Homomorphism Counts as Structural Encodings for Molecular Property Prediction

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Abstract

Graph Transformers are popular neural networks that extend the well-known Transformer architecture to the graph domain. These architectures operate by applying self-attention on graph nodes and incorporating graph structure through the use of positional encodings (e.g., Laplacian positional encoding) or structural encodings (e.g., random-walk structural encoding). The quality of such encodings is critical, since they provide the necessary *graph inductive biases* to condition the model on graph structure. In this work, we propose *motif structural encoding* (MoSE) as a flexible and powerful structural encoding framework based on counting graph homomorphisms. Theoretically, we compare the expressive power of MoSE to random-walk structural encoding and relate both encodings to the expressive power of standard message passing neural networks. Empirically, we observe that MoSE outperforms other well-known positional and structural encodings across a range of architectures, and it achieves state-of-the-art performance on widely studied molecular property prediction datasets.

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AI for New Drug Modalities at NeurIPS 2024.