Graph Symmetry and Graph Spectra

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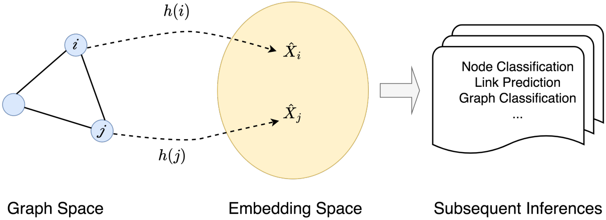
Outline

1. Graph representation learning: spectral vs spatial methods
2. Efficiency: spectral-inspired message-passing networks
3. Expressivity: graph spectra and graph symmetry

Graph Representation Learning

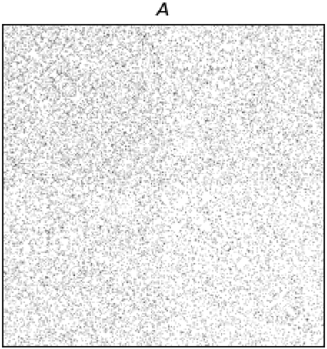


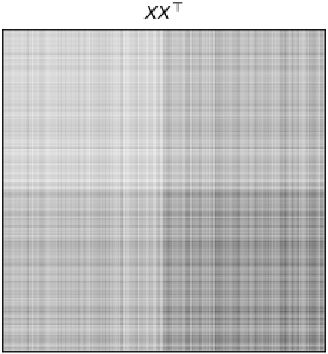
- Learn a finite-dimensional Euclidean embedding of the graph while preserving structural information
- Perform subsequent inferences directly on graph embedding

Testbed: Node Classification/Community Detection

Problem Setup: predict node labels of $Y_{m+1}, \cdots, Y_n$, using

- adjacency matrix $A \in \mathbb{R}^{n \times n}$, node features $X \in \mathbb{R}^{n \times d}$,
- m out of n labels: $Y_1, \cdots, Y_m$





Graph Representation Learning: Methods

Given a graph $G(V, E)$ with a graph operator S

Spectral methods: $S = U\Lambda U^T$

- Spectral graph embedding

$$h^{\text{ASE}} = U_{[:k]}\sqrt{\Lambda}_{[:k]}$$

- Spectral graph neural networks

$$h^{(l+1)} = \sigma(p(S)\, h^{(l)}\, W^{(l)} + b^{(l)})$$

$$\overset{GFT}{\Longrightarrow}\ \hat{h}^{(l+1)} = \sigma(p(\Lambda)\, \hat{h}^{(l)}\, W^{(l)} + \hat{b}^{(l)})$$

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Message-passing algorithms

- Belief propogation

- Message-passing neural networks (MPNNs)

$$h^{(l+1)} = \sigma(S\, h^{(l)}\, W^{(l)} + b^{(l)})$$

$$= \sigma(\sum_{j\in\mathcal{N}(i)} h_j^{(l)} W^{(l)} + b^{(l)}).$$

Injecting Global Information to Local MPNN

Can we compute global information from local MPNNs?

- Functional-calculus spectral filters (Levie et al. 2020; Perlmutter et al. 2019)
- Transformer-based GNNs (Kreuzer et al. 2021; Ying et al. 2021).

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Can we compute global spectra information from local MPNNs?

- `PowerEmbed` (Huang et al. 2022)

PowerEmbed

1. A simple normalization step to express top-k eigenvectors
2. Intermediate embeddings span from local spatial signals to global spectral information

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Algorithm 1 PowerEmbed

Require: a graph operator $S \in \mathbb{R}^{n \times n}$, node features $X \in \mathbb{R}^{n \times k}$, a list $P = [X]$.

Initialize:

$U(t) = X$

for t = 0 to L-1 **do**

$\tilde{U}(t+1) = S\,U(t)$ [Message Passing]

$U(t+1) = \tilde{U}(t+1)[\tilde{U}(t+1)^\top \tilde{U}(t+1)]^{-1}$ [Normalization]

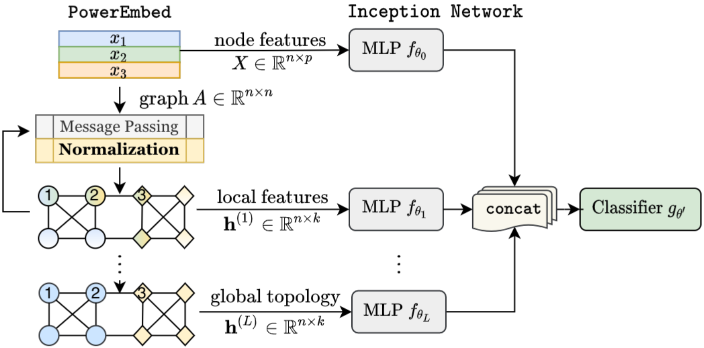
Append $\frac{U(t+1)}{\|U(t+1)[:,k]\|}$ to P

end for

return P

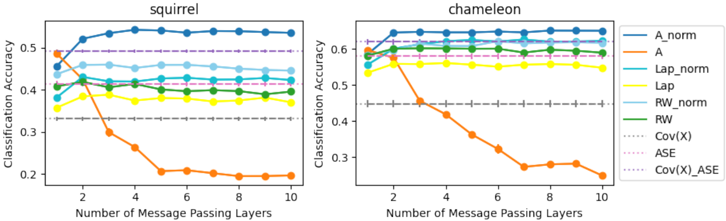
PowerEmbed

1. A simple normalization step to express top-k eigenvectors
2. Representation: intermediate embeddings span from local spatial signals to global spectral information
3. Classification: an inception network



PowerEmbed

✓ Provably avoid over-smoothing (Li et al. 2018) and over-squashing (Topping et al. 2021) in *un-normalized* MPNNs
✓ Computationally efficient to capture both global spectral information and local spatial signals



Expressivity

How powerful are spectral methods compared to spatial methods?

Expressivity: Signal Processing Viewpoint

Spectral GNN: $S = U \Lambda U^T$

$$h^{(l+1)} = \sigma(p(S)\, h^{(l)}\, W^{(l)} + b^{(l)})$$

Spatial MPNN:

$$h^{(l+1)} = \sigma(S\, h^{(l)}\, W^{(l)} + b^{(l)})$$

If we choose $p(\cdot)$ as a degree-k polynomial, then one layer of spectral GNN can be expressed by a k-layer MPNN.

- $p(\cdot)$ can be generalized to rational function (Levie et al. 2021)

Expressivity: Graph Isomorphism Viewpoint

What functions on graphs can be expressed?
Connection to graph isomorphism test.

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Connection to graph isomorphism test.

Definition (Graph Isomorphism)

$G = (V, E, X_V)$ and $G' = (V', E', X'_V)$ are isomorphic if there exists a relabeling of the nodes of G that produce the graph G'.

Definition (Graph Invariant)

A graph invariant i is a function from the set of graphs to some fixed target domain such that this function is invariant under graph isomorphisms, i.e. $i(G) = i(G')$ when G is isomorphic to G'.

Graph Isomorphism and Graph Invariant

Spectral invariants:

- Eigenvalues, graph angles (Cvetković et al. 2010; Van Dam et al. 2003)
- Multiset of the eigen-projectors (Fürer 2010; Rattan et al. 2021)

Graph Isomorphism and Graph Invariant

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Spatial invariants:

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Which invariants are stronger?

Abovementioned Spectral invariants are less powerful than 2-WL (Rattan et al. 2021).

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Spatial invariants:

- Weisfeiler-Lehman (WL) hierarchy
  - 1-WL: MPNN (Morris et al. 2019; Xu et al. 2018)
  - k-WL: k-th order MPNN (Maron et al. 2019)

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Can we design stronger spectral invariants?

Towards Stronger Spectral Invariant: Graph Spectra and Graph Symmetry

Ingredients:

- Spectral-decomposition: $A = \sum_{i=1}^{n} \lambda_i u_i u_i^\top$
- Automorphism: $\Pi A = A\Pi$ for some permutation Π.
- $\text{stabilizer}(u_i) := \{\Pi : \Pi u_i = \pm u_j,\ u_j \in \mathcal{E}(\lambda_i)\}$.

$$\text{aut}(G) = \bigcap_{i=1}^{n} \text{stabilizer}(u_i).$$

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