FINDING GLOBAL HOMOPHILY IN GRAPH NEURAL NETWORKS WHEN MEETING HETEROPHILY

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This paper [1] tries to find global homophily for nodes in graphs with heterophily. Two models (GloGNN and GloGNN++) are proposed, which propagate information over nodes based on a coefficient matrix calculated in each layer, and hence allowing the nodes to aggregate information from all nodes from the graph.

GloGNN uses a decoupled architecture, i.e., the feature $\mathbf{X}$ is first transformed to $\mathbf{H}^{(0)}$ and then the neighborhood aggregation is conducted without feature transformations. Specially, $\mathbf{H}^{(0)}$ is designed to contain the information of both nodes' features and connectivities:

$$\mathbf{H}^{(0)} = (1-\alpha)\mathrm{MLP}_1(\mathbf{X}) + \alpha\mathrm{MLP}_2(\mathbf{A}) \in \mathbb{R}^{n\times c}.$$

The propagation step is similar as in APPNP:

$$\mathbf{H}^{(\ell+1)} = (1-\gamma)\mathbf{Z}^{(\ell)}\mathbf{H}^{(\ell)} + \gamma\mathbf{H}^{(0)}.$$

The coefficient matrix $\mathbf{Z}^{(\ell)}$ is computed from the following optimization problem:

$$\min_{\mathbf{Z}^{(\ell)}} \left\|\mathbf{H}^{(\ell)} - (1-\gamma)\mathbf{Z}^{(\ell)}\mathbf{H}^{(\ell)} - \gamma\mathbf{H}^{(0)}\right\|_F^2 + \beta_1\left\|\mathbf{Z}^{(\ell)}\right\|_F^2 + \beta_2\left\|\mathbf{Z}^{(\ell)} - \sum_{k=1}^{K}\lambda_k\mathbf{A}^k\right\|_F^2,$$

where the first term is similar as the target of APPNP, the second term is to regularize $\mathbf{Z}$, and the third term further regularizing $\mathbf{Z}$ with node's multi-hop reachabilities. The parameters $\lambda_1,\ldots,\lambda_K$ are learnable. This optimization problem has a closed-form solution as follows:

$$\mathbf{Z}^{(\ell)*} = \left[(1-\gamma)\mathbf{H}^{(\ell)}\left(\mathbf{H}^{(\ell)}\right)^T + \beta_2\sum_{k=1}^{K}\lambda_k\mathbf{A}^k - \gamma(1-\gamma)\mathbf{H}^{(0)}\left(\mathbf{H}^{(\ell)}\right)^T\right]\left[(1-\gamma)^2\mathbf{H}^{(\ell)}\left(\mathbf{H}^{(\ell)}\right)^T + (\beta_1+\beta_2)\,\mathbf{I}_n\right]^{-1}.$$

The Woodbury formula is applied to reduce the complexity. GloGNN++ further assigns different weights to different hidden features in $\mathbf{H}^{(\ell)}$.

The grouping effect of $\mathbf{Z}^{(\ell)}$ and $\mathbf{H}^{(\ell)}$ is proved, that is, if two nodes share similar features and local structures, their coefficient vectors and embedding vectors will be close to each other.

References

[1] Xiang Li, Renyu Zhu, Yao Cheng, Caihua Shan, Siqiang Luo, Dongsheng Li, and Weining Qian. Finding global homophily in graph neural networks when meeting heterophily. *arXiv preprint arXiv:2205.07308*, 2022.