Iterative Deep Graph Learning for Graph Neural Networks: Better and Robust Node Embeddings

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This paper [1] proposed an end-to-end graph learning framework, namely Iterative Deep Graph Learning (IDGL), for jointly and iteratively learning graph structure and graph embedding.

The graph structure is learned from node embeddings' similarities based on the multi-head weighted cosine similarity metric function:

$$s_{ij} = \frac{1}{m}\sum_{p=1}^{m} s_{ij}^{p}, \quad s_{ij}^{p} = \cos\left(\mathbf{w} \odot \mathbf{v}_i, \mathbf{w} \odot \mathbf{v}_j\right),$$

where $\mathbf{w}$ is a learnable weight vector. Then, to generate a sparse non-negative adjacency matrix $\mathbf{A}$ from $\mathbf{S}$, those elements in $\mathbf{S}$ which are smaller than a non-negative threshold are masked off (i.e., set to zero). With the mild assumption that the optimized graph structure is potentially a "shift" from the initial graph structure, the learned graph is futher combined with the initial graph and the graph learned from raw node features as follows:

$$\tilde{\mathbf{A}}^{(t)} = \lambda \mathbf{D}^{(0)^{-1/2}} \mathbf{A}^{(0)} \mathbf{D}^{(0)^{-1/2}} + (1-\lambda)\left\{\eta \mathbf{f}\left(\mathbf{A}^{(t)}\right) + (1-\eta)\mathbf{f}\left(\mathbf{A}^{(1)}\right)\right\},$$

where f represents row normalization. Note that if the initial structure is not available, we can use a kNN graph.

To reduce computational complexity, an anchor-based approximation technique can be used. That is, instead of computing similarity scores for all paris of graph nodes, we can randomly sample a set of anchors and only compute the similarity scores between each node with nodes from the anchor set. This will result in a structure that all nodes only connect to the anchors, but we can further transform it to a general structure based on two-step transition probabilities.

The GNN and the structure are optimized alternatively. To improve the quality of the learned graph, a penalty is added to the loss function which controls the smoothness, connectivity and sparsity of the learned graph.

References

[1] Yu Chen, Lingfei Wu, and Mohammed Zaki. Iterative deep graph learning for graph neural networks: Better and robust node embeddings. *Advances in Neural Information Processing Systems*, 33:19314–19326, 2020. (document)