[Openreview 2020] TopoTER: Unsupervised Learning of Topology Transformation Equivariant Representations [paper]

Node/Graph Tasks: Node classification, graph classification

Training Type: pre-training and fine-tuning

Pretext task data: structure
The pretext task here is to train a GNN model such that the representations of nodes under two different graph topology is predictive of the transformation between these two different graph topology.

Initial short summary here
In view that the graph topology transformation is yet fully explored in unsupervised graph representation learning, thie paper proposes the Topology Transformation Equivariant Representation learning to infer unsupervised graph feature representations by estimating topology transformation.

First this paper transforms the original graph adjacency matrix A to $\tilde{A}$ by randomly adding or removing edges from the original edge set. Then by feeding the original and transformed graph topology and the node feature matrix into any GNN based encoder, we get the feature representation $\mathbf{H}, \tilde{\mathbf{H}}$ before and after topology transformation. Then they predict the topology transformation between node i and j through the node-wise feature difference $\Delta\mathbf{H}$ by constructing the edge representation as:

$$\mathbf{e}_{i,j} = \frac{\exp(-(\Delta\mathbf{H}_i - \Delta\mathbf{H}_j) \odot (\Delta\mathbf{H}_i - \Delta\mathbf{H}_j))}{||\exp(-(\Delta\mathbf{H}_i - \Delta\mathbf{H}_j) \odot (\Delta\mathbf{H}_i - \Delta\mathbf{H}_j))||} \tag{71}$$

The edge representation $\mathbf{e}_{ij}$ is then fed into MLP for the prediction of the topology transformation:

$$\tilde{y}_{i,j} = \text{softmax}(\text{linear}(\mathbf{e}_{i,j})) \tag{72}$$

The loss function is trained by minimizing the cross entropy.

Bibtex:
@misc gao2021topoter, title=Topo{TER}: Unsupervised Learning of Topology Transformation Equivariant Representations, author=Xiang Gao and Wei Hu and Guo-Jun Qi, year=2021, url=https://openreview.net/forum?id=9az9VKjOx00