VCU College of Engineering
Computer Science

"Graph Representation Learning & Deep Generative Models on Graphs"

12pm-1pm on September 30, 2022 via Zoom
https://vcu.zoom.us/j/82045305330

Abstract: Graph neural networks (GNNs) utilizing various ways of generalizing the concept of convolution to graphs have been widely applied to many learning tasks, including modeling physical systems, finding molecular representations to estimate quantum chemical computation, etc. Most existing GNNs address permutation invariance by conceiving of the network as a message passing scheme, where each node sums the feature vectors coming from its neighbors. We argue that this scheme imposes a limitation on the representation power of GNNs such that each node loses their identity after being aggregated by summing. Thus, we propose a new general architecture called Covariant Compositional Networks (CCNs) in which the node features are represented by higher order tensors and transform covariantly/equivariantly according to a specific representation of the symmetry group of its receptive field. Experiments show that CCNs can outperform competing methods on standard graph learning benchmarks and on estimating the molecular properties calculated by computationally expensive Density Functional Theory (DFT). This novel machine learning approach allows scientists to efficiently extract chemical knowledge and explore the increasingly growing chemical data.

Understanding graphs in a multiscale perspective is essential for capturing the large-scale structure of molecules, proteins, genomes, etc. For this reason, we introduce Multiresolution Equivariant Graph Variational Autoencoder (MGVAE), the first hierarchical generative model to learn and generate graphs in a multiresolution and equivariant manner. MGVAE is built upon Multiresolution Graph Network (MGN), an architecture which explicitly learns a multilevel hard clustering of the vertices, leading to a true multiresolution hierarchy. MGVAE then employs the hierarchical variational autoencoder model to stochastically generate a graph in multiple resolution levels given the hierarchy of latent distributions. Our proposed framework achieves competitive results with several generative tasks including general graph generation, molecule generation, unsupervised molecular representation learning, link prediction on citation graphs, and graph-based image generation. Future applications of MGVAE range from lead optimization enhancing the most promising compounds in drug discovery to finding stable crystal structures in material science.

Dr. Hy Truong Son is a Postdoctoral Fellow & Lecturer at the Halicioglu Data Science Institute of University of California, San Diego. He obtained a PhD and a MSc in Computer Science from The University of Chicago. He earned a BSc in Computer Science from Eotvos Lorand University in Hungary with a full scholarship from the Hungarian government. His research focuses on graph neural networks, deep generative models on graphs, multiresolution matrix factorization, graph wavelets, group equivariant and multiscale hierarchical models for the purpose of modeling, learning and generating graphs.