Graph Neural Networks with Learnable Structural and Positional Representations

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with

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LoGaG: Learning on Graphs and Geometry Reading Group

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Introduction Summary

!!
Problem

- Nodes in graphs do not have canonical positional information, like words in sentences. This causes limitations such as the lack of (global) structural information when MP-GNNs learn on graphs.
- As a result, these models exhibit low representation power due to their inability to differentiate simple graph symmetries.

In this work, we consider this topic of graph PEs and propose a framework named LSPE that can be used with any MP-GNNs to **learn positional and structural feature representations** at the same time, thus effectively capturing the two properties and tuning these w.r.t. to the task.

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Approach

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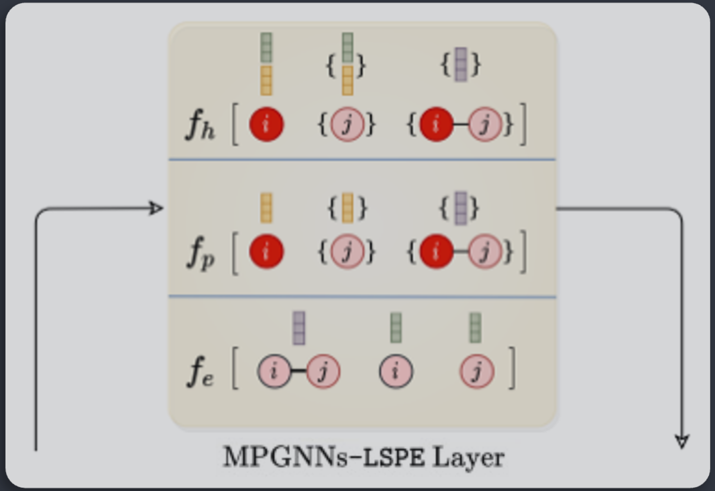
Outline of Presentation

- Motivation
- Background
- Learnable Structural and Positional Encodings (LSPE)
- Numerical Evaluations
- Conclusion



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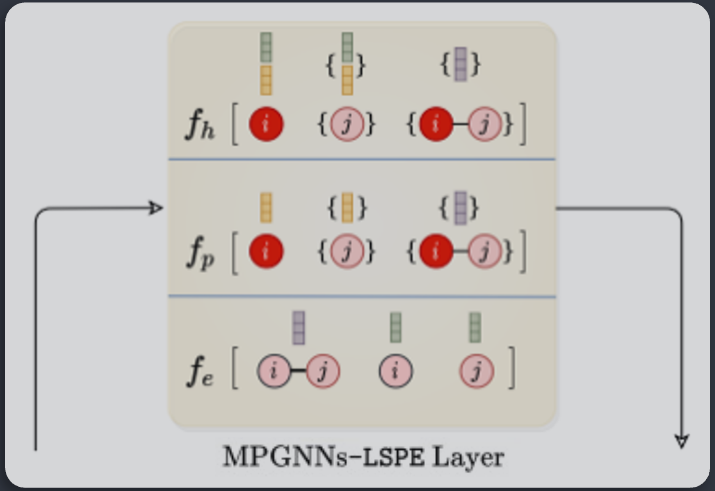
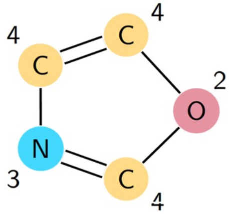
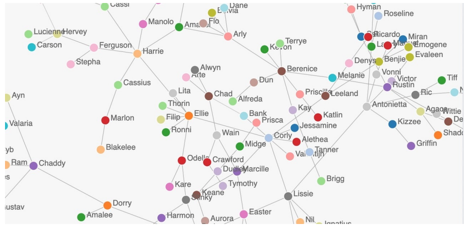


Graph Structured Data

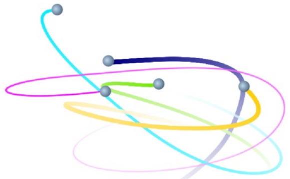
- Graphs are universal language to describe complex systems of bodies and their interactions.



Chemistry
- Learn on molecules and predict chemical properties
- Use in drug repurposing

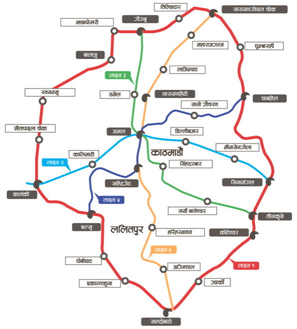


Social networks
- Learn from multi-faceted interactions among users
- Use for commercial and social applications

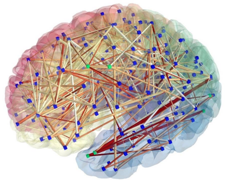


Simple Particles

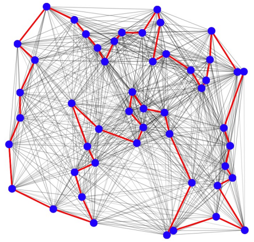
Physics
- Learn from interactions of particles in systems
- Accelerate physics research



Transportation
- Learn from traffic behavior across road networks
- Predict time estimates; efficient transport management



Neuroscience
- Learn functions of brain regions through connectivity
- Accelerate brain-understanding and neuro-disease research



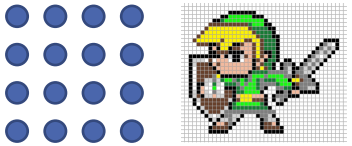
Combinatorial Optimization
- Exploit the fact that most CO problems are rep. as graphs
- Develop better approximated solutions for NP-hard problems

Numerous such examples of graph data and application areas!

Motivation

- Let’s start with some data examples.

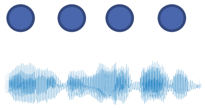
Images



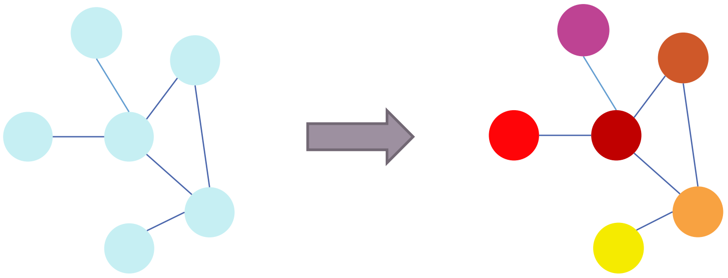
Text

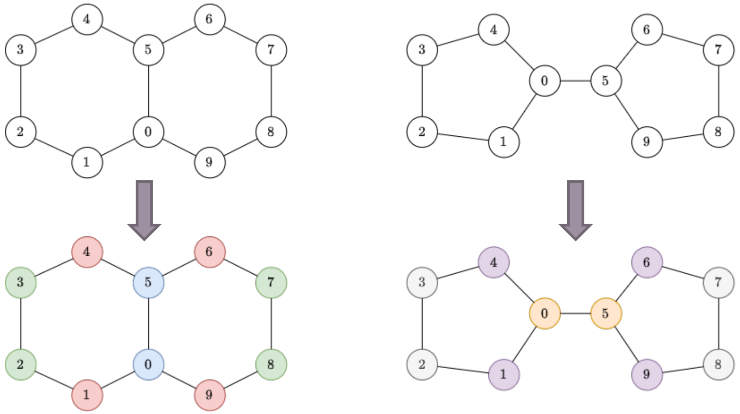
राउर नाँव का ह?

Speech



- CNNs[1] implicitly encode spatial position[2], RNNs build on sequences[3], Transformers use word PE[4].
- What about **graphs** and how GNNs incorporate node positional information?





Decalin

Bicyclopentyl

[1] LeCun, Y., Bottou, L., Bengio, Y. and Haffner, P., 1998. Gradient-based learning applied to document recognition.
[2] Islam, M.A., Jia, S. and Bruce, N.D., 2020. How much position information do convolutional neural networks encode?
[3] Hochreiter, S. and Schmidhuber, J., 1997. Long short-term memory.
[4] Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, Ł. and Polosukhin, I., 2017. Attention is all you need.

Outline of Presentation

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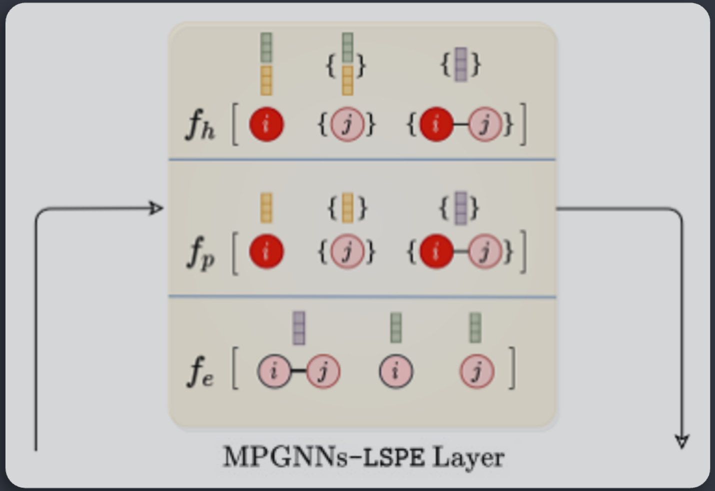
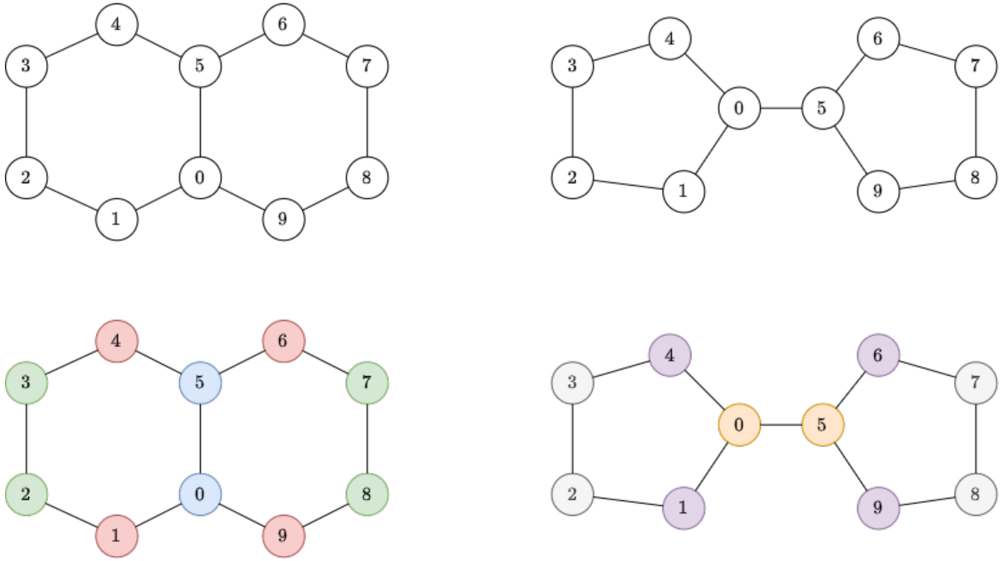


Background

1. GNN’s theoretical **expressivity**



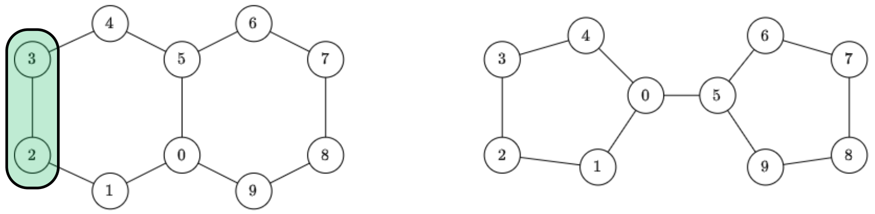
2. Graph **Positional Encoding**

3. **Transformer**-based GNNs

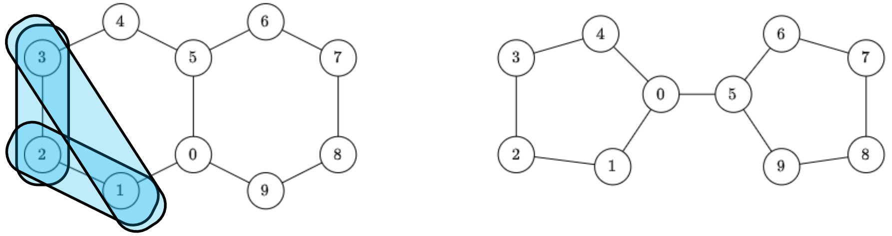
Background

1. GNN's theoretical **expressivity**

- **Message Passing GNNs.**
  -Based on message-passing between nodes [1]
  -Pairwise exchange of information between local neighbors
  -Expressivity bounded by 1-Weisfeiler Leman [2,3]
  -Fail to distinguish simple graphs w.r.t. 1-WL
  -*O(n)* complexity; n: number of nodes



- **Weisfeiler Leman GNNs.**
  -Higher-order GNNs based on the WL test hierarchy (1/2-WL, 3-WL, …, k-WL) [3,4,5,6]
  -Encodes higher-order interactions using k-tuples
  -Can distinguish non-isomorphic graphs w.r.t. k-WL
  -$O(n^2)/O(n^3)$ memory/speed complexity



- Scalable and hybrid WL-GNNs developed recently [6,7]

[1] Gilmer, J., Schoenholz, S.S., Riley, P.F., Vinyals, O. and Dahl, G.E., 2017, July. Neural message passing for quantum chemistry.
[2] Xu, K., Hu, W., Leskovec, J. and Jegelka, S., 2018. How powerful are graph neural networks?
[3] Morris, C., Ritzert, M., Fey, M., Hamilton, W.L., Lenssen, J.E., Rattan, G. and Grohe, M., 2019, July. Weisfeiler and leman go neural: Higher-order graph neural networks.
[4] Maron, H., Ben-Hamu, H., Serviansky, H. and Lipman, Y., 2019. Provably powerful graph networks.
[5] Chen, Z., Villar, S., Chen, L. and Bruna, J., 2019. On the equivalence between graph isomorphism testing and function approximation with gnns.
[6] Morris, C., Rattan, G. and Mutzel, P., 2019. Weisfeiler and Leman go sparse: Towards scalable higher-order graph embeddings.
[7] Bodnar, C., Frasca, F., Otter, N., Wang, Y.G., Liò, P., Montufar, G.F. and Bronstein, M., 2021. Weisfeiler and lehman go cellular: Cw networks.

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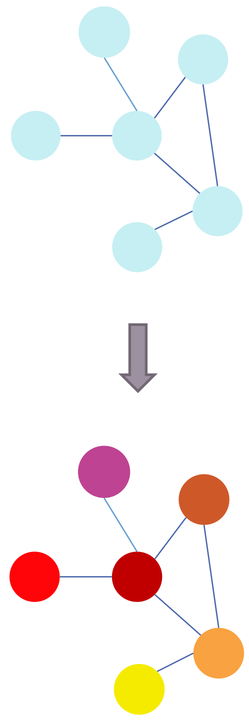
Background

2. Graph **Positional Encoding**

- PE in GNNs help the network disambiguate node symmetries
- MP-GNNs can be more expressive [1] and universal approximators with unique node identifiers [2]



Desired Characteristics:

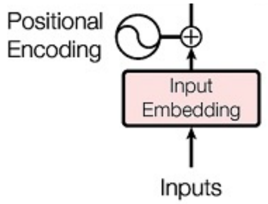
- Unique, Distance-aware, Permutation-equivariant, Efficient/Scalable

Laplacian Positional Encoding [3]

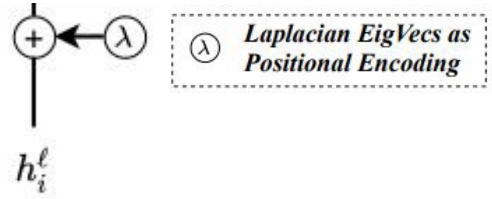
- Based on Laplacian Eigenvectors [4] that embed graphs into a local coordinate system
- Unique and Distance-aware
- Pre-computed from the factorization of the graph Laplacian

$$\Delta = I - D^{-1/2} A D^{-1/2} = U^T \Lambda U$$

- Generalize the PE used in Transformer [5] to graphs



PE in Original Transformer



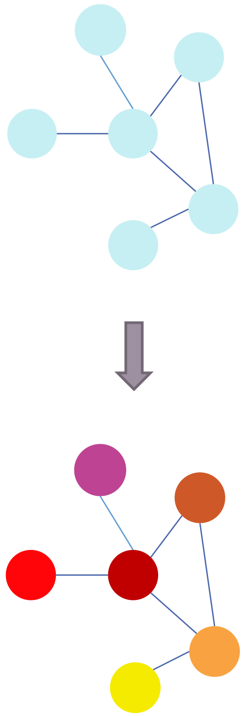
LapPE in GNNs/GraphTransformer

[1] Murphy, R., Srinivasan, B., Rao, V. and Ribeiro, B., 2019, May. Relational pooling for graph representations.
[2] Loukas, A., 2020. What graph neural networks cannot learn: depth vs width.
[3] Dwivedi, V.P., Joshi, C.K., Laurent, T., Bengio, Y. and Bresson, X., 2020. Benchmarking graph neural networks.
[4] Belkin, M. and Niyogi, P., 2003. Laplacian eigenmaps for dimensionality reduction and data representation.
[5] Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, Ł. and Polosukhin, I., 2017. Attention is all you need.

Background

2. Graph **Positional Encoding**

Although **LapPE** shows good empirical performance, there are **limitations**:
- Eigenvectors are defined up to ±1
- When selecting k (<<n) eigenvectors, the number of possibilities is 2^k
- During training, the sign of eigenvectors is randomly flipped [1] for uniform sampling among the 2^k possibilities (less than n! of node indexing)



Other PE based works for GNNs:
- Position aware GNNs that use anchor sets and relative distances [2]
- Distance Encoding w.r.t. a node set used at input layer and as aggregation controllers [3]
- Random walk with Restart as topological embeddings [4]
- PEs used in Transformers for Graphs (next slides →)

[1] Dwivedi, V.P., Joshi, C.K., Laurent, T., Bengio, Y. and Bresson, X., 2020. Benchmarking graph neural networks.
[2] Loukas, A., 2020. What graph neural networks cannot learn: depth vs width.
[3] Li, P., Wang, Y., Wang, H. and Leskovec, J., 2020. Distance Encoding--Design Provably More Powerful GNNs for Structural Representation Learning.
[4] Ahmadi, A.H.K., 2020. Memory-based graph networks.

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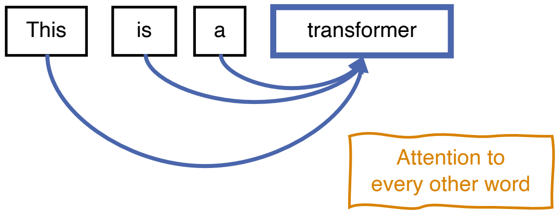
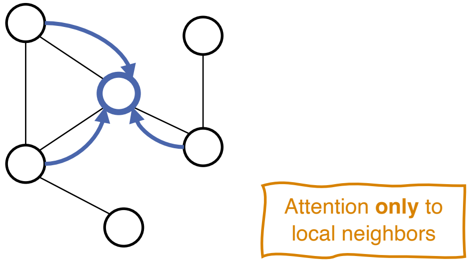
Background



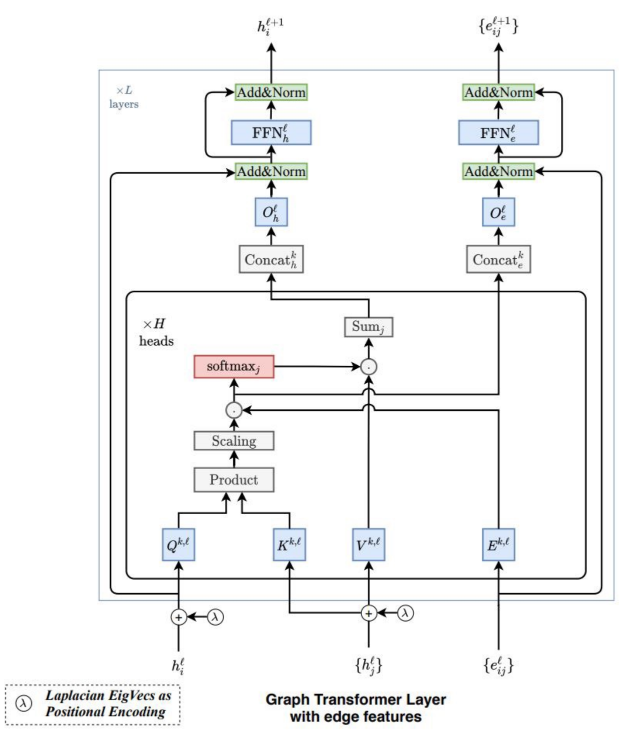
3. Transformer-based GNNs

- Attention based GNNs first proposed in GATs [1]
- Transformers can be viewed as a special case of GNNs on fully connected graph of words [2]
- This **connection** of Transformer and GNNs led to several recent works!



GraphTransformer

- GraphTransformer uses LapPE and local attention to generalize original Transformers to graphs [3]
- However, being similar to MP-GNNs it is susceptible to information bottleneck [4]
- Direct use of full attention without the use of appropriate positional and structural encodings does not work well [3]



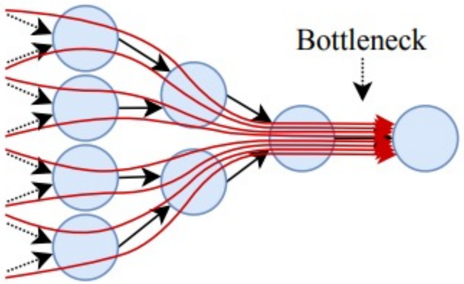


Image from [4]

[1] Veličković, P., Cucurull, G., Casanova, A., Romero, A., Lio, P. and Bengio, Y., 2017. Graph attention networks.
[2] Joshi, C., 2020. Transformers are graph neural networks.
[3] Dwivedi, V.P. and Bresson, X., 2020. A generalization of transformer networks to graphs.
[4] Alon, U. and Yahav, E., 2020. On the bottleneck of graph neural networks and its practical implications.

Background

3. Transformer-based GNNs

- Fully connected Transformer-GNNs recently proposed which perform better thanks to **PE-focused** innovations!

Spectral Attention Networks (SAN) [1]

- SAN use a Learnable PE module that applies a Transformer encoder on a sequence of eigenvalues/vectors to generate a fixed sized PE
- During full-attention in the main Transformer, separate learnable parameters are maintained for real and non-real edges

← Injecting PE at node inputs

GraphiT [2]

- Use of diffusion geometry to capture short and long-range information
- The diffusion distance is multiplied with attention score

← Injecting PE with attention score

Graphormer [3]

- Use of centrality, spatial and edge encoding to improve node inputs and attention.

← Injecting PE with node inputs as well as attention score

Note: Other previous works such as Graph-BERT [4] use a combination of structural and relative encodings after a link-less subgraph batching

[1] Kreuzer, D., Beaini, D., Hamilton, W.L., Létourneau, V. and Tossou, P., 2021. Rethinking Graph Transformers with Spectral Attention.
[2] Mialon, G., Chen, D., Selosse, M. and Mairal, J., 2021. GraphiT: Encoding Graph Structure in Transformers.
[3] Ying, C., Cai, T., Luo, S., Zheng, S., Ke, G., He, D., Shen, Y. and Liu, T.Y., 2021. Do Transformers Really Perform Bad for Graph Representation?
[4] Zhang, J., Zhang, H., Xia, C. and Sun, L., 2020. Graph-bert: Only attention is needed for learning graph representations.

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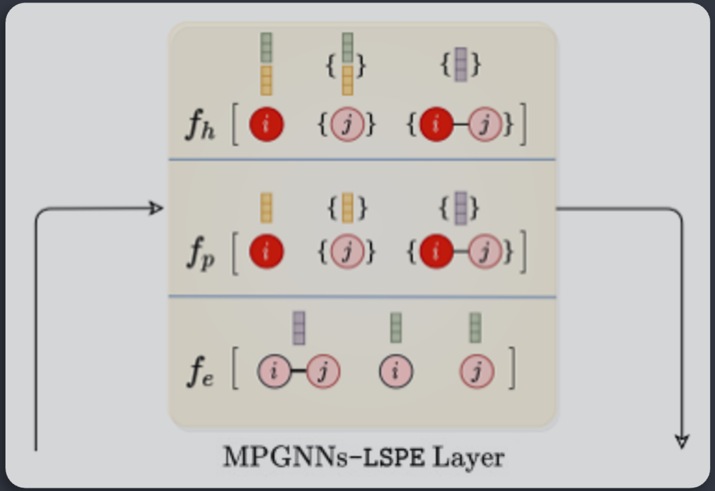


Learnable Structural and Positional Encodings

1. Standard MP-GNNs

$$\text{MP-GNNs}: \quad h_i^{\ell+1} = f_h\left(h_i^{\ell}, \{h_j^{\ell}\}_{j\in\mathcal{N}_i}, e_{ij}^{\ell}\right),\ h_i^{\ell+1}, h_i^{\ell} \in \mathbb{R}^d,$$
$$e_{ij}^{\ell+1} = f_e\left(h_i^{\ell}, h_j^{\ell}, e_{ij}^{\ell}\right),\ e_{ij}^{\ell+1}, e_{ij}^{\ell} \in \mathbb{R}^d,$$

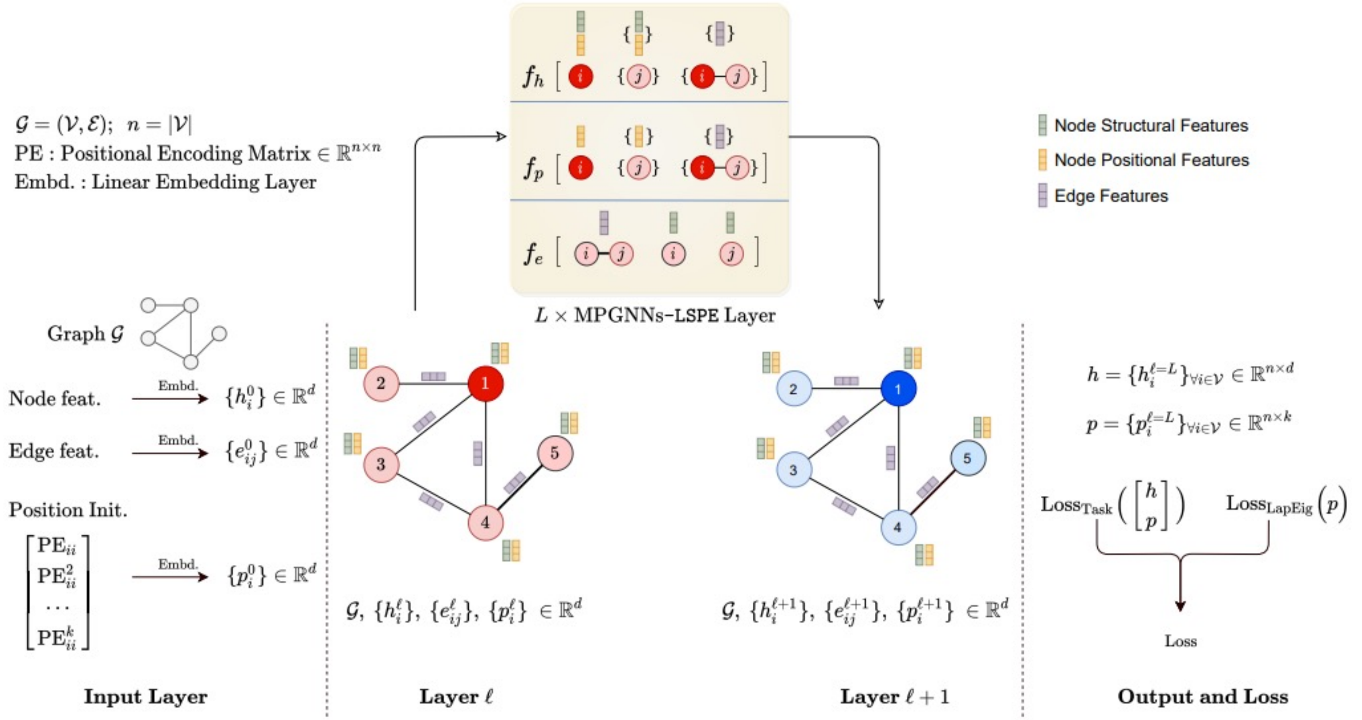
2. MP-GNNs with PE injected with the input node features

$$\text{with initial } h_i^{\ell=0} = \text{LL}_h\left(\begin{bmatrix} h_i^{\text{in}} \\ p_i^{\text{in}} \end{bmatrix}\right) = D^0 \begin{bmatrix} h_i^{\text{in}} \\ p_i^{\text{in}} \end{bmatrix} + d^0 \in \mathbb{R}^d,$$
$$\text{and } e_{ij}^{\ell=0} = \text{LL}_e(e_{ij}^{\text{in}}) = B^0 e_{ij}^{\text{in}} + b^0 \in \mathbb{R}^d,$$

3. **[Proposed] Learning structural and positional representations** at every layer

$$\text{MP-GNNs-LSPE}: \quad h_i^{\ell+1} = f_h\left(\begin{bmatrix} h_i^{\ell} \\ p_i^{\ell} \end{bmatrix}, \left\{\begin{bmatrix} h_j^{\ell} \\ p_j^{\ell} \end{bmatrix}\right\}_{j\in\mathcal{N}_i}, e_{ij}^{\ell}\right),\ h_i^{\ell+1}, h_i^{\ell} \in \mathbb{R}^d,$$
$$e_{ij}^{\ell+1} = f_e\left(h_i^{\ell}, h_j^{\ell}, e_{ij}^{\ell}\right),\ e_{ij}^{\ell+1}, e_{ij}^{\ell} \in \mathbb{R}^d,$$
$$p_i^{\ell+1} = f_p\left(p_i^{\ell}, \{p_j^{\ell}\}_{j\in\mathcal{N}_i}, e_{ij}^{\ell}\right),\ p_i^{\ell+1}, p_i^{\ell} \in \mathbb{R}^d,$$

- We decouple positional and structural representations and learn each separately
- Initial PE to be chosen (next slide →)
- The proposed modification is generic and applies to any model that fits to MP-GNNs
- Additionally, a positional loss can be used for tuning final positional representations



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Learnable Structural and Positional Encodings

Initial PE

- Choice of initial PE to be used in MP-GNNs-LSPE is critical
- If we use LapPE which can provide unique node representation, it brings the limitations as discussed

$$p_i^{\text{LapPE}} = [\ U_{i1}, U_{i2}, \cdots, U_{ik}\ ] \in \mathbb{R}^k$$

- We propose **RWPE** based on the Random Walk diffusion process

$$p_i^{\text{RWPE}} = [\ \text{RW}_{ii}, \text{RW}_{ii}^2, \cdots, \text{RW}_{ii}^k\ ] \in \mathbb{R}^k$$

- We use RW_{ii} from every k^{th} step to construct RWPE of node i
- Thus, RWPE **encodes** the landing probability of a node to itself in 1 to k steps of random walk
- RWPE closely based on Distance Encoding (DE) [1] but we do not consider all relative RW_{ij} as in DE

Meaningful higher-order structure information!

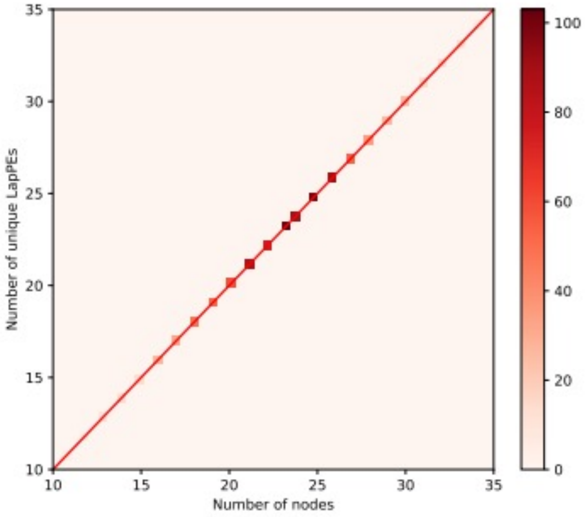
[1] Li, P., Wang, Y., Wang, H. and Leskovec, J., 2020. Distance Encoding--Design Provably More Powerful GNNs for Structural Representation Learning.

Learnable Structural and Positional Encodings

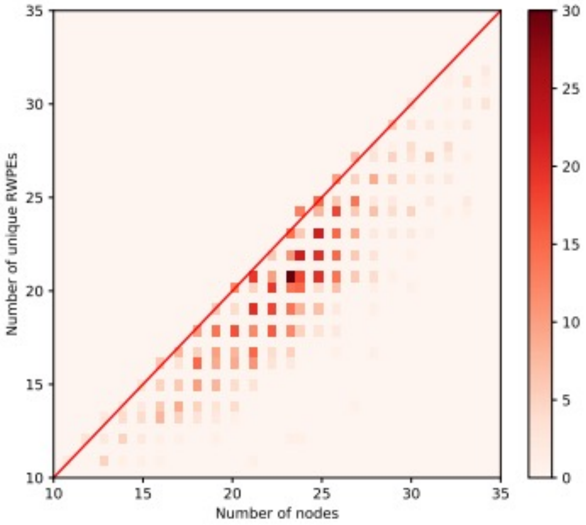
Initial PE: RWPE

Characteristics of RWPE

- Unique representation for a node “given a distinct k-hop” neighborhood when considering a sufficient k

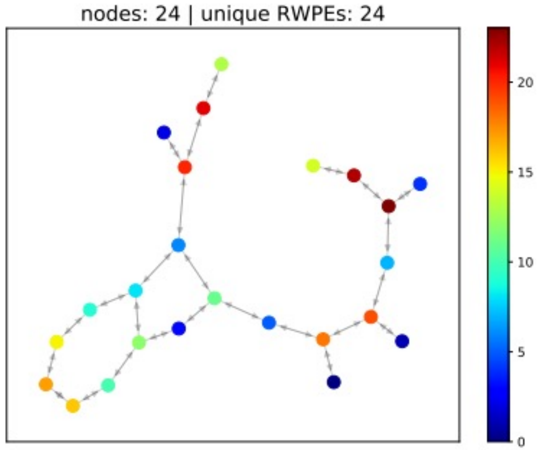


(a) LapPE, $k = 36$

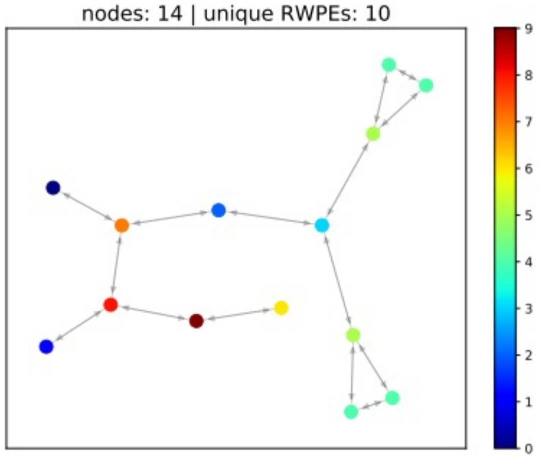


(b) RWPE, $k = 24$

ZINC valset: number of nodes vs. number of unique PE
the point intensity is the number of graphs



(a) ZINC molecule (val index 91)



(b) ZINC molecule (val index 212)

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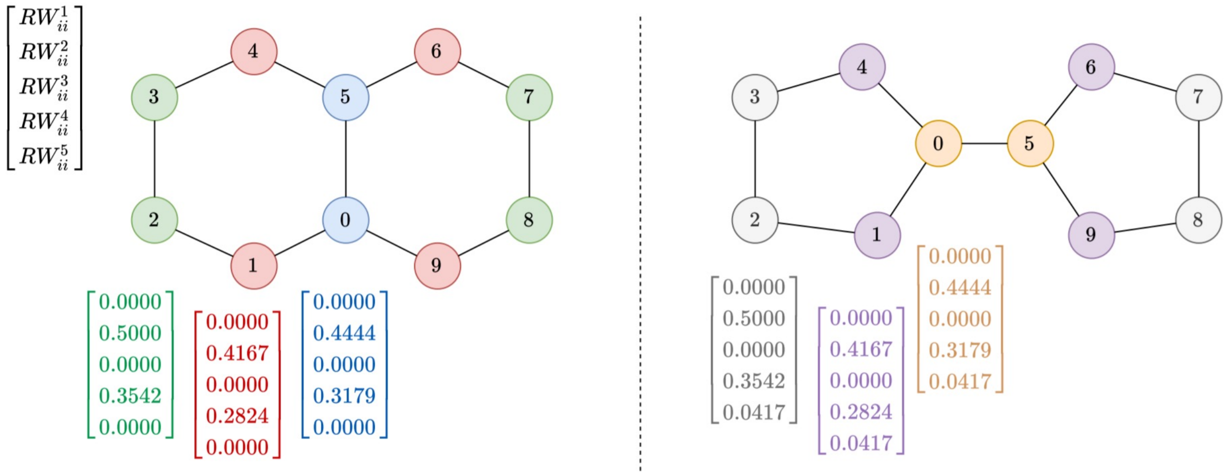
Learnable Structural and Positional Encodings

Initial PE: RWPE

Characteristics of RWPE

- No sign ambiguity as in LapPE
- Can distinguish graph-pairs that failed to be classified correctly by MP-GNNs (1-WL)



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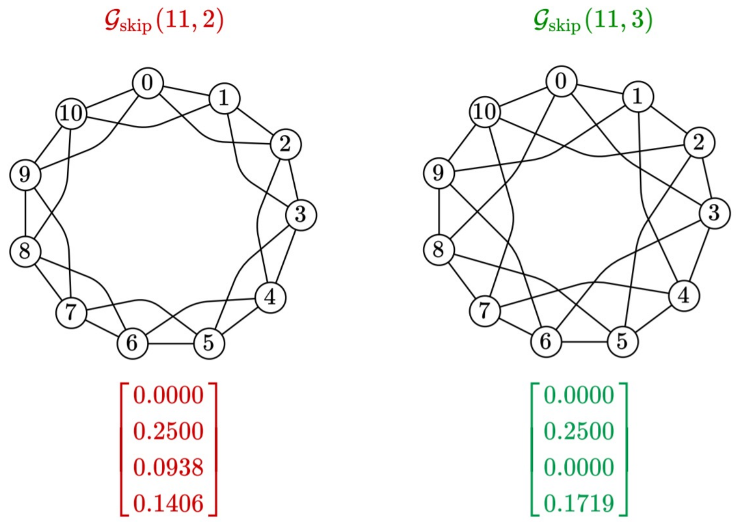

A pair of Circular Skip Link Graphs

Learnable Structural and Positional Encodings

A. Instantiation of LSPE with sparse MP-GNNs

$$\text{MP-GNNs-LSPE}: \quad h_i^{\ell+1} = f_h\left(\begin{bmatrix} h_i^\ell \\ p_i^\ell \end{bmatrix}, \left\{\begin{bmatrix} h_j^\ell \\ p_j^\ell \end{bmatrix}\right\}_{j\in\mathcal{N}_i}, e_{ij}^\ell\right),\ h_i^{\ell+1}, h_i^\ell \in \mathbb{R}^d,$$
$$e_{ij}^{\ell+1} = f_e\left(h_i^\ell, h_j^\ell, e_{ij}^\ell\right),\ e_{ij}^{\ell+1}, e_{ij}^\ell \in \mathbb{R}^d,$$
$$p_i^{\ell+1} = f_p\left(p_i^\ell, \{p_j^\ell\}_{j\in\mathcal{N}_i}, e_{ij}^\ell\right),\ p_i^{\ell+1}, p_i^\ell \in \mathbb{R}^d,$$

1. GatedGCN [1] -LSPE

$$h^{\ell+1}, e^{\ell+1}, p^{\ell+1} = \text{GatedGCN-LSPE}\left(h^\ell, e^\ell, p^\ell\right),\ h \in \mathbb{R}^{n\times d}, e \in \mathbb{R}^{E\times d}, p \in \mathbb{R}^{n\times d},$$
$$\text{with}\ \ h_i^{\ell+1} = h_i^\ell + \text{ReLU}\left(\text{BN}\left(A_1^\ell \begin{bmatrix} h_i^\ell \\ p_i^\ell \end{bmatrix} + \sum_{j\in\mathcal{N}(i)} \eta_{ij}^\ell \odot A_2^\ell \begin{bmatrix} h_j^\ell \\ p_j^\ell \end{bmatrix}\right)\right),$$
$$e_{ij}^{\ell+1} = e_{ij}^\ell + \text{ReLU}\left(\text{BN}\left(\hat{\eta}_{ij}^\ell\right)\right),$$
$$p_i^{\ell+1} = p_i^\ell + \tanh\left(C_1^\ell p_i^\ell + \sum_{j\in\mathcal{N}(i)} \eta_{ij}^\ell \odot C_2^\ell p_j^\ell\right),$$
$$\text{and}\ \ \eta_{ij}^\ell = \frac{\sigma\left(\hat{\eta}_{ij}^\ell\right)}{\sum_{j'\in\mathcal{N}(i)} \sigma\left(\hat{\eta}_{ij'}^\ell\right) + \epsilon},$$
$$\hat{\eta}_{ij}^\ell = B_1^\ell h_i^\ell + B_2^\ell h_j^\ell + B_3^\ell e_{ij}^\ell,$$

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[1] Bresson, X. and Laurent, T., 2017. Residual gated graph convnets.

Learnable Structural and Positional Encodings

A. Instantiation of LSPE with sparse MP-GNNs

$$\text{MP-GNNs-LSPE}: \quad h_i^{\ell+1} = f_h\left(\begin{bmatrix} h_i^\ell \\ p_i^\ell \end{bmatrix}, \left\{\begin{bmatrix} h_j^\ell \\ p_j^\ell \end{bmatrix}\right\}_{j\in\mathcal{N}_i}, e_{ij}^\ell\right), \; h_i^{\ell+1}, h_i^\ell \in \mathbb{R}^d,$$

$$e_{ij}^{\ell+1} = f_e\left(h_i^\ell, h_j^\ell, e_{ij}^\ell\right), \; e_{ij}^{\ell+1}, e_{ij}^\ell \in \mathbb{R}^d,$$

$$p_i^{\ell+1} = f_p\left(p_i^\ell, \{p_j^\ell\}_{j\in\mathcal{N}_i}, e_{ij}^\ell\right), \; p_i^{\ell+1}, p_i^\ell \in \mathbb{R}^d,$$

2. PNA [1] -LSPE

$$h^{\ell+1}, p^{\ell+1} = \text{PNA-LSPE}\left(h^\ell, e^0, p^\ell\right), \; h \in \mathbb{R}^{n\times d}, e^0 \in \mathbb{R}^{E\times d}, p \in \mathbb{R}^{n\times d},$$

$$\text{with } h_i^{\ell+1} = h_i^\ell + \text{LReLU}\left(\text{BN}\left(U_h^\ell\left(\begin{bmatrix} h_i^\ell \\ p_i^\ell \end{bmatrix}, \bigoplus_{j\in\mathcal{N}(i)} M_h^\ell\left(\begin{bmatrix} h_i^\ell \\ p_i^\ell \end{bmatrix}, e_{ij}^0, \begin{bmatrix} h_j^\ell \\ p_j^\ell \end{bmatrix}\right)\right)\right)\right),$$

$$p_i^{\ell+1} = p_i^\ell + \tanh\left(U_p^\ell\left(p_i^\ell, \bigoplus_{j\in\mathcal{N}(i)} M_p^\ell\left(p_i^\ell, e_{ij}^0, p_j^\ell\right)\right)\right),$$

$$\text{and } \bigoplus = \begin{bmatrix} I \\ S(D, \alpha=1) \\ S(D, \alpha=-1) \end{bmatrix} \otimes \begin{bmatrix} \mu \\ \sigma \\ \max \\ \min \end{bmatrix},$$

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[1] Corso, G., Cavalleri, L., Beaini, D., Liò, P. and Veličković, P., 2020. Principal neighbourhood aggregation for graph nets.

Learnable Structural and Positional Encodings

B. Instantiation of LSPE with Transformer-GNNs*

1. SAN [1] -LSPE

$$h^{\ell+1}, p^{\ell+1} = \text{SAN-LSPE}\left(h^\ell, e^0, p^\ell\right),\ h \in \mathbb{R}^{n\times d}, e^0 \in \mathbb{R}^{n\times n\times d}, p \in \mathbb{R}^{n\times d},$$

$$\text{with}\ h_i^{\ell+1} = \text{BN}\left(\bar{h}_i^{\ell+1} + W_2^\ell\, \text{ReLU}\left(W_1^\ell\, \bar{h}_i^{\ell+1}\right)\right) \in \mathbb{R}^d$$

$$\bar{h}_i^{\ell+1} = \text{BN}\left(h_i^\ell + \hat{h}_i^{\ell+1}\right) \in \mathbb{R}^d,$$

$$\hat{h}_i^{\ell+1} = O^\ell\left(\Big\Vert_{k=1}^{H} \sum_{j\in\mathcal{V}} \frac{w_{ij}^{k,\ell}}{\sum_{j'\in\mathcal{V}} w_{ij'}^{k,\ell}}\, v_j^{k,\ell}\right) \in \mathbb{R}^d,$$

$$w_{ij}^{k,\ell} = \begin{cases} \frac{1}{1+\gamma}\cdot \exp(A_{ij}^{k,\ell}) & \text{if } ij \in E \\ \frac{\gamma}{1+\gamma}\cdot \exp(\bar{A}_{ij}^{k,\ell}) & \text{if } ij \notin E \end{cases},$$

$$\begin{cases} A_{ij}^{k,\ell} = q_i^{k,\ell^T} \text{diag}(c_{ij}^{k,\ell}) k_j^{k,\ell} / \sqrt{d_k} \in \mathbb{R} & \text{if } ij \in E \\ \bar{A}_{ij}^{k,\ell} = \bar{q}_i^{k,\ell^T} \text{diag}(\bar{c}_{ij}^{k,\ell}) \bar{k}_j^{k,\ell} / \sqrt{d_k} \in \mathbb{R} & \text{if } ij \notin E \end{cases}$$

$$Q^{k,\ell} = \begin{bmatrix} h^\ell \\ p^\ell \end{bmatrix} W_Q^{k,\ell},\ K^{k,\ell} = \begin{bmatrix} h^\ell \\ p^\ell \end{bmatrix} W_K^{k,\ell},\ V^{k,\ell} = \begin{bmatrix} h^\ell \\ p^\ell \end{bmatrix} W_V^{k,\ell} \in \mathbb{R}^{n\times d_k}$$

$$\bar{Q}^{k,\ell} = \begin{bmatrix} h^\ell \\ p^\ell \end{bmatrix} \bar{W}_Q^{k,\ell},\ \bar{K}^{k,\ell} = \begin{bmatrix} h^\ell \\ p^\ell \end{bmatrix} \bar{W}_K^{k,\ell},\ \bar{V}^{k,\ell} = \begin{bmatrix} h^\ell \\ p^\ell \end{bmatrix} \bar{W}_V^{k,\ell} \in \mathbb{R}^{n\times d_k}$$

$$C^{k,0} = e^0 W_e^k,\ \bar{C}^{k,0} = e^0 \bar{W}_e^k \in \mathbb{R}^{n\times n\times d_k}$$

$$\text{and}\ p_i^{\ell+1} = p_i^\ell + \tanh\left(O_p^\ell\left(\Big\Vert_{k=1}^{H} \sum_{j\in\mathcal{V}} \frac{w_{p,ij}^{k,\ell}}{\sum_{j'\in\mathcal{V}} w_{p,ij'}^{k,\ell}}\, v_{p,j}^{k,\ell}\right)\right) \in \mathbb{R}^d,$$

2. GraphiT [2] –LSPE

Here we use SAN based architecture for separate parameters for real and non-real edges and modify the weight-score using GraphiT as:

$$w_{ij}^{k,\ell} = \begin{cases} K_{ij}\cdot \exp(A_{ij}^{k,\ell}) & \text{if } ij \in E \\ K_{ij}\cdot \exp(\bar{A}_{ij}^{k,\ell}) & \text{if } ij \notin E \end{cases}$$

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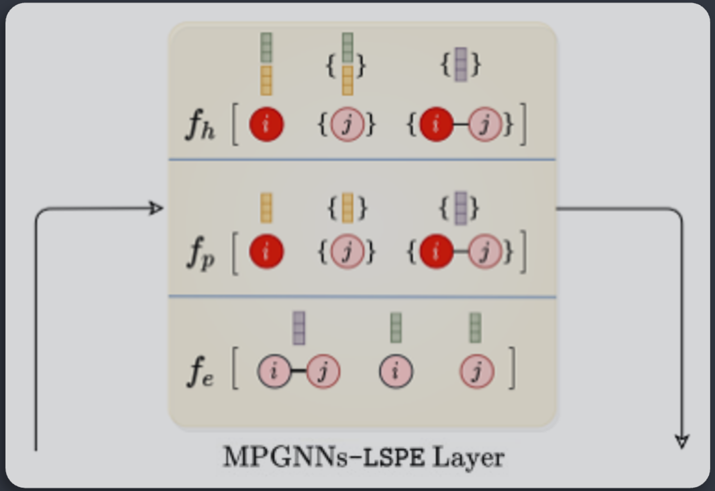
[1] Kreuzer, D., Beaini, D., Hamilton, W.L., Létourneau, V. and Tossou, P., 2021. Rethinking Graph Transformers with Spectral Attention.
[2] Mialon, G., Chen, D., Selosse, M. and Mairal, J., 2021. GraphiT: Encoding Graph Structure in Transformers.

Footnote: * with modifications

Outline of Presentation

- ❑ Motivation
- ❑ Background
- ❑ Learnable Structural and Positional Encodings (LSPE)
- ❑ **Numerical Evaluations**
- ❑ Conclusion



Numerical Evaluations

Step by step empirical evaluation towards the final GNN-LSPE architecture

Instance: GatedGCN-LSPE **Dataset:** ZINC **Metric:** MAE (lower is better)

Insights:

- Adding PE improves performance against not using one
- RWPE outperforms LapPE while simply injecting these at the input
- Use of PE at the input layer as opposed with final learnt representations

- Simply adding RWPE leads to overfit
- Using LSPE alleviates this overfit and improves performance significantly

	Model	Init PE	LSPE	Final h	L	#Param	Test MAE±s.d.	Train MAE±s.d.	#Epochs	Epoch/Total
1	GatedGCN	x	x	h^L	16	504309	0.251±0.009	0.025±0.005	440.25	8.76s/1.08hr
2	GatedGCN	LapPE	x	h^L	16	505011	0.202±0.006	0.033±0.003	426.00	8.91s/1.22hr
3	GatedGCN	RWPE	x	h^L	16	505947	0.122±0.003	0.013±0.003	436.25	9.14s/1.28hr
4	GatedGCN	x	x	$[h^L, \textbf{RWPE}]$	16	515249	0.249±0.012	0.024±0.002	437.50	10.05s/1.55hr
5	GatedGCN	LapPE	✓	h^L	16	516722	0.202±0.008	0.032±0.005	405.25	15.10s/1.84hr
6	GatedGCN	LapPE	✓	$[h^L, p^L]$	16	520734	0.196±0.008	0.023±0.004	454.00	15.22s/2.06hr
7	GatedGCN	RWPE	✓	h^L	16	518150	0.100±0.006	0.018±0.012	395.00	15.09s/1.73hr
8	GatedGCN	RWPE	✓	$[h^L, p^L]$	16	522870	0.093±0.003	0.014±0.003	440.75	15.17s/1.99hr

- **At last**, using the final layer positional and structural features for the task with LSPE gives the best performance

Numerical Evaluations

All experiments on 3 molecular datasets

Insights:

- LSPE consistently enhances the capabilities of existing GNNs on the 4 instances evaluated
- On these datasets, sparse GNNs show better performance compared to fully-connected Transformer GNNs
- Positional Loss improves test score on ZINC slightly while in general it leads to overfit on training data

Dataset	Model	Init PE	LSPE	PosLoss	L	#Param	TestMAE±s.d.	TrainMAE±s.d.	Epochs	Epoch/Total
ZINC	GatedGCN	x	x	x	16	504309	0.251±0.009	0.025±0.005	440.25	8.76s/1.08hr
ZINC	GatedGCN	**LapPE**	x	x	16	505011	0.202±0.006	0.033±0.003	426.00	8.91s/1.22hr
ZINC	GatedGCN	**RWPE**	✓	x	16	522870	0.093±0.003	0.014±0.003	440.75	15.17s/1.99hr
ZINC	GatedGCN	**RWPE**	✓	✓	16	522870	**0.090±0.001**	0.013±0.004	460.50	33.06s/4.39hr
ZINC	PNA	x	x	x	16	369235	0.141±0.004	0.020±0.003	451.25	79.67s/10.03hr
ZINC	PNA	**RWPE**	✓	x	16	503061	**0.101±0.003**	0.026±0.012	443.75	126.06s/15.77hr
ZINC	SAN	x	x	x	10	501314	0.181±0.004	0.017±0.004	433.50	74.33s/9.23hr
ZINC	SAN	**RWPE**	✓	x	10	588066	**0.104±0.004**	0.016±0.002	462.50	134.74s/17.23hr
ZINC	GraphiT	x	x	x	10	501313	0.181±0.006	0.021±0.003	493.25	63.54s/9.37hr
ZINC	GraphiT	**RWPE**	✓	x	10	588065	**0.106±0.002**	0.028±0.002	420.50	125.39s/14.84hr
	Model	**Init PE**	**LSPE**	**PosLoss**	L	**#Param**	**TestAUC±s.d.**	**TrainAUC±s.d.**	**Epochs**	**Epoch/Total**
MOLTOX21	GatedGCN	x	x	x	8	1003739	0.772±0.006	0.933±0.010	304.25	5.12s/0.46hr
MOLTOX21	GatedGCN	**LapPE**	x	x	8	1004355	0.774±0.007	0.921±0.006	275.50	5.23s/0.48hr
MOLTOX21	GatedGCN	**RWPE**	✓	x	8	1063821	**0.775±0.003**	0.906±0.003	246.50	5.99s/0.63hr
MOLTOX21	PNA	x	x	x	8	5244849	0.755±0.008	0.876±0.014	214.75	6.25s/0.38hr
MOLTOX21	PNA	**RWPE**	✓	x	8	5357393	**0.781±0.013**	0.901±0.013	249.75	9.87s/0.73hr
MOLTOX21	PNA	**RWPE**	✓	✓	8	5357393	0.778±0.006	0.906±0.012	245.00	24.09s/1.70hr
MOLTOX21	SAN	x	x	x	10	957871	**0.744±0.007**	0.915±0.015	279.75	18.06s/1.44hr
MOLTOX21	SAN	**RWPE**	✓	x	10	1051017	0.744±0.008	0.918±0.018	281.75	30.82s/2.84hr
MOLTOX21	GraphiT	x	x	x	10	957870	0.743±0.003	0.919±0.023	276.50	16.73s/1.36hr
MOLTOX21	GraphiT	**RWPE**	✓	x	10	1051788	**0.746±0.010**	0.934±0.016	279.75	27.92s/2.57hr
	Model	**Init PE**	**LSPE**	**PosLoss**	L	**#Param**	**TestAP±s.d.**	**TrainAP±s.d.**	**Epochs**	**Epoch/Total**
MOLPCBA	GatedGCN	x	x	x	8	1008263	0.262±0.001	0.401±0.057	190.50	149.10s/7.91hr
MOLPCBA	GatedGCN	**LapPE**	x	x	8	1008879	0.266±0.002	0.391±0.003	177.00	152.94s/8.29hr
MOLPCBA	GatedGCN	**RWPE**	✓	x	8	1068721	**0.267±0.002**	0.403±0.006	181.00	206.43s/11.64hr
MOLPCBA	PNA	x	x	x	4	6550839	0.279±0.003	0.448±0.004	129.25	174.75s/6.34hr
MOLPCBA	PNA	**RWPE**	✓	x	4	6521029	**0.287±0.003**	0.392±0.002	334.50	202.59s/23.68hr

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Numerical Evaluations

Comparison with baselines and state-of-the-art GNNs

(a) ZINC

Model	Test MAE
GCN	0.367±0.011
GAT	0.384±0.007
GatedGCN-LapPE	0.202±0.006
GT	0.226±0.014
SAN	0.139±0.006
Graphormer	0.122±0.006
GatedGCN-LSPE	**0.090±0.001**

(b) OGBG-MOLTOX21

Model	Test ROC-AUC
GCN	0.7529±0.0069
GCN-VN	0.7746±0.0086
GIN	0.7491±0.0051
GIN-VN	0.7757±0.0062
GatedGCN-LapPE	0.7743±0.0073
PNA-LSPE	**0.7808±0.0130**

(c) OGBG-MOLPCBA

Model	Test AP
GIN	0.2266±0.0028
GIN-VN	0.2703±0.0023
DeeperGCN-VN	0.2781±0.0038
PNA	0.2838±0.0035
DGN	0.2885±0.0030
PHC-GNN	**0.2947±0.0026**
PNA-LSPE	0.2873±0.0027

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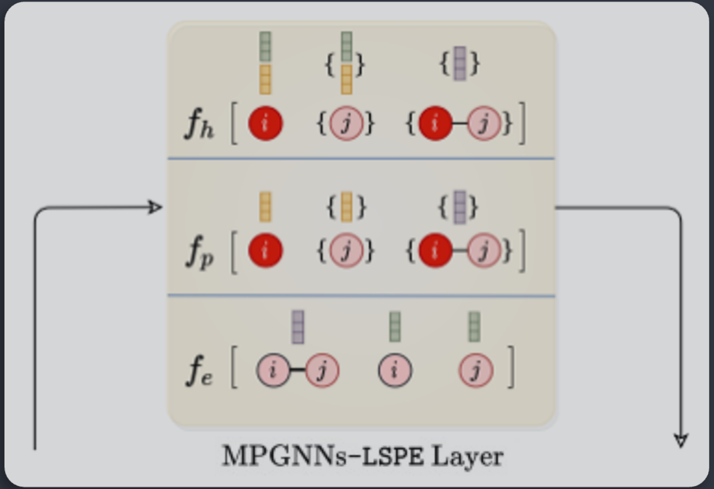

Conclusion

- Decoupling and learning structural and positional representations at every layer improves existing GNNs – both sparse and fully-connected.
- The initialization of PE is critical and contributes greatly towards improving a GNN.
- LSPE helps the feature representations to be tuned for the task and improves generalization performance.
- Compared to fully-connected Transformer-GNNs, the sparse GNNs perform better on the molecular datasets that we considered for evaluation and are efficient at the same time.
- The proposed LSPE architecture is a general framework that can be applied to improve any GNN that fits in the message-passing framework.

Questions?

Thank you!

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