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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 analyze 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 views 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 data-efficient and well-generalized models. These symmetry-aware models are highly suitable to fit into problems of chemistry, biology and some 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 easy 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 a goal, we introduce both invariant and equivariant features in node representations, and design an equivariant message-passing scheme and an equivariant decoding strategy that can preserve the invariance and equivariance throughout. The resulting model named 3DLinker auto-regressively generates new atoms (invariant atom types, edge types and equivariant atom coordinates) utill hitting the stop node. Empirically, 3DLinker brings significant improvements in graph recovery rate and coordinate prediction compared to previous works. See [1] for the paper.

Cycle counting power of graph neural networks. Expressive power is an important topic of graph neural networks (GNNs) research. The expressive power is usually measured by the discriminative power in comparison to the 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 the 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 to 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, the ability to count certain substructures gives a more intuitive and precise description of the 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 is 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 has good scalability, i.e. linear complexity w.r.t. the 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

One of the main directions 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 a 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 into an equivariant one shrinks the size of the function class and may damage the expressive power, since it brings redundant and unexpected symmetry to the weights. For instance, a graph neural network, as a special permutation equivariant network, 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 an equivariant probability distribution. There is 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 equivariant neural networks. Data in these fields usually have complex geometry and inspire new methodology for 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 the group of Professor **Siamak Ravanbakhsh**, Professor **Jian Tang**, and Professor **Guillaume Rabusseau**. Prof. Siamak Ravanbakhsh participated in many renowned 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 the development of machine learning models, e.g. graph neural networks [9], since graphs essentially express interaction/relation between nodes. In sum, I hope that I can join Mila, work with outstanding professors and contribute to the development of AI.

References

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