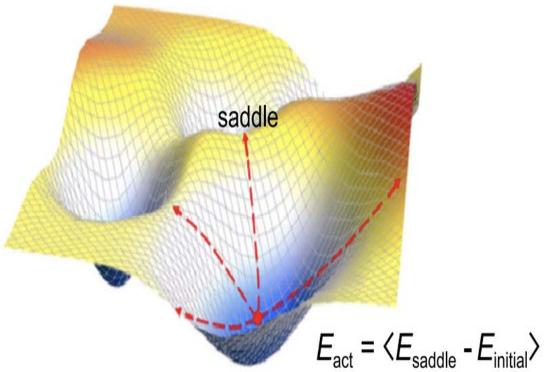


Individual Atom



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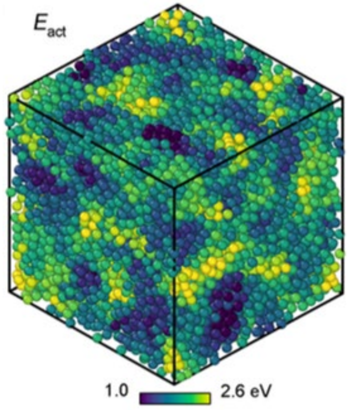
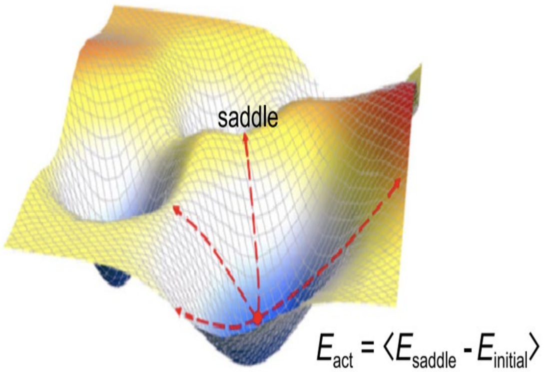


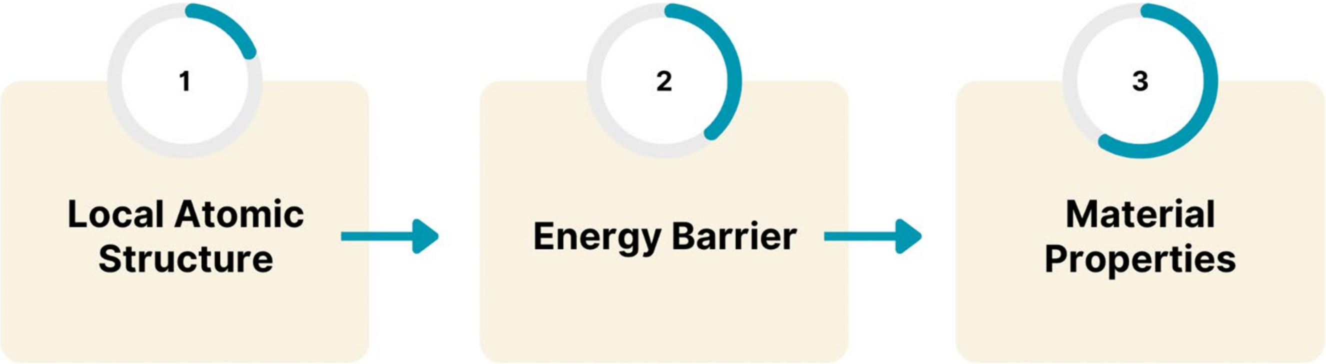
Individual Atom



- Energy barriers can be computed from the local atomic structure, but the computation is **slow.**

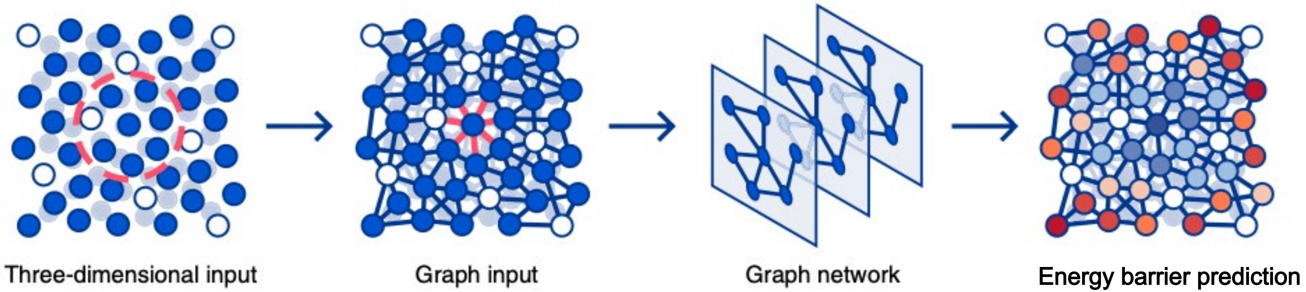
Project Goal

- Using AI models to **efficiently** predict the energy barrier from the local atomic structure.



A Graph Machine Learning Formulation of Energy Barrier Prediction

- We phrase energy barrier prediction as a ***graph node regression problem***



- Atoms ⇒ Nodes, Connecting close atoms ⇒ Edges, Energy Barriers ⇒ Numeric labels
- Atom Type ⇒ Node Feature, Relative distance in 3D coordinates ⇒ Edge Feature

Image credit: Bapst, V., Keck, T., Grabska-Barwińska, A., Donner, C., Cubuk, E. D., Schoenholz, S. S., ... & Kohli, P. (2020). Unveiling the predictive power of static structure in glassy systems. *Nature Physics*, *16*(4), 448-454.

Challenges and Solutions

- Energy barriers are ***invariant under orthogonal transformations,*** e.g. reflection and rotation, of the atomic structure

- Existing AI models ***cannot*** capture this invariance thus lead to poor prediction performance

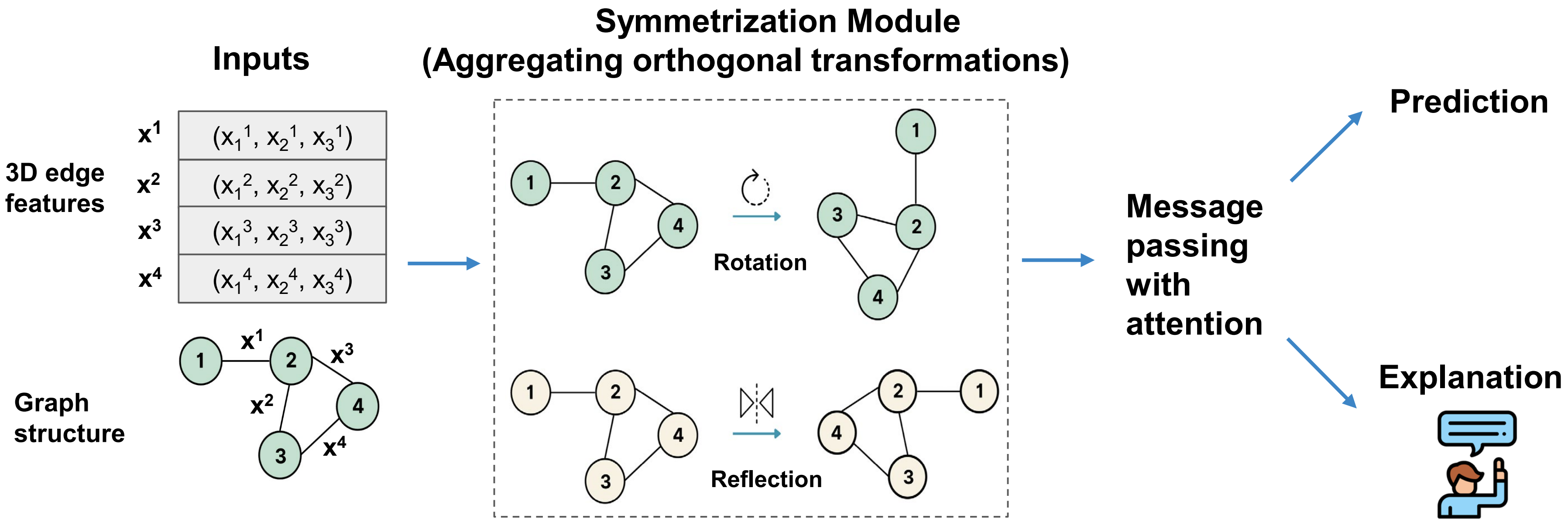
- We propose SymGNN

  Symmetrization module + message-passing module

  Symmetrization by aggregating orthogonal transformations of the graph

  Message-passing with attention on symmetrized edge features

SymGNN Model Architecture



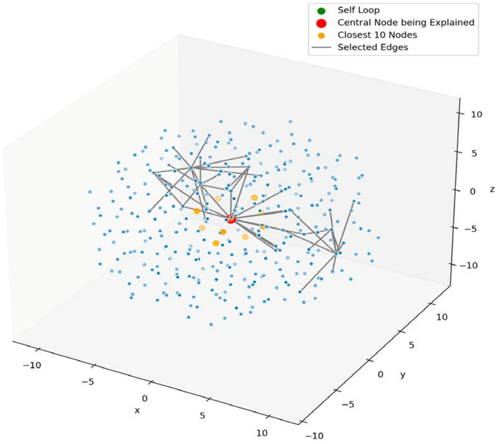
Experiments: Prediction Correlation

	Training Score	Testing Score
SymGNN (Ours)	**0.85**	**0.78**
GCN	0.15	0.10
GCN with Edge Features	0.80	0.71
Equivariant GNN	0.65	0.45
MLP	0.05	0.03

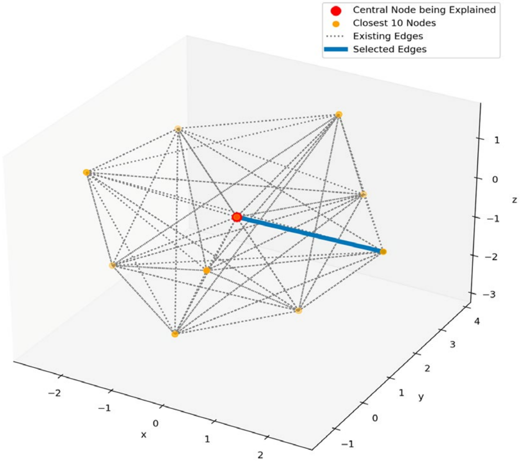
Interpreting Energy Barrier Predictions

- We explain the energy barrier predictions by identifying the important edges
  - Find edges that can maximize the mutual information

Global Version



Local Version



Q & A

Extra Slides

Experiments: Datasets and Evaluation Metrics

- 6 Train Graphs, 1 Validation Graph, 2 Test Graphs. Each graph has ~8000 nodes and ~260000 edges. Edge are constructed between nodes with Euclidean distance less than a threshold.
    - Collecting energy barrier data is challenging because simulating the true measurement is time consuming.

- Model is trained on <u>MSE loss</u>, and performance is measured by the <u>Pearson correlation</u> between the predicted energy barriers and the true energy barriers.

Ablation Studies

- We remove the symmetrization module to observe its effectiveness

	Training Score	Testing Score
SymGNN	0.85	0.78
SymGNN with no symm module	0.87	0.71

Best model on validation set

- Significant performance dropped when we remove the symmetrization layer