MSGNN: A Spectral Graph Neural Network Based on a Novel Magnetic Signed Laplacian

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LOG CONFERENCE

Motivation

- Many important and interesting phenomena are naturally modeled as signed and/or directed graphs, i.e., graphs in which objects may have either positive or negative relationships, and/or in which such relationships are not necessarily symmetric. Examples:
  - In the analysis of social networks, positive and negative edges could model friendship or enmity, and directional information could model the influence of one person on another [1,2].
  - Signed/directed networks also arise when analyzing time-series data with lead-lag relationships [3], detecting influential groups in social networks [4], and computing rankings from pairwise comparisons [5].
- Many signed networks are directed.
- Graph neural networks (GNNs) can be broadly classified into spatial or spectral.
- Most existing works on signed directed networks are spatial, such as SDGNN [2], SiGAT [6], SNEA [7], and SSSNET [8].
- A principal challenge for spectral GNNs: need to design a notion for signed directed Laplacian matrix.

Problem Definition

We consider a graph (network) $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with:

- The node set $\mathcal{V}$ is a set of n nodes.
- The edge set $\mathcal{E}$, which can be divided in positive and negative parts $\mathcal{E}^+$and $\mathcal{E}^-$so that $\mathcal{E} = \mathcal{E}^+ \cup \mathcal{E}^-$.
- The node feature matrix $\boldsymbol{X} \in \mathbb{R}^{n \times din}$.
- The adjacency matrix is denoted as $\boldsymbol{A}$, which is *asymmetric* for a directed graph.
- A **clustering** into K clusters: a partition of the node set into disjoint sets $\mathcal{V} = \mathcal{C}_0 \cup \dots \cup \mathcal{C}_{K-1}$.
- *Semi-supervised*: seed nodes in each cluster, with label supervision during training.
- *Self-supervised*: no label supervision during training.
- **Link prediction** tasks considered:
  - **Link sign prediction (SP):** predict the edge sign of pairs of vertices u, v for which either $(u, v) \in \mathcal{E}^+$ or $(u, v) \in \mathcal{E}^-$.
  - **Direction prediction (DP):** predict the edge direction of pairs of vertices u, v for which either $(u, v) \in \mathcal{E}$ or $(v, u) \in \mathcal{E}$.
  - **Three-class classification (3C):** classify an edge $(u, v) \in \mathcal{E}, (v, u) \in \mathcal{E}$, or $(u, v), (v, u) \notin \mathcal{E}$.
  - **Four-class classification (4C):** classify an edge $(u, v) \in \mathcal{E}^+, (v, u) \in \mathcal{E}^+, (u, v) \in \mathcal{E}^-$, or $(v, u) \in \mathcal{E}^-$.
  - **Five-class classification (5C):** in addition to the classes in (4C), add a class $(u, v), (v, u) \notin \mathcal{E}$.
- We evaluate the link prediction performance by **accuracy**.

Our Contributions

- We devise a novel magnetic signed Laplacian, which can naturally be applied to signed and directed networks. The magnetic signed Laplacian is Hermitian, positive semidefinite, and the eigenvalues of its normalized counterpart lie in [0,2]. They reduce to existing Laplacians when the network is unsigned and/or undirected.
- We propose an efficient spectral GNN architecture, MSGNN, based on this magnetic signed Laplacian, which attains leading performance on extensive node clustering and link prediction tasks, including novel tasks that consider edge sign and directionality jointly.
- We introduce a novel synthetic model for signed and directed networks, called Signed Directed Stochastic Block Model (SDSBM), and also contribute a number of new real-world data sets constructed from lead-lag relationships of financial time series data.

Signed Directed Stochastic Block Models (SDSBMs)

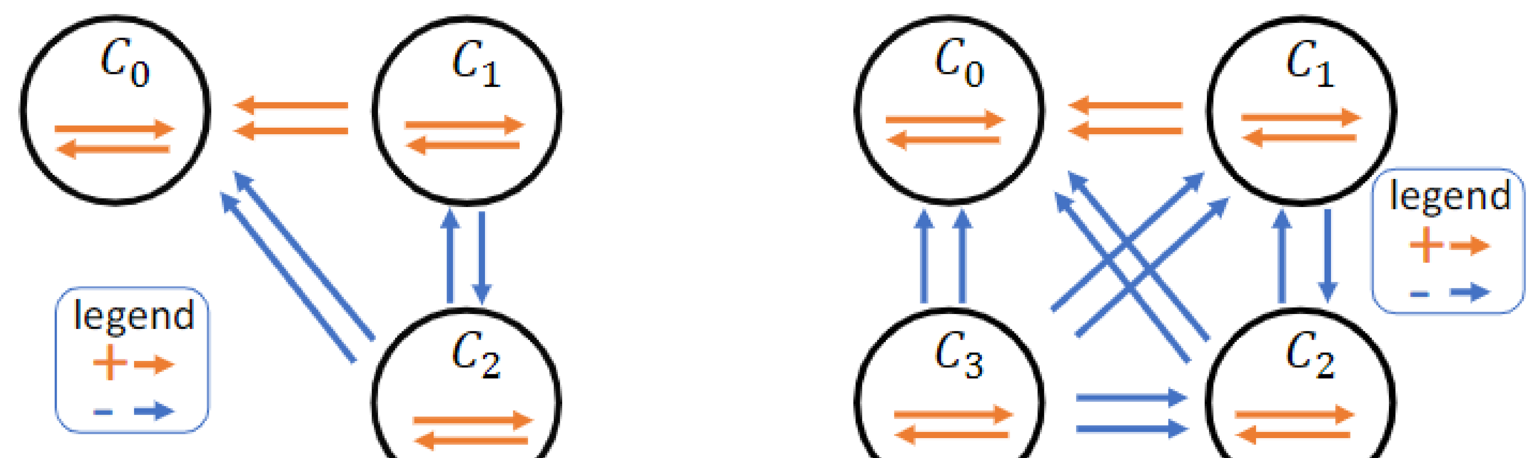

Figure 1: This toy example models groups of athletes and sports fans on social media. Here, signed, directed edges represent positive or negative mentions. $\mathcal{C}_0$: players of a sports team; $\mathcal{C}_1$: a group of their fans who typically say positive things about the players; $\mathcal{C}_2$: a group of fans of a rival team; $\mathcal{C}_3$: a group of fans of a third, less important team.

Hermitian Adjacency Matrix

- Phase matrix for direction distinguishment $\boldsymbol{\Theta}^{(q)}_{i,j} := 2\pi q(\mathbf{A}_{i,j} - \mathbf{A}_{j,i}), q \geq 0$

$$\exp(i\boldsymbol{\Theta}^{(q)})_{i,j} := \exp(i\boldsymbol{\Theta}^{(q)}_{i,j})$$

- Hermitian adjacency matrix and the absolute degree matrix

$$\tilde{\mathbf{A}}_{i,j} := \frac{1}{2}(\mathbf{A}_{i,j} + \mathbf{A}_{j,i}), \quad 1 \leq i, j \leq n,$$

$$\tilde{\mathbf{D}}_{i,i} := \frac{1}{2}\sum_{j=1}^{n}(|\mathbf{A}_{i,j}| + |\mathbf{A}_{j,i}|), \quad 1 \leq i \leq n,$$

$$\mathbf{H}^{(q)} := \tilde{\mathbf{A}} \odot \exp(i\boldsymbol{\Theta}^{(q)})$$

Magnetic Signed Laplacian

- Magnetic Signed Laplacian $\mathbf{L}_U^{(q)} := \tilde{\mathbf{D}} - \mathbf{H}^{(q)} = \tilde{\mathbf{D}} - \tilde{\mathbf{A}} \odot \exp(i\boldsymbol{\Theta}^{(q)})$,
- Normalized Magnetic Signed Laplacian

$$\mathbf{L}_N^{(q)} := \mathbf{I} - \left(\tilde{\mathbf{D}}^{-1/2}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-1/2}\right) \odot \exp(i\boldsymbol{\Theta}^{(q)}).$$

Theorem 1
For all $q \geq 0$, both $\mathbf{L}_U^{(q)}$ and $\mathbf{L}_N^{(q)}$ are positive semidefinite.

Theorem 2
For all $q \geq 0$, the eigenvalues of $\mathbf{L}_N^{(q)}$ are contained in the interval $[0, 2]$.

MSGNN

- MSGNN in ChebNet form [9] $\quad Z = \sum_{k=0}^{K} T_k(\tilde{\mathbf{L}})\mathbf{X}\Theta_k, \quad \tilde{\mathbf{L}} = \mathbf{L}_N^{(q)} - \mathbf{I}$
- The computation complexity is comparable with GCN [10]

Conclusion

For signed directed networks, we propose a spectral graph neural network based on a novel magnetic signed Laplacian matrix, introduce a novel synthetic network model and new real-world data sets, and conduct experiments on node clustering and link prediction tasks that are not restricted to considering either link sign or directionality alone. MSGNN performs as well or better than leading GNNs, while being considerably faster on real-world data sets.

References

[1] Kumar, S., Spezzano, F., Subrahmanian, V. S., & Faloutsos, C. (2016, December). Edge weight prediction in weighted signed networks. In 2016 IEEE 16th International Conference on Data Mining (ICDM) (pp. 221-230). IEEE.
[2] Huang, J., Shen, H., Hou, L., & Cheng, X. (2021, May). SDGNN: Learning node representation for signed directed networks. In Proceedings of the AAAI Conference on Artificial Intelligence (Vol. 35, No. 1, pp. 196-203).
[3] Bennett, S., Cucuringu, M., & Reinert, G. (2022). Detection and clustering of lead-lag networks for multivariate time series with an application to financial markets.
[4] He, Y., Reinert, G., & Cucuringu, M. (2021). DIGRAC: Digraph Clustering Based on Flow Imbalance. arXiv preprint arXiv:2106.05194.
[5] He, Y., Gan, Q., Wipf, D., Reinert, G. D., Yan, J., & Cucuringu, M. (2022, June). GNNRank: Learning global rankings from pairwise comparisons via directed graph neural networks. In International Conference on Machine Learning (pp. 8581-8612). PMLR.
[6] Huang, J., Shen, H., Hou, L., & Cheng, X. (2019, September). Signed graph attention networks. In International Conference on Artificial Neural Networks (pp. 566-577). Springer, Cham.
[7] Li, Y., Tian, Y., Zhang, J., & Chang, Y. (2020, April). Learning signed network embedding via graph attention. In Proceedings of the AAAI Conference on Artificial Intelligence (Vol. 34, No. 04, pp. 4772-4779).
[8] He, Y., Reinert, G., Wang, S., & Cucuringu, M. (2022). SSSNET: Semi-Supervised Signed Network Clustering. In Proceedings of the 2022 SIAM International Conference on Data Mining (SDM) (pp. 244-252). Society for Industrial and Applied Mathematics.
[9] Defferrard, M., Bresson, X., & Vandergheynst, P. (2016). Convolutional neural networks on graphs with fast localized spectral filtering. Advances in neural information processing systems, 29.
[10] Kipf, T. N., & Welling, M. (2016). Semi-supervised classification with graph convolutional networks. arXiv preprint arXiv:1609.02907.