Geometric Deep Learning with Graph Neural Networks

Sergei Grudinin, Kliment Olechnovic, Rémi Vuillemot, Dmitrii Zhemchuzhnikov

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1. GNN Course: An Introduction to Graph Neural Networks in 3 Tutorials

Tutorial 1: Pytorch-geometric, Graph Notations, and Simple GCN

1. Introduction to Graphs
2. Setting up Pytorch-geometric
3. Graph Representation in Pytorch-geometric 4. Simple Graph Network Implementation

Tutorial 2: Graph Isomorphism and Custom MPNNs

1. Graph Isomorphism
2. Introduction to Message Passing Neural Networks (MPNNs)
3. Custom MPNNs using Pytorch-geometric

Tutorial 3: Spatial Graphs and SE(3)-equivariance

1. Introduction to Spatial Graphs
2. SE(3)-equivariance in Neural Networks
3. Implementing SE(3)-equivariant Neural Networks
4. Applications

2. Molecular graphs and node-based regression tasks

The purpose of this part will be constructing and testing GNN architectures that can predict node-level probabilities in molecular graphs constructed from protein molecules. The ultimate goal of the project is to compare multiple equivariant SE3 architectures and multiple representations and node embeddings for a specific task of predicting protein pocket identification.

1. The dataset for the node-based regression task is provided and described at https://github.com/kliment-olechnovic/apo-to-holo.

2. The preprocessing step requires some knowledge of C++ and computational geometry. The machine-learning task will be performed with Pytorch-Geometric.

3. The project requires weekly in-person meetings, and progressively written technical report (Latex, in English).