Statement of Purpose
of Yinan Huang (CS Master/PhD applicant for Fall–2023)

My research interests are theories and methodologies of graph neural networks, geometric deep learning and equivariant neural networks, and their applications in sciences such as computational chemistry and combinatorial optimization. I find it particularly fascinating to analyse and develop deep learning models on data with certain "structures", such as combinatorial structures on graphs and Euclidean structures on point clouds. They are closely related to a key concept called **equivariance** in geometric deep learning, which view the data as fields distributed on a space with certain symmetries and studies the classes of models preserving these symmetries. The equivariance essentially emerges in the form of parameter sharing, resulting in a data-efficient and well-generalized models. These symmetry-aware models are highly suitable to fit into problems of chemistry, biology and some of combinatorial optimizations, since symmetries arise naturally in these fields. In short, geometric deep learning is intriguing to me as it is an interdisciplinary direction that uses **geometric and algebraic** tools to develop computational deep models, and has wide applications in scientific problems. Below I list a few relevant projects that I worked on.

Equivariant generative models for 3D linker design. Deep learning has achieved tremendous success in designing novel chemical compounds with desirable pharmaceutical properties. But they usually generate the whole molecule from scratch. In our work, we focus on a new drug design problem called linker design: generate a linker molecule that integrates two given fragment molecules. Previous relevant works model it as either graph completions or text translations, ignoring the rich information in molecules' 3D geometry. To this end, we propose to integrate the encoding and decoding of 3D coordinates into the graph generative models, resulting in a 3D graph completion problem. It brings several advantages: one is that 3D information hopefully helps better supervise the reconstruction of the molecular graphs; another is that the generated 3D molecules are easily to be adapted to downstream 3D tasks. Regarding the methodology, a key observation is that generated coordinates should be equivariant to rigid body transformations of input fragments, while the generated graphs are invariant. To achieve such goal, we introduce both invariant and equivariant features in node representations, design an equivariant message passing scheme and an equivariant decoding strategy that can preserve the invariance and equivariance throughout. The resulting model named 3DLinker autogressively generate new atoms (invariant atom types, edge types and equivaraint atom coordinates) utill hitting the stop node. Empirically, 3DLinker brings significant improvements on graph recovery rate and coordinate prediction compared to previous works. See [1] for the paper.

Cycle counting power of graph neural networks. The expressive power is a important topic of graph neural networks (GNNs) research. The expressive power are usually measured by the discriminative power in comparison to k-dimensional Weisfeiler-Lehman test (k-WL), a classic graph isomorphism test heuristic. A widely used class of GNNs are message passing neural networks (MPNNs), whose discriminative power is bounded by 1-WL test. Many variants of GNNs are proposed to lift the discriminative power to be stronger than 1-WL and bounded by 3-WL, including a recent popular class of GNNs dubbed Subgraph MPNNs. The core idea of Subgraph MPNNs is to factorize a graph into a bag of subgraphs, each of which is tied with one specific node. The final graph representation is aggregated from subgraph representations. In our work, we propose to understand the expressive power of Subgraph MPNNs via their counting power of cycles and paths. On one hand, ability to count certain substructures give a more intuitive and precise description of model's expressive power, compared to lower and upper bounds of discriminative power; On the other hand, cycles play crucial roles in chemistry, e.g., ring systems. We prove that Subgraph MPNNs cannot count cycles with more than 4 nodes, indicating their bad cycle representation power. To further boost the counting power, we observe that Subgraph MPNNs' extra expressive power are from their node identifier. Thus We generalize Subgraph MPNNs to use a pair of node identifiers, resulting in a novel model named I^2-GNNs with strictly stronger expressive power. Remarkably, we prove that I^2-GNNs can count at least 6-cycles, covering common ring systems such as benzene rings. Moreover, given constant node degree, I^2-GNNs have a good scalability, i.e. linear complexity w.r.t. number of nodes. The manuscript is submitted to ICLR 2023 and is currently under review. Based on my research experiences, there are several topics I feel attractive and would like to explore during my PhD study.

Graph representation learning

A main direction of graph representation learning is to design expressive and scalable invariant/equivariant graph neural networks. The basic MPNNs have good scalability, i.e., linear complexity, but their expressiveness is limited. High-order GNNs, such as [2, 3], and some permutation-invariant universal architectures, such as [4], are provably expressive but computationally unaffordable for large-scale graphs. Thus how to balance the trade-off between expressiveness and scalability is an challenging as well as practical topic. Particularly, there are attempts to leverage the graph sparsity for better scalability, but the design space and the impact of such localization on theoretical expressiveness are still unclear or not fully understood.

Equivariant neural networks

Generally, turning an arbitrary network in an equivariant one shrinks the size of function class and may damage the expressive power, since it brings redudant and unexpected symmetry to the weights. For instance, graph neural network, as a special permutation equivariant networks, is not universal regardless of the hidden dimension. Thus further characterizing the expressive power of varieties of equivariant neural networks is an interesting topic. On the other hand, it is an exciting challenge to adapt equivariance to generative models, i.e., modeling a equivariant probability distribution. There are still a lot to do to understand the design space and the theory of equivariant generative models.

Machine learning for science

The applications of deep learning in computational chemistry and drug design are closely related to graph representation learning and equivaraint neural networks. Data in these fields usually has complex geometry and inspire new methodology of developing geometric deep models. On the other hand, it would be exciting to explore the possibility of using graph neural networks to solve combinatorial optimization such as mixed integer linear programming.

I am applying to M.S. in Mila due to its leading position in deep learning research. I am particularly interested in joining of group of Professor **Siamak Ravanbakhsh**, Professor **Jian Tang** and Professor **Guillaume Rabusseau**. Prof. Siamak Ravanbakhsh participated in many renown works on equivariant neural networks (e.g., DeepSets [5], Equivariance Through Parameter sharing [6]), which aligns with my interests. Prof. Jian Tang's works on network embedding, graph neural networks for drug design and geometric deep learning also match my research interests. His recent works [7, 8] on molecular conformation generation are really impressive. The generative model (probability distribution) is well adapted to preserve E(3) equivariance. Prof. Guillaume Rabusseau mainly studies tensor networks, an important computational tool in many-body quantum physics. Interestingly, it can also be applied to development of machine learning models, e.g. graph neural networks [9], since graphs essentially express interaction/relation between nodes. In sum, I really hope that I can join Mila, work with outstanding professors and contribute to the development of AI.

References

[1] **Yinan Huang**, Xingang Peng, Jianzhu Ma, and Muhan Zhang. 3DLinker: An E (3) Equivariant Variational Autoencoder for Molecular Linker Design. In *International Conference on Machine Learning*, pages 9280–9294. PMLR, 2022.

[2] Christopher Morris, Martin Ritzert, Matthias Fey, William L Hamilton, Jan Eric Lenssen, Gaurav Rattan, and Martin Grohe. Weisfeiler and leman go neural: Higher-order graph neural networks. In *Proceedings of the AAAI conference on artificial intelligence*, volume 33, pages 4602–4609, 2019.

[3] Haggai Maron, Heli Ben-Hamu, Nadav Shamir, and Yaron Lipman. Invariant and equivariant graph networks. *arXiv preprint arXiv:1812.09902*, 2018.

[4] Ryan Murphy, Balasubramaniam Srinivasan, Vinayak Rao, and Bruno Ribeiro. Relational pooling for graph representations. In *International Conference on Machine Learning*, pages 4663–4673. PMLR, 2019.

[5] Manzil Zaheer, Satwik Kottur, Siamak Ravanbakhsh, Barnabas Poczos, Russ R Salakhutdinov, and Alexander J Smola. Deep sets. *Advances in neural information processing systems*, 30, 2017.

[6] Siamak Ravanbakhsh, Jeff Schneider, and Barnabas Poczos. Equivariance through parameter-sharing. In *International conference on machine learning*, pages 2892–2901. PMLR, 2017.

[7] Minkai Xu, Wujie Wang, Shitong Luo, Chence Shi, Yoshua Bengio, Rafael Gomez-Bombarelli, and Jian Tang. An end-to-end framework for molecular conformation generation via bilevel programming. In *International Conference on Machine Learning*, pages 11537–11547. PMLR, 2021.

[8] Minkai Xu, Lantao Yu, Yang Song, Chence Shi, Stefano Ermon, and Jian Tang. Geodiff: A geometric diffusion model for molecular conformation generation. *arXiv preprint arXiv:2203.02923*, 2022.

[9] Chenqing Hua, Guillaume Rabusseau, and Jian Tang. High-order pooling for graph neural networks with tensor decomposition. *arXiv preprint arXiv:2205.11691*, 2022.