MagNet: A Neural Network for Directed Graphs

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Neural Information Processing Systems, 2021

Introduction

Endowing a collection of objects with a graph structure allows one to encode pairwise relationships among its elements. These relations often possess a natural notion of direction. Such datasets are naturally modeled by **directed graphs**.

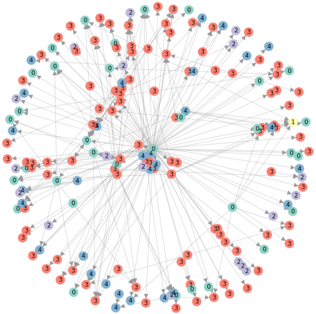
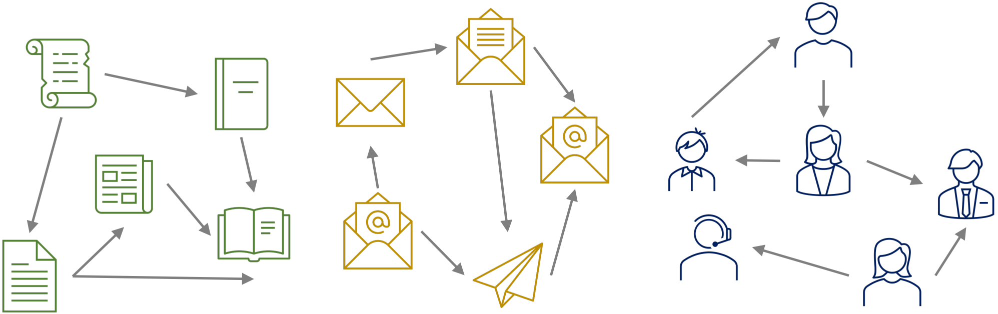


Figure: Visualization of WebKB-Cornell.

Introduction

- The directed graph is a ubiquitous data structure in the real world.
- The inherent relations are **asymmetric**.



(a) Citation networks (b) Email networks (c) Social networks

Figure: Some popular directed structures.

Graph Neural Networks

- One of the popular forms of graph neural networks, GCN (Kipf, et al. 2017)

$$Z = \widetilde{\mathrm{D}}^{-\frac{1}{2}} \widetilde{\mathrm{A}} \widetilde{\mathrm{D}}^{-\frac{1}{2}} \mathrm{X} \Theta,$$

$$\widetilde{\mathrm{A}} = \mathrm{A} + \mathrm{I}_N, \quad \widetilde{\mathrm{D}}(u,u) = \sum_{v \in \mathcal{N}(u)} \widetilde{\mathrm{A}}(u,v),$$

$$\mathrm{X} \in \mathbb{R}^{N \times d}, \quad \Theta \in \mathbb{R}^{d \times d'}$$

- GCN is obtained from the approximation from the spectral graph convolution on undirected graphs.

Spectral Graph Convolution on Undirected Graphs

- Consider a simple spectral convolution on the undirected graph,

$$g_\theta \star x = \mathrm{U}\mathrm{diag}(\theta)\mathrm{U}^\top x,$$

$$\mathrm{L} = \mathrm{I}_N - \mathrm{D}^{-\frac{1}{2}}\mathrm{A}\mathrm{D}^{-\frac{1}{2}} = \mathrm{U}\Lambda\mathrm{U}^\top, x \in \mathbb{R}^N, \theta \in \mathbb{R}^N$$

- $\mathrm{U}^\top x$ is the graph Fourier transform of x.
- Spectral graph convolution requires a **symmetric** Laplacian matrix to get a complete set of eigenvectors.
- It is a popular step to **symmetrize the adjacency matrix** first to handle directed graphs.

Graph Convolution on Directed Graphs (Digraphs)

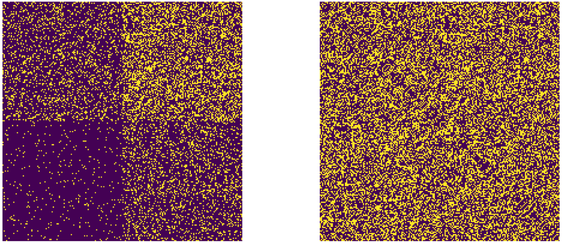
- Existing graph convolution for directed graphs also creates **symmetric Laplacian** matrices.
- Digraph Convolution based on approximated personalized PageRank (Tong, et al. 2020)

$$Z = \frac{1}{2}\left(P + P^{\top}\right) X\Theta$$

$$P = \Pi_{appr}^{\frac{1}{2}} \widetilde{P} \Pi_{appr}^{-\frac{1}{2}}, \quad \widetilde{P} = \widetilde{D}^{-1}\widetilde{A}, \quad \widetilde{A} = A + I_N$$

Symmetric Representation

Symmetric representation may lose critical information for downstream tasks.



(a) Directed adjacency (b) Symmetrized adjacency

Figure: The asymmetric adjacency matrix (a) and its symmetrized version (b).

Motivation

There are four types of edges in directed graphs:

- Undirected edges
- Incoming edges
- Outgoing edges
- No edge

A proper Laplacian for directed graphs should distinguish information from the four types of edges and have a complete set of eigenvectors.

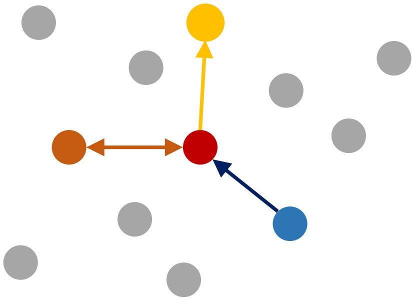


Figure: Different types of edges.

Motivation

- To get a complete set of eigenvectors, the Laplacian matrix can be **complex-valued Hermitian** besides symmetric.
- Encoding edge weights information in the **magnitude** matrix.
- Encoding direction information in the **phase** matrix.
- **Magnetic Laplacian** is one of the proper choices. The name originates from its interpretation as a quantum mechanical Hamiltonian of a particle under magnetic flux.
- Magnetic Laplacian is constructed based on **Hermitian adjacency** matrix.

Hermitian Adjacency Matrix

- Phase matrix for direction distinguishment

$$\Theta^{(q)}(u,v) := 2\pi q(\mathrm{A}(u,v) - \mathrm{A}(v,u)), q \geq 0$$
$$\exp\left(i\Theta^{(q)}\right)(u,v) := \exp\left(i\Theta^{(q)}(u,v)\right)$$

- Hermitian adjacency matrix

$$\mathrm{H}^{(q)} := \mathrm{A}_s \odot \exp\left(i\Theta^{(q)}\right),\ \mathrm{A}_s = \frac{1}{2}(\mathrm{A} + \mathrm{A}^\top)$$

Representation Capability of Hermitian Adjacency Matrix

In Hermitian adjacency matrix:

- Incoming and outgoing edges are complex conjugate.

$$\mathrm{H}^{(q)}(u,v) = a + ib,\ \mathrm{H}^{(q)}(v,u) = a - ib,$$
$$\text{for } (u,v) \in E \text{ and } (v,u) \notin E$$

- Undirected edges are all 1s.

$$\mathrm{H}^{(q)}(u,v) = \mathrm{H}^{(q)}(v,u) = 1$$

- No edge is 0.

$$\mathrm{H}^{(q)}(u,v) = 0$$

Special Forms of Hermitian Adjacency Matrix

- Hermitian adjacency matrix is symmetric when $q = 0$.

$$\mathrm{H}^{(0)} = \mathrm{A}_s$$

- Directed edges in Hermitian adjacency matrix are pure imaginary when $q = 0.25$.

$$\mathrm{H}^{(.25)}(u, v) = -\mathrm{H}^{(.25)}(v, u) = \frac{i}{2},$$
$$\text{for } (u, v) \in E \text{ and } (v, u) \notin E$$

Magnetic Laplacian

- Regular Laplacian

$$\mathrm{L}_U := \mathrm{D}_s - \mathrm{A}_s; \quad \mathrm{L}_N := \mathrm{I}_N - \mathrm{D}_s^{-\frac{1}{2}} \mathrm{A}_s \mathrm{D}_s^{-\frac{1}{2}}$$

- Magnetic Laplacian

$$\mathrm{L}_U^{(q)} := \mathrm{D}_s - \mathrm{H}^{(q)} = \mathrm{D}_s - \mathrm{A}_s \odot \exp\left(i\Theta^{(q)}\right)$$

- Normalized Magnetic Laplacian

$$\mathrm{L}_N^{(q)} := \mathrm{I}_N - \left(\mathrm{D}_s^{-\frac{1}{2}} \mathrm{A}_s \mathrm{D}_s^{-\frac{1}{2}}\right) \odot \exp\left(i\Theta^{(q)}\right)$$

Magnetic Laplacian

Theorem 1

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

Theorem 2

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

MagNet

- MagNet in ChebNet form (Defferrard, et al. 2016)

$$Z = \sum_{k=0}^{K} T_k(\widetilde{\mathrm{L}})\mathrm{X}\Theta_k, \quad \widetilde{\mathrm{L}} = \mathrm{L}_N^{(q)} - \mathrm{I}Wen$$

- MagNet in GCN form (Kipf, et al. 2017)

$$Z = \widetilde{\mathrm{D}}_s^{-\frac{1}{2}}\widetilde{\mathrm{A}}_s\widetilde{\mathrm{D}}_s^{-\frac{1}{2}} \odot \exp\left(i\Theta^{(q)}\right)\mathrm{X}\Theta$$

- The computation complexity is comparable with GCN (Kipf, et al. 2017).

Architectures

- Complex activation function

$$\sigma(z) = \begin{cases} z & \text{if } -\pi/2 \leq \arg(z) < \pi/2 \\ 0 & \text{otherwise} \end{cases}$$

- Framework

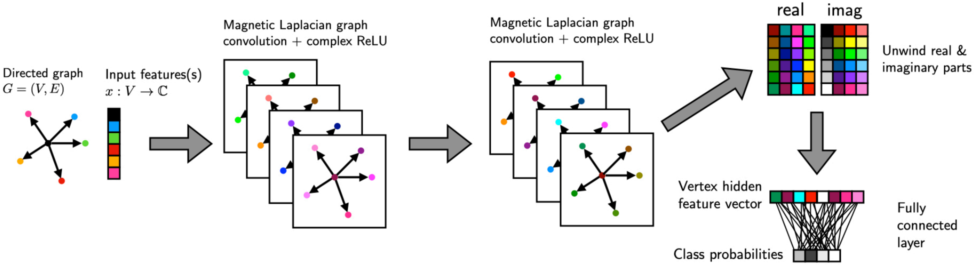
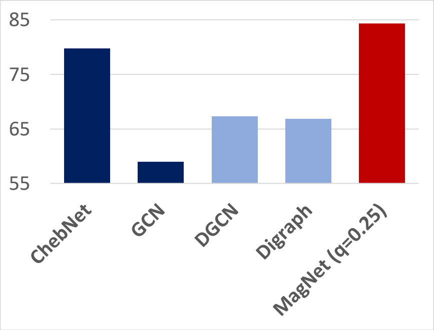


Figure: MagNet with two layers applied to node classification.

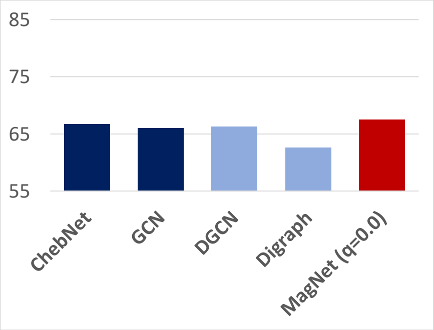
Experiment Settings

- We evaluate MagNet on both node classification and link prediction tasks.
- We select the MagNet in ChebNet form and set $K = 1$.
- Parameter q in the Hermitian adjacency matrix is selected based on cross-validation.
- MagNet reduces to ChebNet when $q = 0$.

Node Classification Results



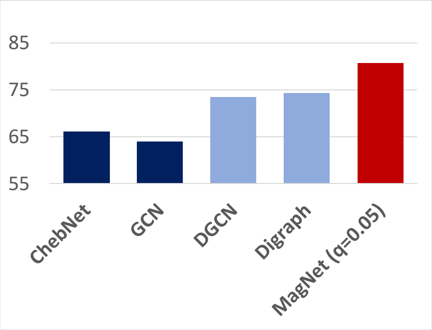
(a) WebKB/Cornell



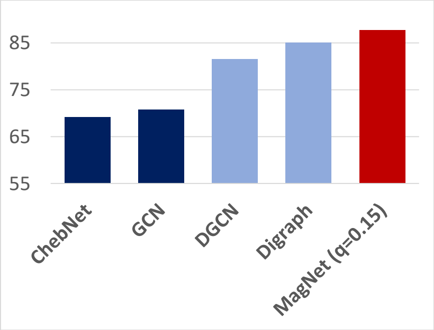
(b) Citeseer

Figure: Testing accuracy of node classification.

Link Prediction Results



(a) Existence Prediction



(b) Direction Prediction

Figure: Testing accuracy of link prediction on Citeseer.

Summary

- We have introduced MagNet, a neural network for directed graphs based on the magnetic Laplacian.
- This network can be viewed as the natural extension of spectral graph convolutional networks to the directed graph setting.
- We demonstrate the effectiveness of our network by node classification and link prediction tasks.

References

- Kipf, Thomas N. and Welling, Max. "Semi-Supervised Classification with Graph Convolutional Networks" International Conference on Learning Representations (2017).
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- Defferrard, Michaël, Xavier Bresson, and Pierre Vandergheynst. "Convolutional neural networks on graphs with fast localized spectral filtering." Advances in neural information processing systems 29 (2016): 3844-3852.