[Openreview 2020] Motif-Driven Contrastive Learning of Graph Representations [paper]

Node/Graph Tasks: Graph classification

Training Type: comparing the pretraining-fine tuning and pre-training and linear classifier

Pretext task data: subgraph structure
The pretext task here is to optimize the GNN encoder by maximizing the similarity between positive pairs while minimizing the similarity between negative pairs. The positive pairs correspond to graph and motifs extracted from it while the negative pairs correspond to graph and motifs extracted from other graphs. Another novice is that the subgraph here is the motif which has the physical meaning in the specific task settings.

Initial short summary here
The general idea is to learn graph motifs as prototypical cluster centers of subgraph embeddings encoded by GNNs. The learned motifs can help generate more informative subgraphs for graph-to-subgraph contrastive learning. Given a dataset with M graphs $\mathbb{G} = \{\mathcal{G}_1, ..., \mathcal{G}_M\}$, the differentiable clustering learning is to learn the GNN-based graph encoder that maps input graphs to an embedding vector and to learn a K-slot embedding table where each slot is a motif vector corresponding to a cluster center of embeddings of frequently occurred subgraphs.

First subgraphs are generated by performing segmentation on a node affinity matrix A. Specifically GNN encoder is used to generate node embeddings of all nodes in the graph. Then we compute the node affinity matrix A as:

$$A_{s,t} = \text{softmax}(\phi(\mathbf{n}_s)^{\mathrm{T}}\phi(\mathbf{n}_t)/\tau_n), \tag{62}$$

where τ_n is the temperature, $\mathbf{n}_s$ is the node embedding of the node s. Then we perform spectral clustering on this affinity matrix to generate different groups, in which the connected components that have more than three nodes are collected as our sampled subgraphs and the their embeddings are generated by performing any permutation-invariant operation on all nodes belonging to those subgraphs.

The extracted subgraphs are then feed to the Motify learner to learn motifs by applying an Expectation-maximization style clustering algorithm. For each graph g_j, we calculate its cosine similarity with each of the K motif vectors. Then we get a similarity metric $S \in \mathbb{R}^{K\times N}$encoding all similarity information between each subgraph to each motif. Denoting the assignment matrix as $Q \in \mathbb{R}^{K\times N}$, we find the optimal Q by optimizing the following:

$$\max_{Q\in\mathcal{Q}} Tr(Q^{\mathrm{T}}S) + \frac{1}{\lambda}H(Q), \tag{63}$$

which is to maximize similarities between embeddings and its assigned motif and $H(Q) = -\sum_{i,j} Q_{ij} \log Q_{ij}$ which is to avoid all representations collapsing to a single cluster center. Then we maximize the log-likelihood of our data given the cluster assignment matrix Q by updating parameters in GNN encoder and the motif embedding table, which is equivalent to a supervised K-class classification problem with labels Q and predictions scores S. A columnwise softmax normalization with temperature τ_g is first applied to S to get the probabilities and then the negative likelihood is used as the loss function:

$$\mathcal{L}_m = -\frac{1}{N} \sum_{j=1}^{N} \sum_{k=1}^{K} Q_{k,j} \log \tilde{S}_{k,j} \tag{64}$$

The next step is to train our encoder through contrastive learning between subgraph views (motif) and the whole graph representation generated by performing any permutation invariant function on all nodes belonging to that graph. Assuming that we have graph representation $\mathbf{h}_i$ and the subgraph representation $\mathbf{e}_j$, the whole graph and subgraphs sampled from it is deemed as the positive pairs while the whole graph and subgraphs sampled from other graphs is deemed as the negative pairs. Then the contrastive objective function is:

$$\mathcal{L}_c = -\frac{1}{M} \sum_{i=1}^{M} \sum_{j=1}^{N} \log W_{ij} \cdot \mathbf{1}\{g_j \in \mathcal{G}_i\} \tag{65}$$

Bibtex:
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