CRACK: Contrastive Relational-Aware Compression of Knowledge for Machine Learning Force Fields

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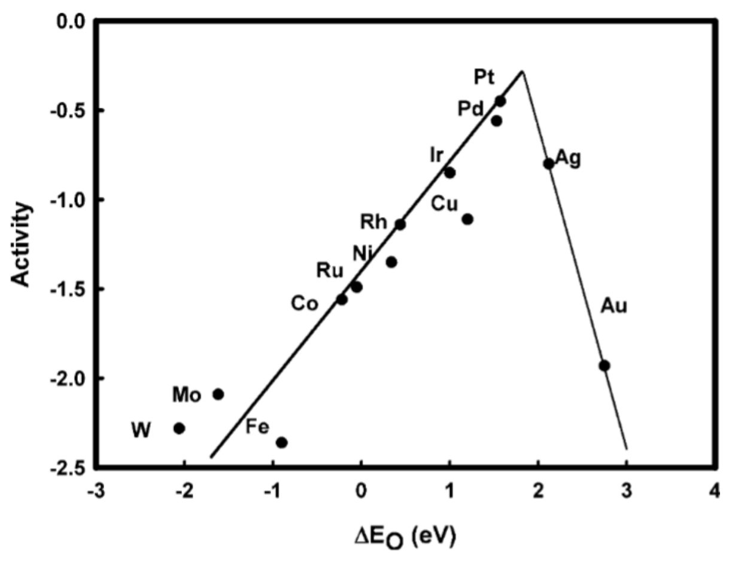
Introduction

Application Domain:

- Accelerating the **discovery of novel catalyst materials** for the **oxygen reduction reaction (ORR)** which is critical in fuel cells.

Governing Problem:

- Developing a **high-performance, low-cost catalyst** for the ORR is a critical challenge to overcome the limitations of platinum (Pt).
  (Nørskov, J. K., et al. JPCB 108.46 (2004): 17886-17892.)



Barrier to Discovery:

- Screening **vast materials search space** to find optimal catalyst.
- Density Functional Theory (DFT) are accurate, but have **infeasible computational cost** for large-scale screening.
- Fundamental **trade-off**: simulation accuracy & scope of the search.
- Research on Machine Learning Force Fields (MLFFs) to break this trade-off by providing both **high accuracy & speed.**
  (Unke, O. T., et al. Chemical Reviews 121.16 (2021): 10142-10186.)

Motivation

Problem Domain:

- Knowledge distillation for Machine Learning Force Fields (MLFFs) to enable efficient molecular simulations.

Existing Challenges:

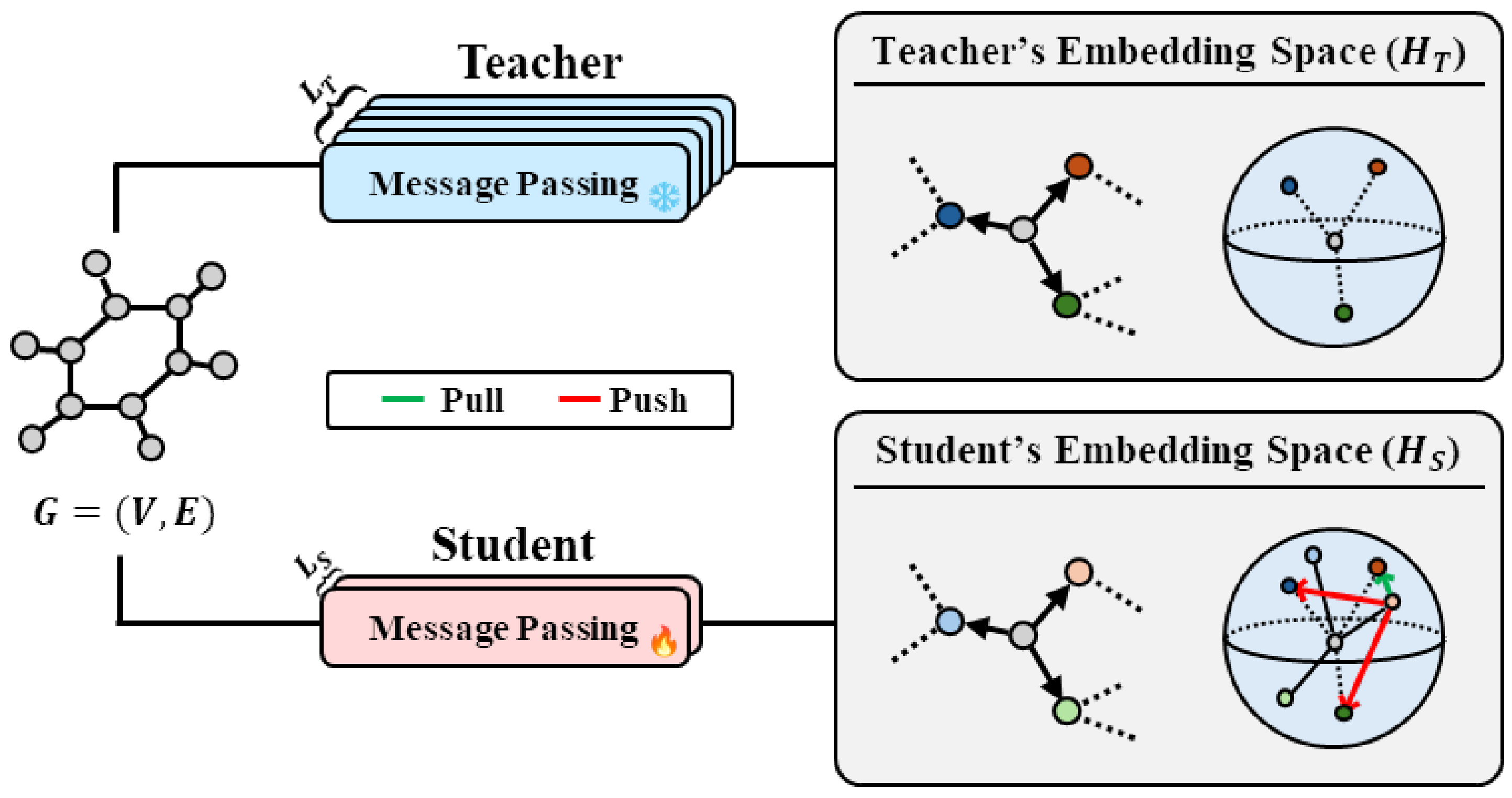
- Trade-off between accuracy and computational efficiency in molecular dynamics simulations.
- State-of-the-art equivariant GNNs (like EquiformerV2) achieve high accuracy but have **substantial computational cost.**
  (Liao, Y., et al. The Twelfth International Conference on Learning Representations (2024))
- This limits adoption in large-scale molecular dynamics, **high-throughput materials screening**, and drug discovery.

Limitation of Previous Approaches:

- Simplistic atom-wise feature matching that treats atoms as independent entities.
- Missing the crucial physics: how atoms **interact with neighbors** to define the potential energy surface (PES).

Methods

CRACK Architecture:



Key Components:

1. **Relational Vectors:**
   - Derived from learned atomic embeddings of bonded atom pairs ($\boldsymbol{z}_{src} - \boldsymbol{z}_{dst}$).
   - Serve as proxies for teacher's learned representation of interatomic potentials.
2. **Contrastive Learning:**
   - InfoNCE loss trains student to generate relational vectors uniquely identifiable with teacher counterparts.
   - Each teacher relational vector forms positive pair with corresponding student vector.
   - All other student vectors in batch serve as negatives.

Advantages:

Physics-Informed

O(E) Scalability

Applicability

Results

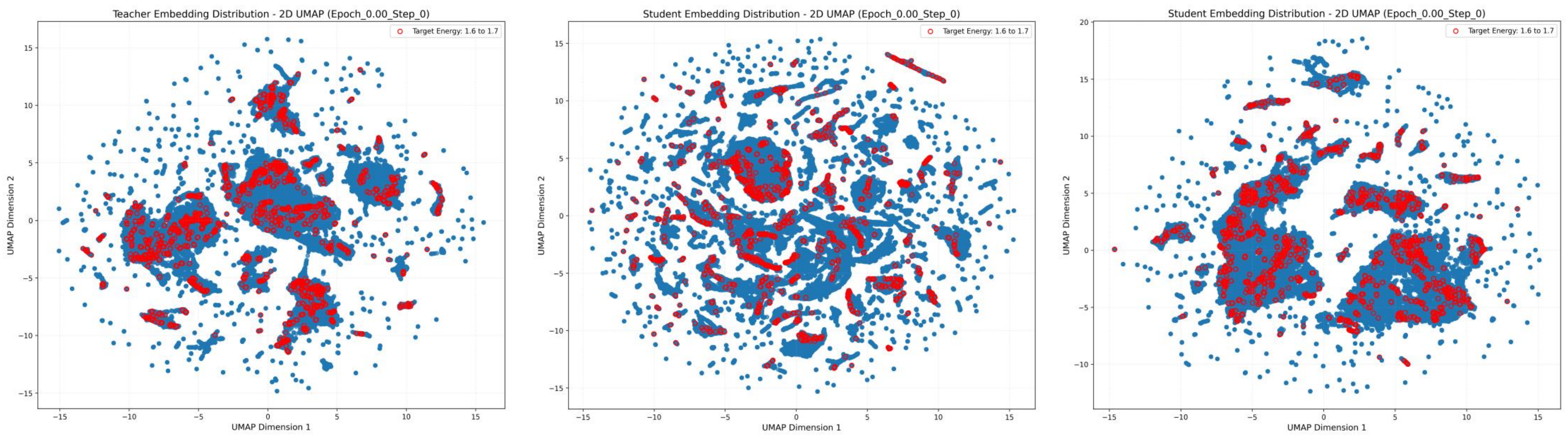
O* Subset of OC20 dataset:

Method	Params	Embedding		Energy	Force
		MAE	Cosine Similarity	MAE ↓ (meV)	MAE ↓ (mev/Å)
Teacher	**153M**	**-**	**-**	**39.8**	**5.8**
vanilla	22M	0.217	0.205	294.5	5.9
pretrained	22M	0.311	0.271	263.6	6.1
n2n	22M	0.078	0.839	252.9	5.8
Hessian	22M	1.062	0.073	363.5	26.1
Ours	**22M**	**0.282**	**0.230**	**234.1**	**6.1**
Ours (w/ n2n)	**22M**	**0.082**	**0.820**	**231.7**	**5.8**

200K Subset of OC20 dataset:

Method	Params	Embedding		Energy	Force
		MAE	Cosine Similarity	MAE ↓ (meV)	MAE ↓ (mev/Å)
Teacher	**153M**	**-**	**-**	**171.5**	**12.4**
vanilla	22M	0.309	0.233	474.9	51.8
pretrained	22M	0.181	0.460	410.8	37.6
n2n	22M	0.096	0.816	412.8	34.8
Hessian	22M	0.351	0.180	419.3	48.6
Ours	**22M**	**0.190**	**0.424**	**373.8**	**35.8**
Ours (w/ n2n)	**22M**	**0.097**	**0.811**	**371.1**	**34.1**

Visualization of Embeddings for O* Subset:



Teacher **n2n** **CRACK**

Conclusion & Future Work

Key Contributions:

- First KD framework to directly distill **first-order interatomic relational knowledge** for MLFFs.
- Novel **relational-contrastive loss** that captures geometry of teacher's learned PES.
- **State-of-the-art performance** on OC20, significantly outperforming baselines.

Future Directions:

- More **sophisticated relational descriptors** incorporating higher-order structural features.
- Application to **high-throughput materials discovery** by enabling rapid screening of large material databases with compressed yet accurate models.

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