Beyond Sparse Graphs: Graph Transformers

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CS598: Deep Learning with Graphs, 2024 Fall

https://ulab-uiuc.github.io/CS598/

Logistics: Updated Submission Task

- **1 DDL:** The deadline for the submission task is **Nov 21 (Thu), 11:59 PM CT**. Please plan the progress of your project reasonably.
  - We will kick off the peer-review session right after the submission. We will also give instructions on review and response on Nov 22 (Fri).
  - The fall break begins from Nov 23 (Sat). Enjoy your break after submitting your paper :)
- **2 Length:** We expect a minimum length of **6 pages** in ICLR 2025 format for the **draft submission**.
  - For the draft version, you are expected to include at least sections such as related work, methods, and experiment settings.
  - We will use the OpenReview to receive submissions, which will be announced on Canvas by this weekend.

Logistics: Updated Submission Task

- **3 Grading:** The submission task counts towards **15% (writing) + 15% (implementation) = 30%** of your final grade.
  - For the 15% of writing, **only 5%** is determined by the **draft version** (**due on Nov 21**) and **10%** is determined by the **final version** (**due on Dec 8**).
  - The 15% of implementation is determined by the code you provide for the **final version** (**due on Dec 8**).
  - You can revise your draft version during the review and response as well as the presentation stage based on others' feedback.
  - However, we encourage you to complete as much as possible for your submission to receive more comprehensive feedback.

Logistics: Updated Schedule

12	Nov 13 Wed	No class	Paper Writing		
	Nov 15 Fri	GNN applications: graph mining (remote)	Paper Writing		Assignment 4, due on Nov 17
13	Nov 20 Wed	GNN applications: science	Paper Writing		Submission task, due on Nov 21 (only draft required)
	Nov 22 Fri	Conclusion	Review & Response	Review & response task, out	
14	Nov 27 Wed	No class (fall break)	Review & Response		
	Nov 29 Fri	No class (fall break)	Review & Response		

- **No class and office hour on Nov 13 (Wed)**
- **Remote session on Nov 15 (Fri)**
  - Zoon link will be announced on Canvas and Slack.

Logistics: Coding Homework

- **Assignment 3 due**
  - Please submit your code and written answers to Canvas.
  - The submission deadline is **Nov 3 (Sun) 11:59 PM, CT**.
- **Assignment 4 out**
  - Assignment will be released on Canvas today.
  - Implement graph transformers
  - Submit your code and written answers downloaded from Colab to Canvas by **Nov 17 (Sun) 11:59 PM, CT**.

Today's Lecture

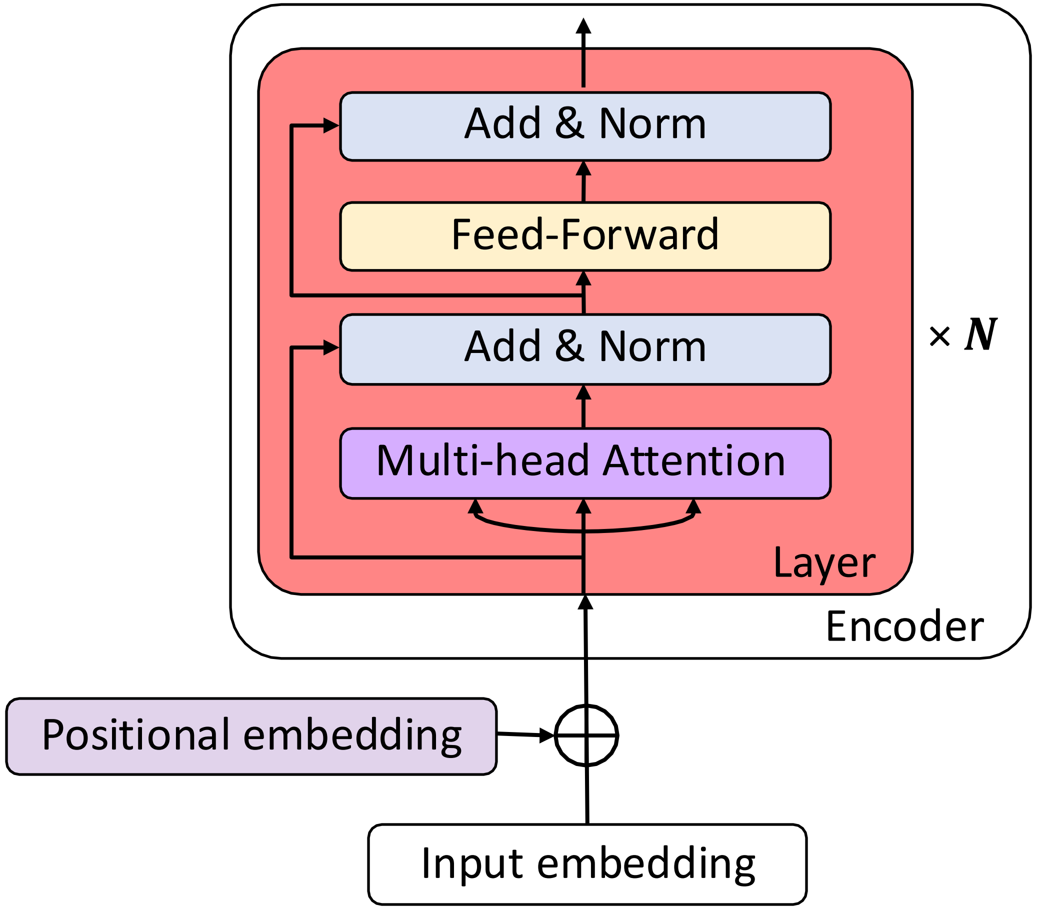
- Graph attention is **closely related** to transformers
- Graph learning techniques can **make transformers more efficient**
- Transformer can **inspire GNN architectures**

Beyond Sparse Graphs: Graph Transformers

Self-Attention and Transformers

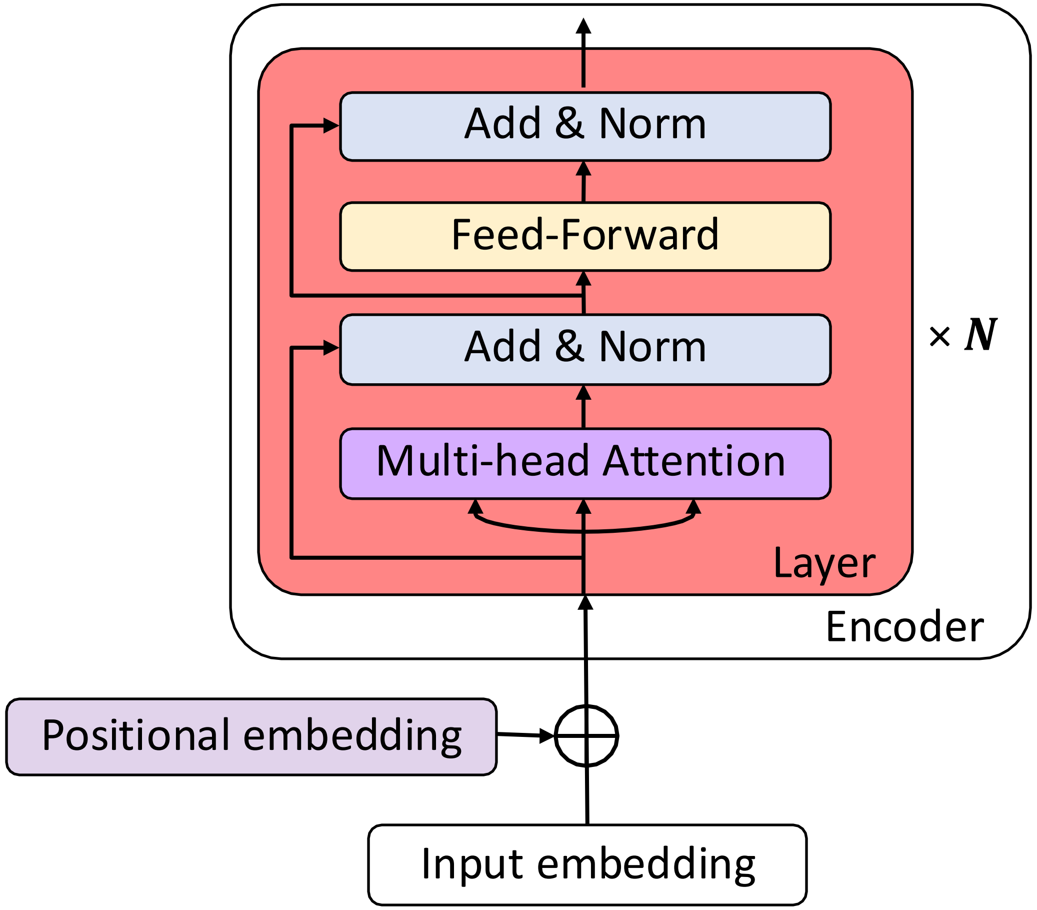
Transformers: Overview

- **Original paper**: Attention is all you need [Vaswani et al., 2017].
- **Key component**: Multi-head self-attention
- **Other components** of a transformer layer: layer normalization, skip connection, position- wise feed-forward layer (FFN, or MLP)



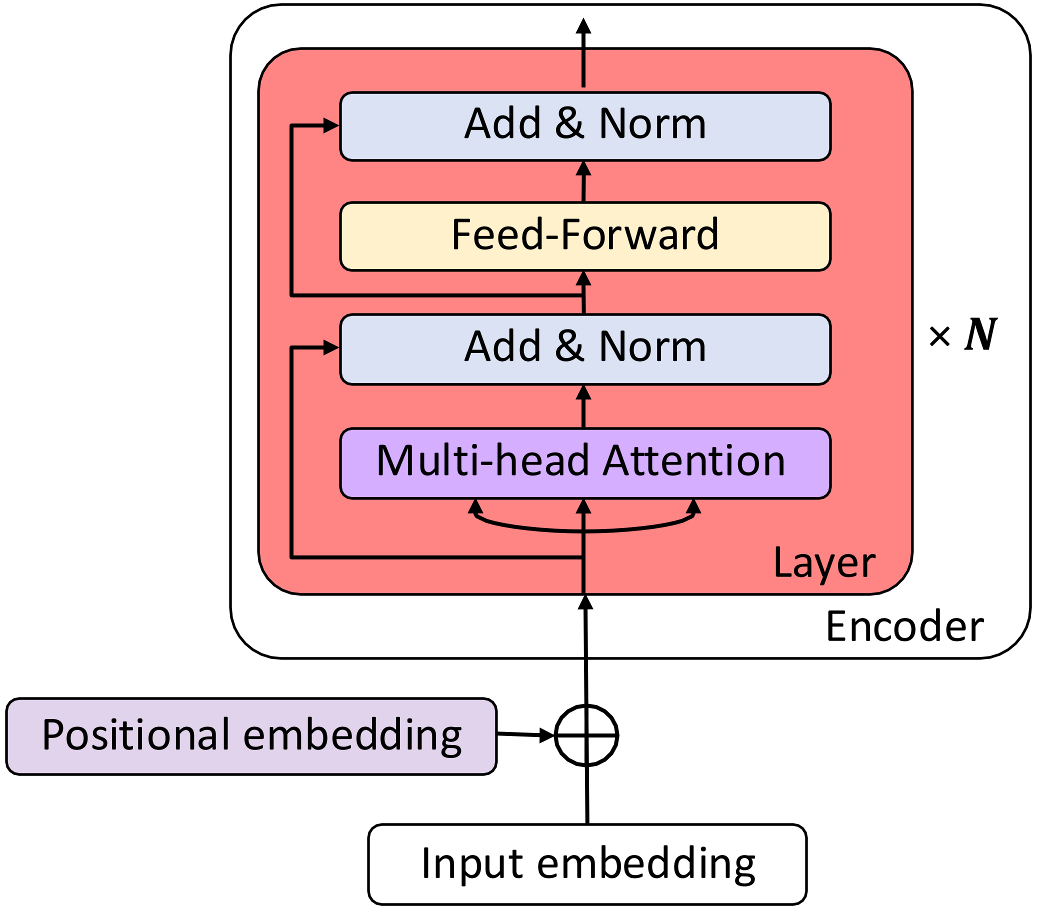
Transformers: Overview

- **Model usage**: Pre-training followed by fine- tuning. The transferred model can be:
  - Encoder-only (e.g BERT)
    - Many-to-one classification / regression
    - Sentiment classification, document classification ...
    - Word / Sentence embeddings for downstream tasks (e.g. recommender system)
  - Encoder-Decoder (e.g BART)
  - Decoder-only (e.g GPT)

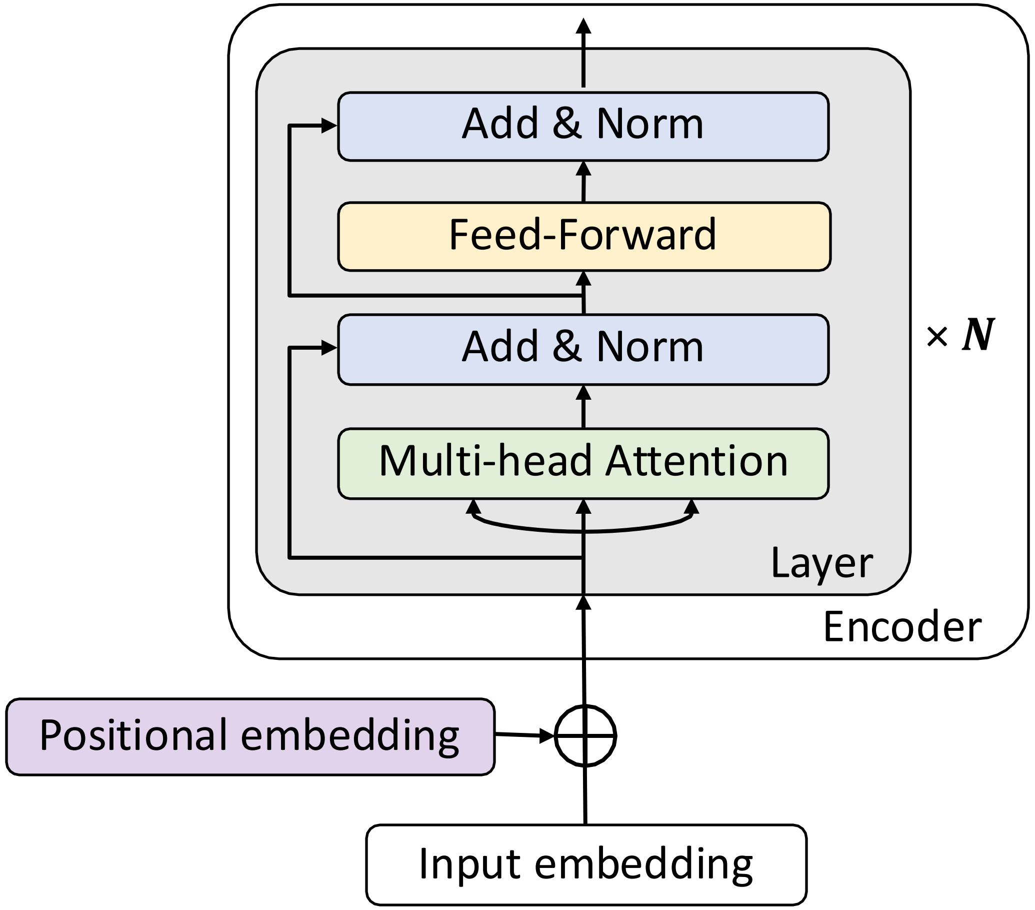


Transformers: Overview

- **Model usage**: Pre-training followed by fine- tuning. The transfered model can be:
  - Encoder-only (e.g BERT)
  - Encoder-Decoder (e.g [BART])
    - Many-to-many use cases
    - Summarization, translation, style transfer ...
  - Decoder-only (e.g OpenAI GPT)
    - One-to-many use cases
    - Image / text / code generation, dialogue systems ...
    - GPT-3/4 based [apps]



Transformers: Overview

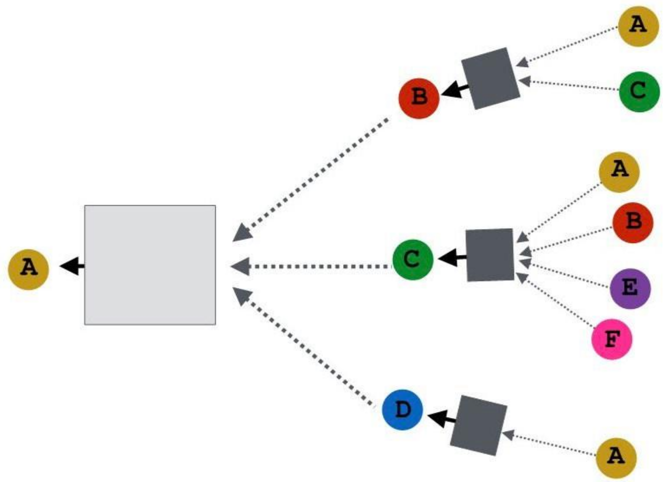


Design choices of transformers: (there are many papers on this topic for those interested in transformer architectures)

- Absolute/relative position, equivariant embedding (for graph)
- Sparse attention, low-rank attention, attention with prior, KV cache compression…
- Placement, substitutes, normalization-free
- Cross-block connections, recurrence/hierarchy, other architecture

Recap: Graph Attention Mechanism

- Message Aggregation: Review



Non-linearity

Embedding of u at layer l

$$\boldsymbol{h}_v^{(l)} = \sigma\Big(\sum_{u \in N(v)} \alpha_{vu} \boldsymbol{W}^{(l)} \boldsymbol{h}_u^{(l-1)}\Big)$$

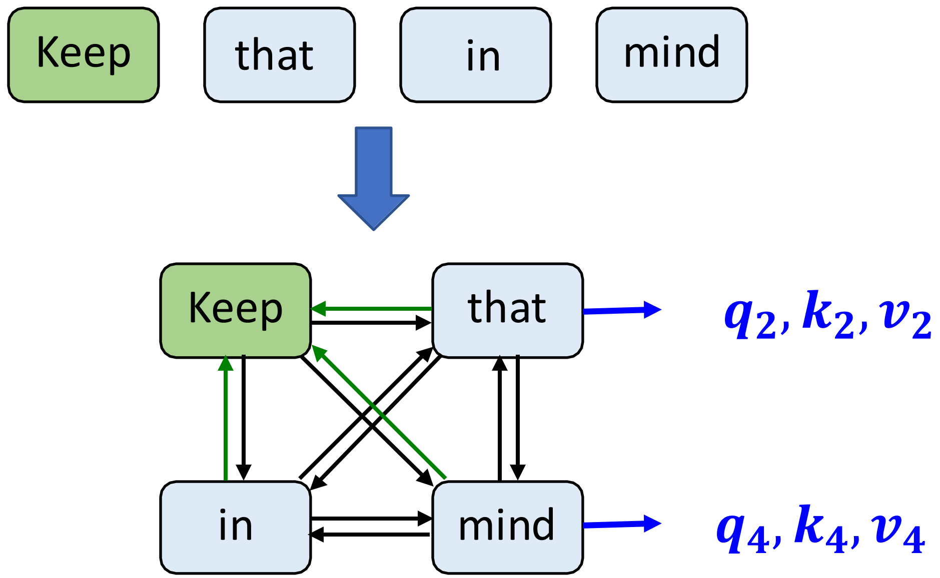
Neighbors of v

Learnable parameter

Weighting factor of u's message to v

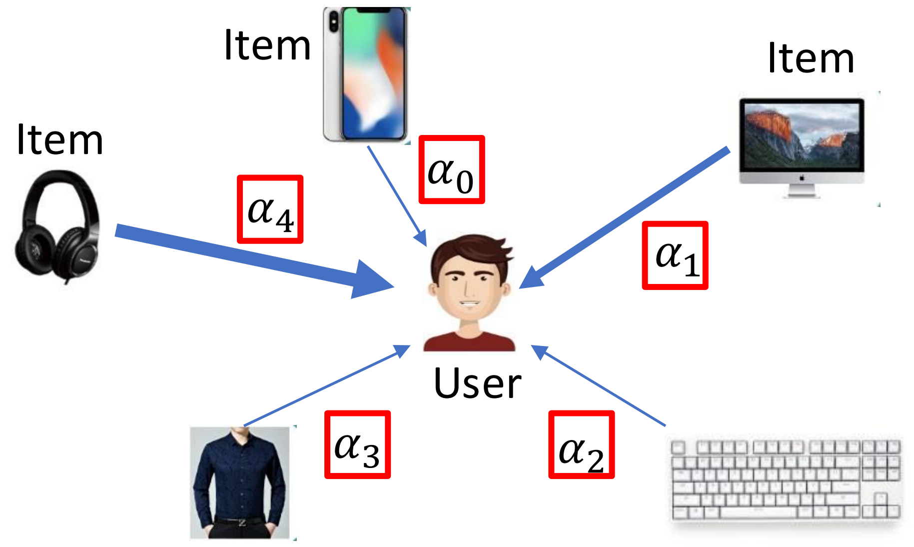
Transformers: in the Language of Graphs

Transformers



Step ① Mapping: Each node feature $\boldsymbol{x_i}$ is projected to $\boldsymbol{q_i}, \boldsymbol{k_i}, \boldsymbol{v_i}$.

GATs

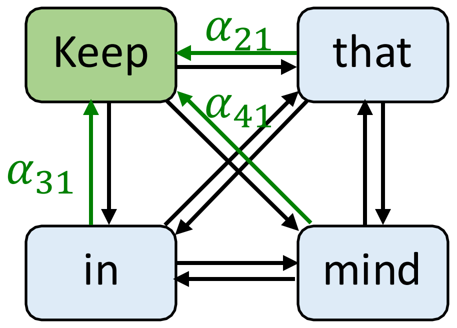


Message computing: transform information of neighbor node to a message.

$$m_u^{(l)} = \boldsymbol{W}^{(l)} \boldsymbol{h}_u^{(l-1)}, u \in N_v$$

Transformers: in the Language of Graphs

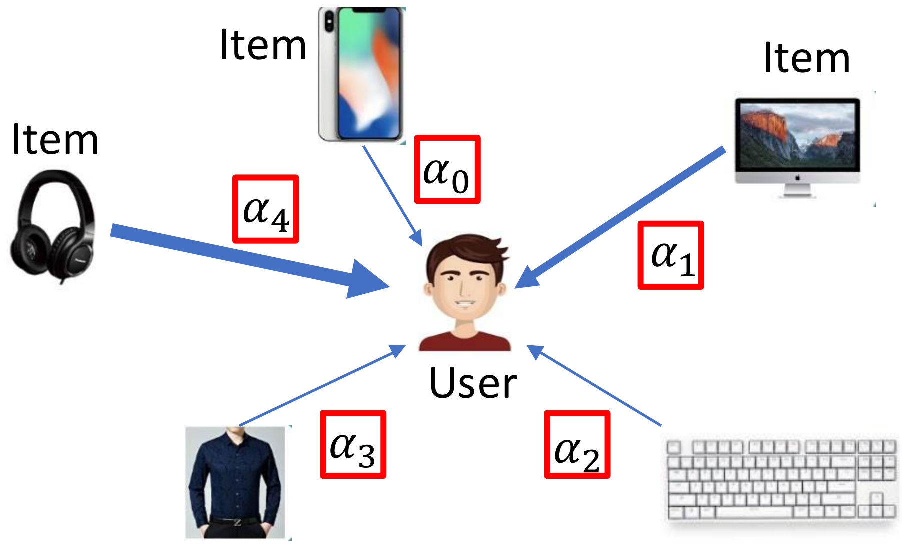
Transformers



Step ② Attention: Calculate the edge weights using q_i, k_j of the two endpoints node i and node j as $e_{ij} = \frac{q_i^T k_j}{\sqrt{d}}$, then normalizing it by neighbors of node i,

$$\alpha_{ij} = \mathrm{softmax}_i(e_{ij}) = \frac{\exp(e_{ij})}{\sum_{k \in N_i} \exp(e_{ik})}$$

GATs

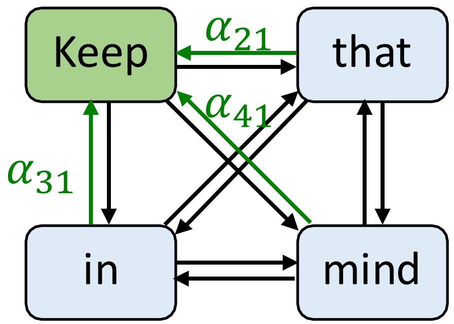


Attention computation: calculate the importance of neighbors

$$\alpha_{vu} = att(\boldsymbol{h}_v^{(l-1)}, \boldsymbol{h}_u^{(l-1)})$$

Transformers: in the Language of Graphs

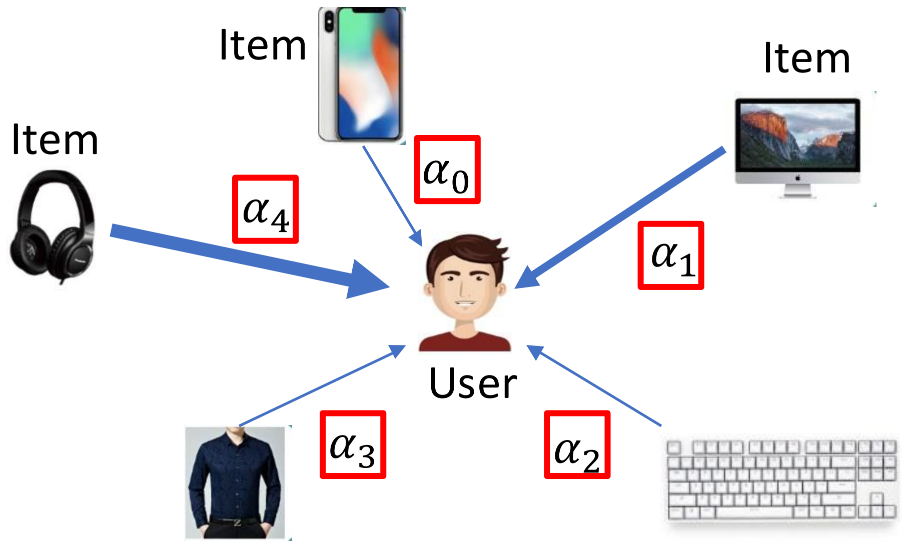
Transformers



Step ③ Update: Update each node feature according to its neighbors as

$$\boldsymbol{x}_i' = \sum_{k \in N_i} \alpha_{ij} \boldsymbol{x}_j$$

GATs



Aggregate message: aggregate messages from neighbor nodes

$$\boldsymbol{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \alpha_{vu} \boldsymbol{m}_u^{(l)}\right)$$

Transformers: in the Language of Graphs

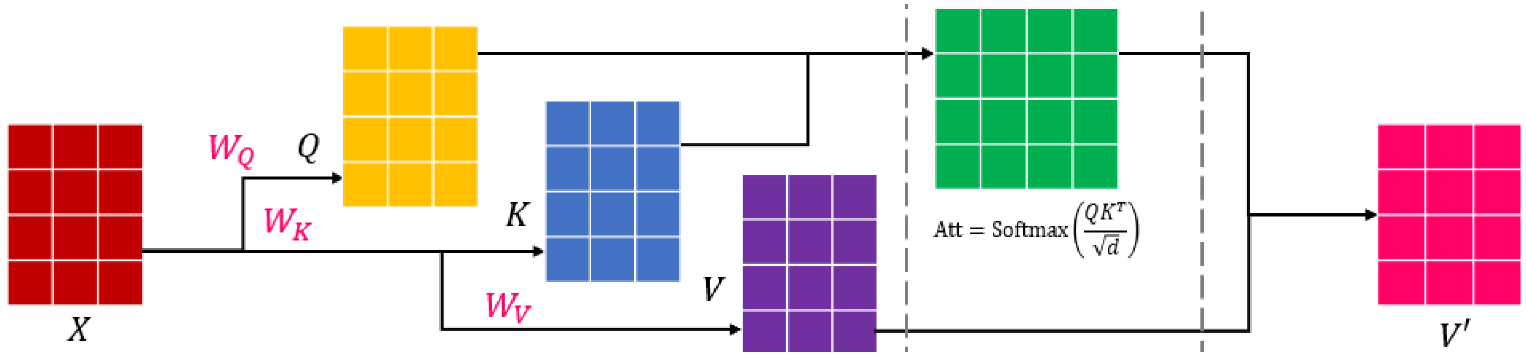
- Summary: Comparison of **Self-attention (SA)** and **Graph Attention Networks (GAT)**
  - Step ① Mapping
    - **SA**: **different** weights for q, k, v. $q = w_q x, k = w_k x, v = w_v x$.
    - **GAT**: **shared** weights for q, k, v. $q = wx, k = wx, v = wx$.
  - Step ② Attention: **SA** uses dot-product attention, while (the original) **GAT** uses concatenation with MLP
    - Dot-product: $e_{ij} = \frac{q_i^T k_j}{\sqrt{d}}$.
    - Concat: $e_{ij} = \mathrm{act}(W[q_i \parallel k_j])$, where is a weight vector and act is the activation function like $\mathrm{LeakyReLU}$

Transformers: in the Language of Graphs

- The above computations do not require the assumption of the **complete graph**.
  - We assume full connectivity, mostly because we do not want to miss any potential token correlations.
- **Self-attention can be easily adapted to graph-structured** input data where the token correlations are given by the **adjacency matrix**, by replacing the **complete graph** with the **input graph**.
  - $\text{Self-Att}(X) = \text{Softmax}(\frac{(\boldsymbol{W}_k\boldsymbol{X})(\boldsymbol{W}_q\boldsymbol{X})^T)}{\sqrt{d}} \odot \boldsymbol{A_G} \odot \boldsymbol{W}_E E)V$.
  - A_G is the adjacency matrix of graph E is the edge weights of the graph is any.
- The complexity is no longer $O(n^2 d)$ but is linear to the edge number $O(E)$.

Sparse Transformers for Efficiency

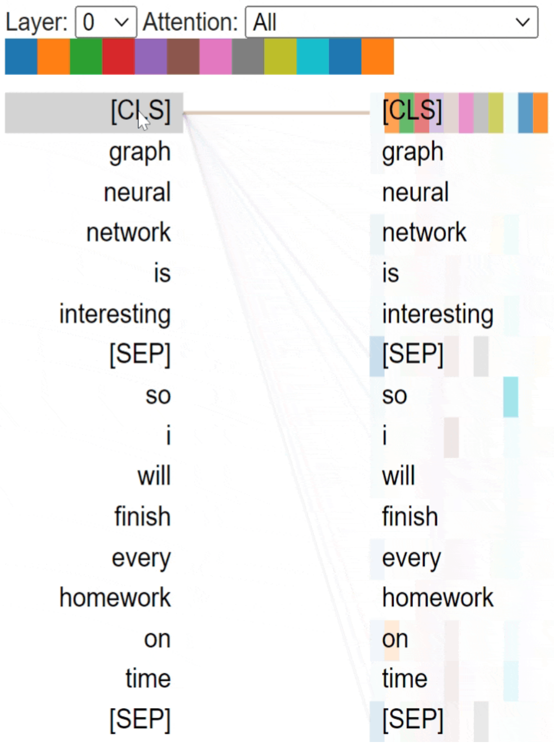
- Conventional Transformers cannot scale to **long sequences** due to $\boldsymbol{O(n^2)}$ complexity from the full-attention
  - The $\boldsymbol{QK^T}$ matrix multiplication, $\mathrm{Softmax}()$, $\mathrm{Att}V$ value updates all consume n^2 time and memory.



Complexity: $O(ndd_X)$ $O(n^2d)$ $O(n^2d)$

Sparse Transformers for Efficiency

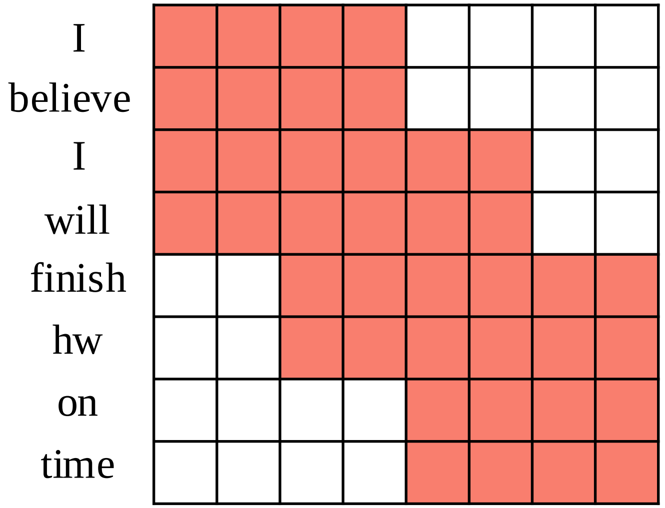
- **Observation 1**: Although every attention is calculated, most of them are close to 0, the resulting attention maps are usually **sparse**.
- **Observation 2**: non-zero attention mostly appear between the node and its local neighbors. (**local** attention).
- **Observation 3**: some key words like “so” almost attend to every token in the sentence. (**global** attention)
- **Can we simplify self-attention (full-attention) using graph?**



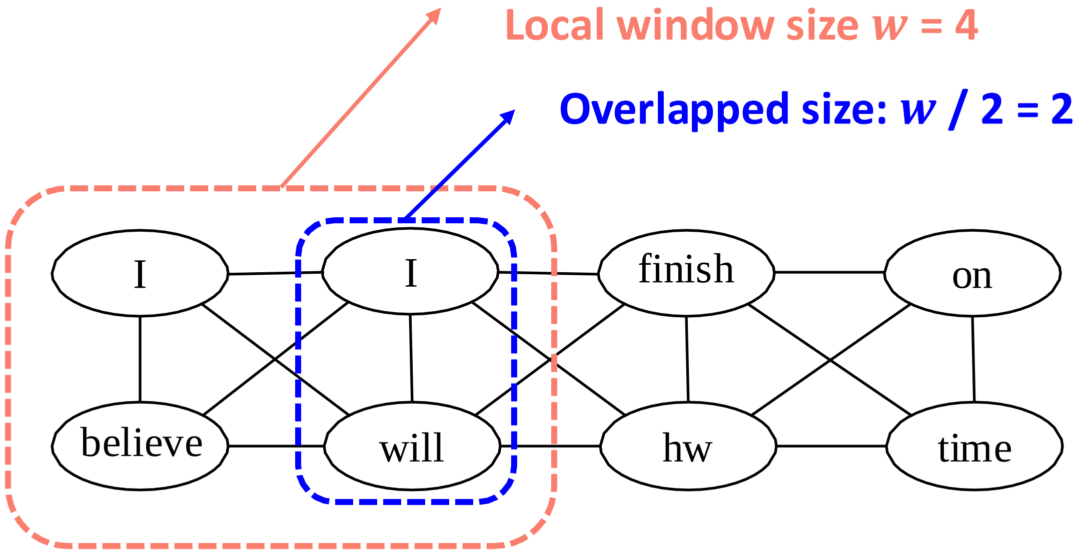
Try yourself!
https://github.com/jessevig/bertviz

Sparse Transformers: Longformer

- Applying overlapped local window attention to approximate the full-attention, only calculating attentions shaded in red



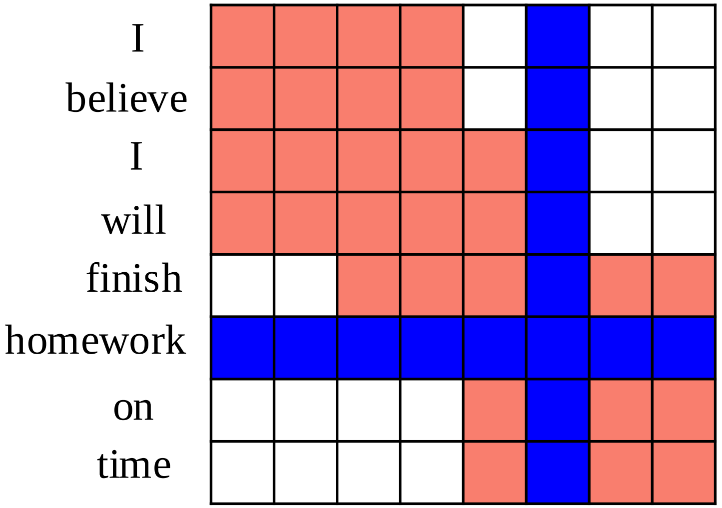
Masked Attention Pattern
(adjacency matrix)



Associated graph structure

Sparse Transformers: Longformer

- Longformer is based on the assumption that adjacent words have stronger correlations

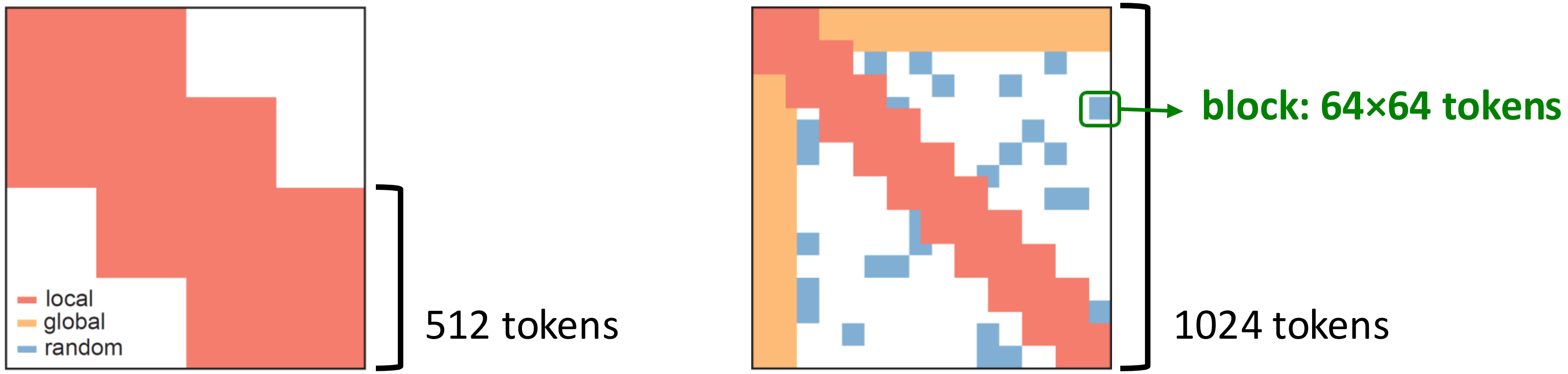


Masked Attention Pattern
(adjacency matrix)

- **Local window** is overlapped in half to enable cross- window attention (to ensure the graph is connected so that every pair of tokens can attend by stacking layers).
- **Global attention** is further introduced for specific down-stream task
  - Select a subset of random tokens as global tokens
  - Use special token such as beginning-of-sentence token
- Complexity is now $O(nw)$ compared to $O(n^2)$.
- Longformer can handle long sequences like 4096 tokens, by specifying local window size to be 512

Sparse Transformers — BigBird

- BigBird model further introduces **Random Attention** to better approximate the full- attention.
- The smallest unit in BigBird is called a **block** (64 adjacent tokens)
- "Blockifying" is used to accelerate the sparse attention computation



(a) Longformer (b) BigBird

Beyond Sparse Graphs: Graph Transformers

Graph Transformers

Graph Transformers: Overview

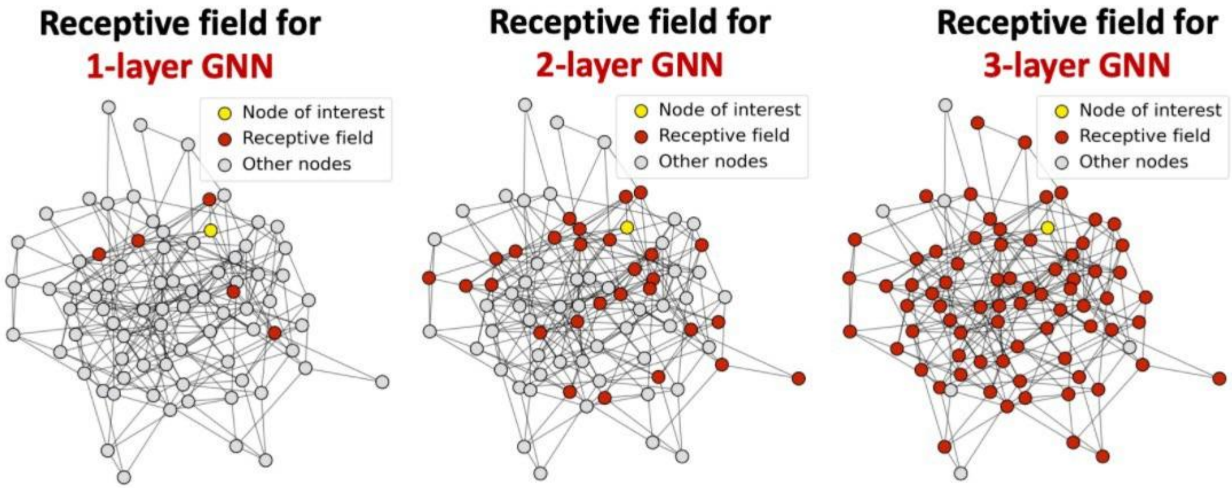
- Motivation of Graph Transformers
- Challenges for Building Graph Transformers
- Encodings: Positional & Structural
  - Laplacian Positional Encoding
  - Random Walk Structural Encoding
- Token Construction
- Forward Propagation
- Empirical Verification

Message Passing Drawbacks

- **Expressiveness**: 1-order Message passing GNNs (**MPNN**) have limited expressiveness (at most as powerful as 1-WL test)

Non-isomorphic graphs that cannot be distinguished by MPNN

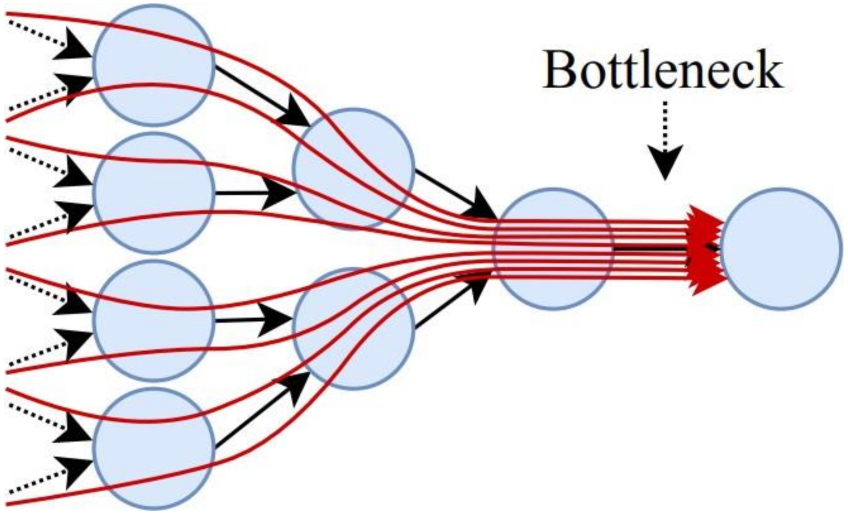
- **Over-smoothing:** node features tend to converge to the same value with the increasing number of message passing layers



Receptive field quickly **covers the entire graph as the number of layers increases**

Message Passing Drawbacks

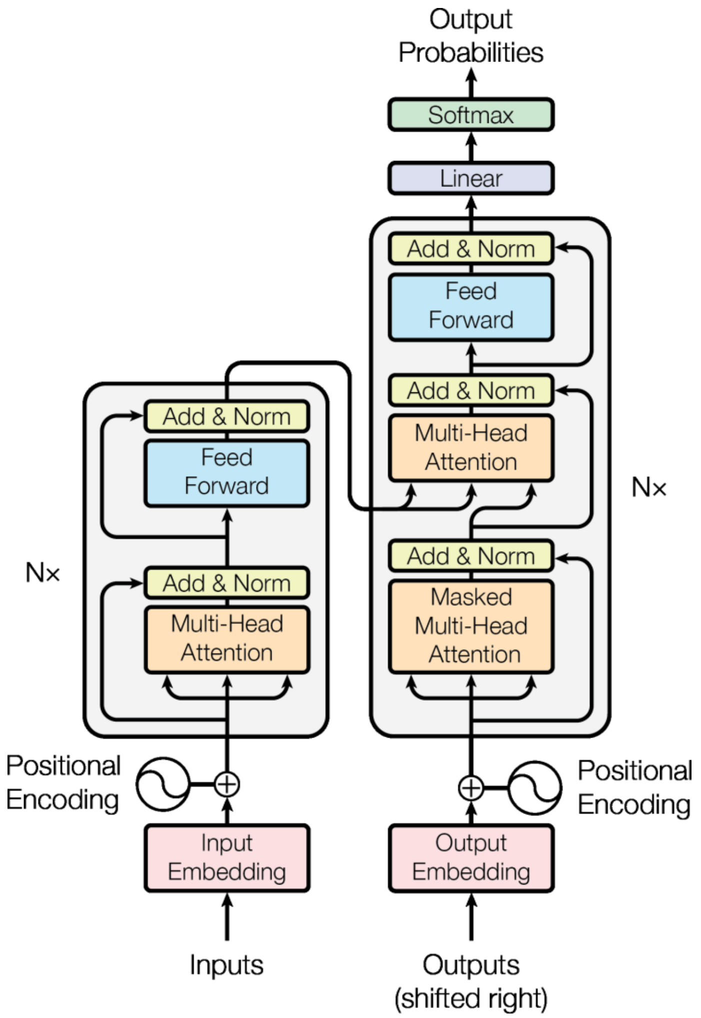
- **Over-squashing**: In tasks relying on long-distance interactions, an **exponentially-growing** amount of information from distant nodes is squashed into a fixed-size vector.
- Message Passing Layers cannot **capture long-range dependencies effectively**.



The bottleneck of graph neural networks

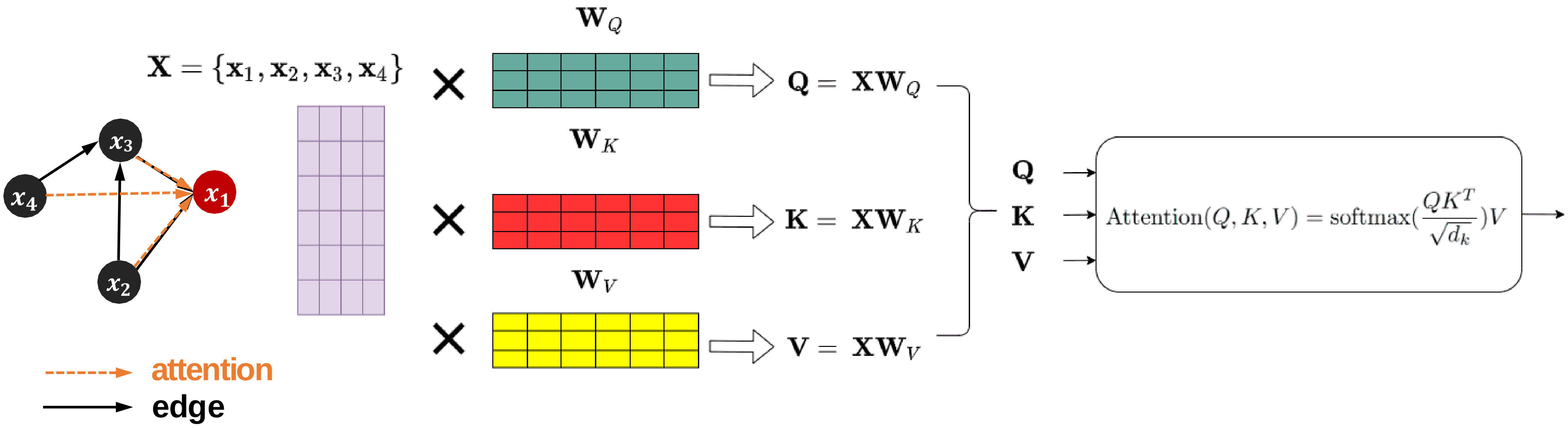
Motivation of Graph Transformer

- **Transformer is powerful in modelling sequential data**, such as natural language, speech, computer vision.
- Transformer **enables long-range connections** as all tokens attend to each other
- **Motivation**: Can Transformer architectures be used to model graphs and improve graph representation learning?
  - **Expressiveness**
  - **Over-smoothing**
  - **Over-squashing (long-range)**



Attention in Graph Transformers

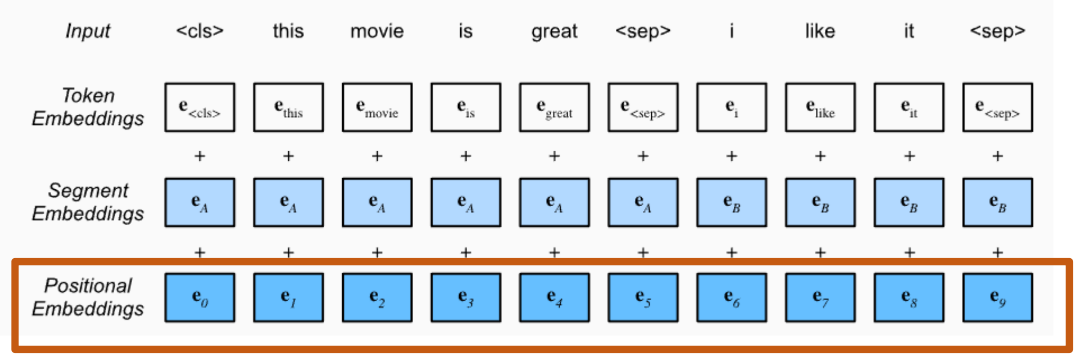
- Naïve full attention on node set:

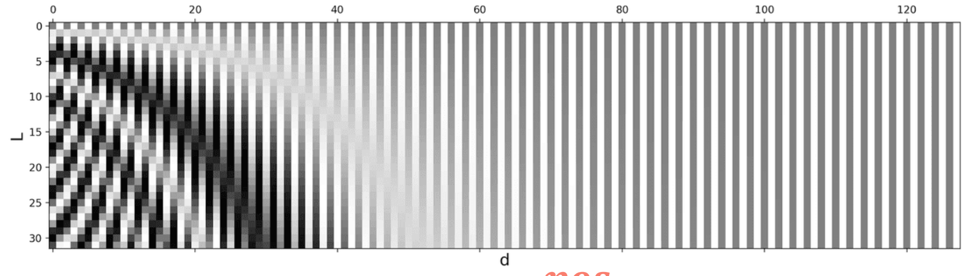


- Naturally capture **long-range dependencies**

Challenges for Graph Transformers

- Language has natural sequential order, while graphs are permutation invariant to node ordering.





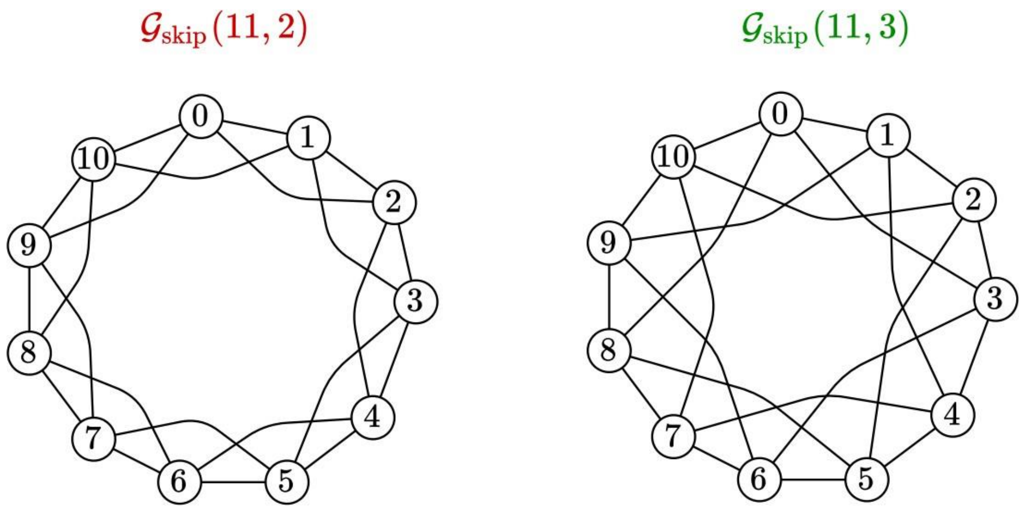
$$PE_{(pos,2i)} = \sin\left(\frac{pos}{10000^{2i/d_{model}}}\right),$$

$$PE_{(pos,2i+1)} = \cos\left(\frac{pos}{10000^{2i/d_{model}}}\right)$$

- Positional Encoding for sequential input fails to identify nodes in a graph
- How to better **indicate the position of the node in a graph** ⇒ **Positional Encoding (PE)**

Challenges for Graph Transformers

- Message passing GNNs suffer from **limited expressiveness** (1-WL test)
- Message passing GNNs cannot capture **local structure information** sufficiently.
- How to **better incorporate neighborhood information** in graph transformers ⇒ **Structural Encoding (SE)**

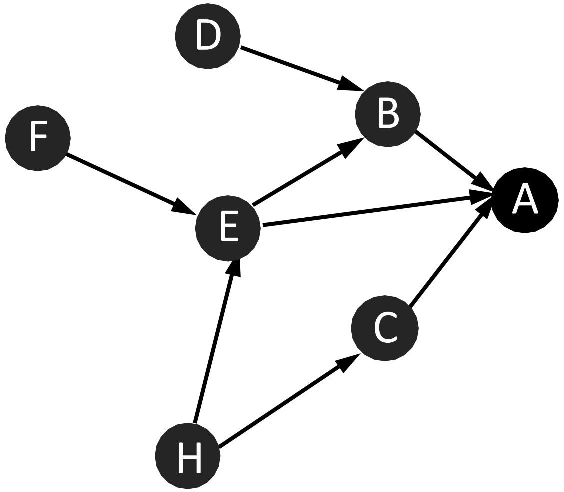


Circular Skip Links (CSL) Graphs

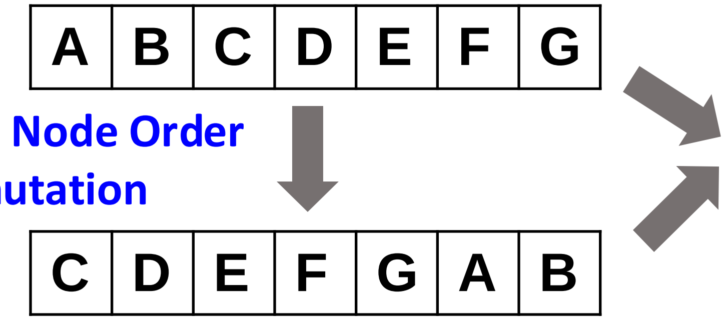
- Message passing GNNs fail to distinguish Circular Skip Links (CSL) graph pair
- Structural Encoding (which captures local substructure) can distinguish graph pairs

Why traditional PE fails?

- Graphs **do not have a natural node ordering** like sequences.
- **Permutation equivariance** should be preserved by positional encoding.



No natural node ordering within a graph



After Node Order Permutation

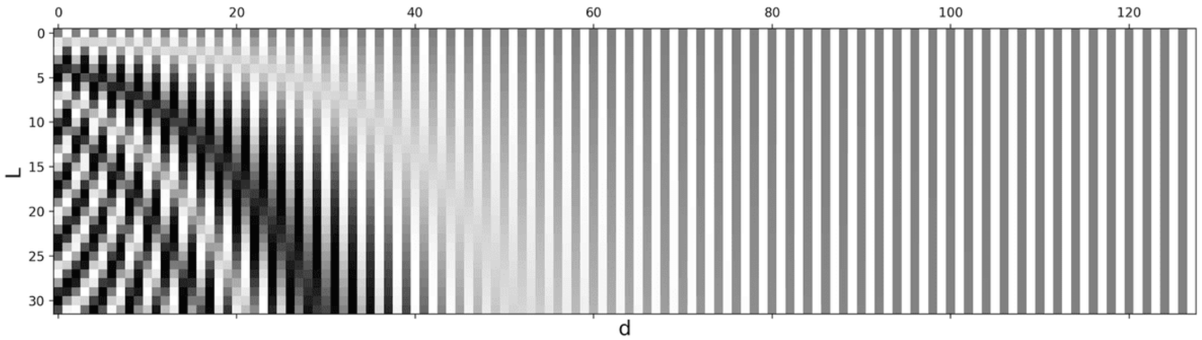
Should have the same output

Differences between PE and SE

- **Positional Encodings (PE)**
  - Provide **an embedding of the position of a given node within the graph**
  - **Assumption**: when two nodes are close to each other within a graph or subgraph, their PE should also be close.
  - Recall: Positional-aware GNN. In practice: pair-wise shortest path distance
- **Structural Encodings (SE)**
  - Provide **an embedding of the structure of neighborhoods or subgraphs** to help increase the expressiveness and the generalizability of GNNs
  - **Assumption**: when two nodes share similar subgraphs, or when two graphs are similar, their SE should also be close.
  - Recall: Identity-aware GNN. **Next:** Laplacian & Random walk

Why Sin/Cos as Positional Encoding

- The positional encoding for sequential input:



$$PE_{(pos,2i)} = \sin\left(\frac{pos}{10000^{\frac{2i}{d_{model}}}}\right),$$

$$PE_{(pos,2i+1)} = \cos\left(\frac{pos}{10000^{\frac{2i}{d_{model}}}}\right)$$

- **Question**: Why we use sin/cos functions as positional encoding?
- In Euclidean space, **sin/cos functions are the eigenfunctions of the Laplacian operator** f, *i.e.*, $Lf = \lambda f$ with some λ.

Definition of Laplacian Operator:

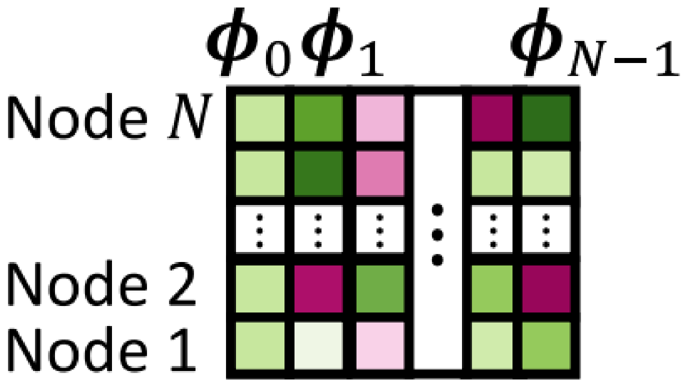
$$Lf = \text{div}(\nabla f)$$

Laplacian in Graph Domain

- In graph domain, the **eigenvectors** of the graph Laplacian naturally encode the structural information of the given graph

$$L = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}} = U^T \Lambda U$$

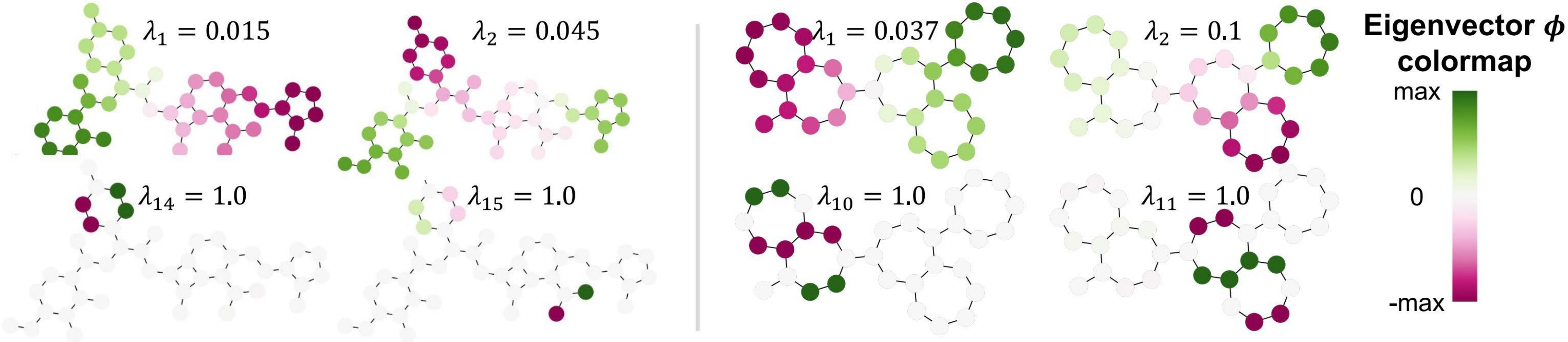
- $U = [\phi_0, \dots, \phi_{N-1}]^T$, where ϕ_i indicates the i-th eigenvector.



Each column represents an eigenvector
One row per node.

Eigenvectors Reflect Graph Substructures

- Eigenvectors can be used to discriminate between different graph structures and sub-structures



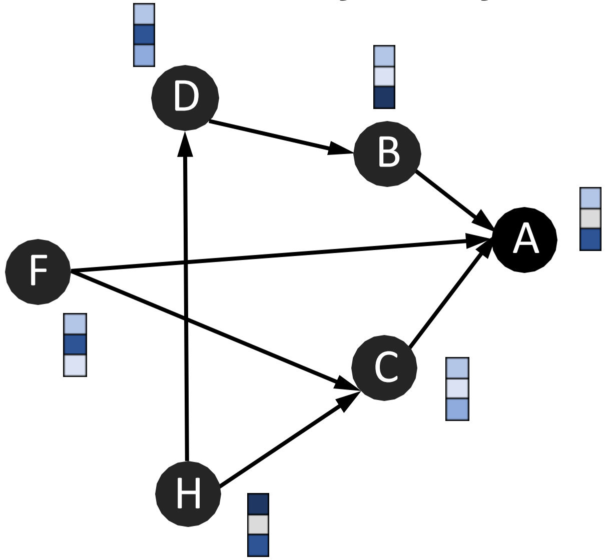
The **low-frequency** eigenvectors ϕ_1, ϕ_2 are **spread across the graph**

The **high-frequency** eigenvectors ϕ_i $(i > 10)$ **resonate in local structures**

Laplacian Positional Encoding

- Use Laplacian eigenvectors as node positional encoding (usually select m eigenvectors with m-lowest eigenvalues)
- The Laplacian positional Encoding **for the *j*-th node**:

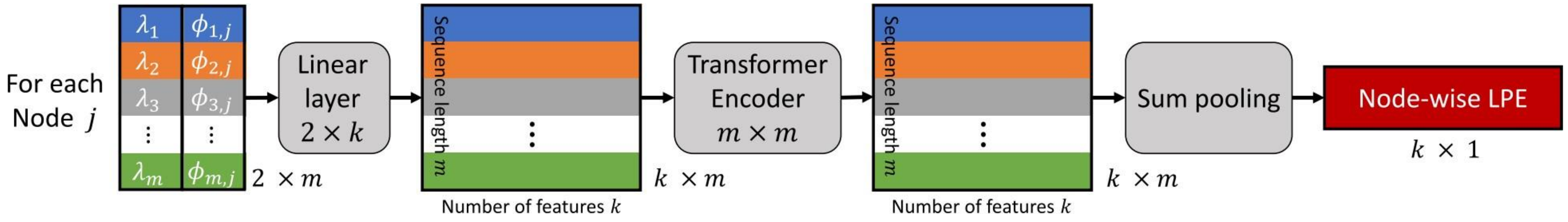
$$p_j^{\text{LapPE}} = [\phi_{1j}, \phi_{2j}, \dots, \phi_{mj}]$$



Node-level Positional Encoding
(associated with each node)
($m = 3$)

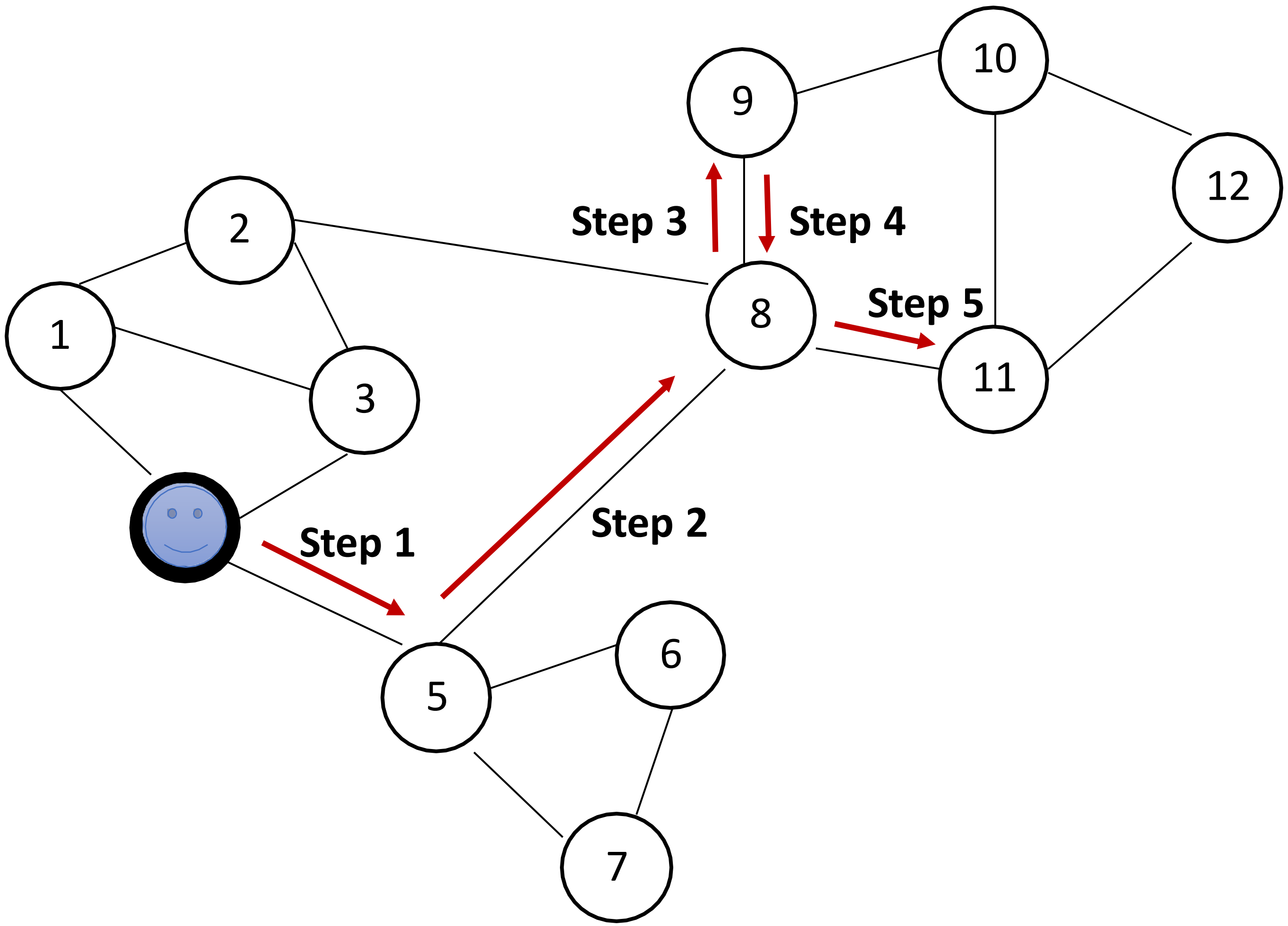
Laplacian Positional Encoding

- Advance version:
  - concatenate with the corresponding eigenvalues
  - learn the potential positional encoding by neural networks



LPE: **L**earned **P**ositional **E**ncoding

Random Walk



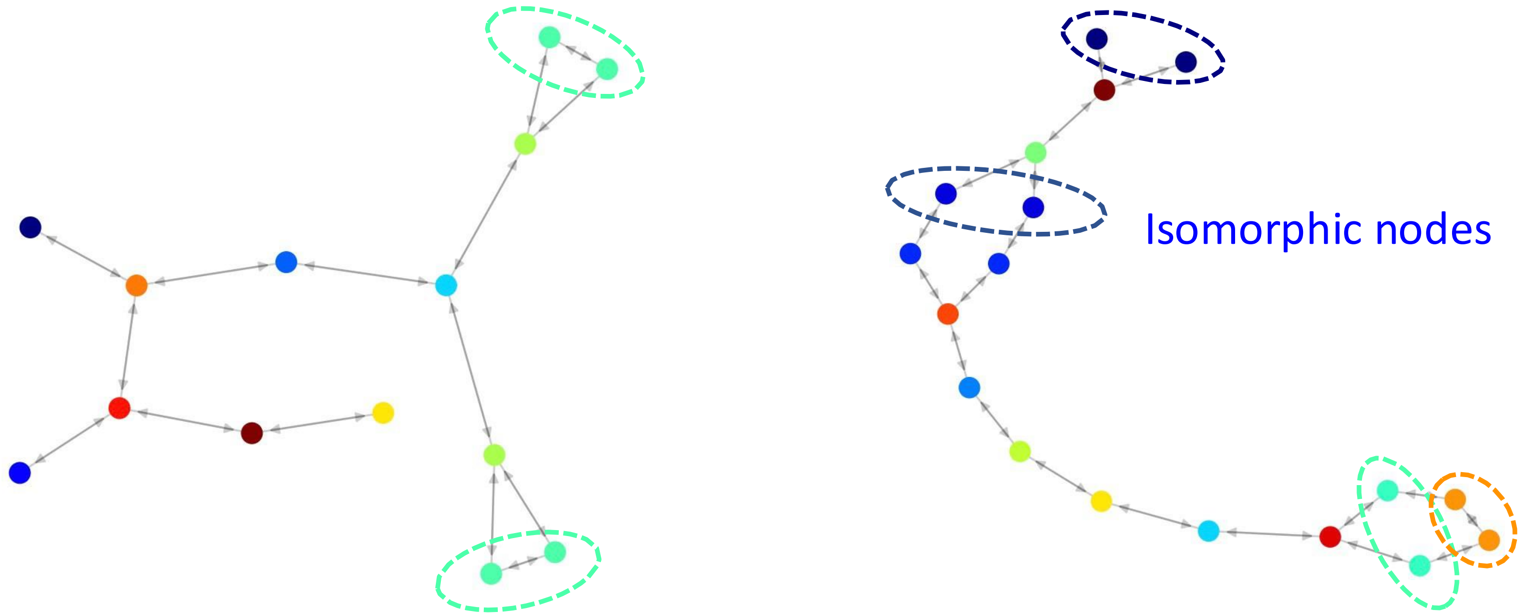
- Given a *graph* and a *starting point*, we **select a neighbor** of it at **random**
- Move to this neighbor
- Select a neighbor of this point at random and move to it.
- The (random) sequence of points visited this way is a **random walk on the graph**.

Random Walk Encoding

- $\mathrm{RW} = AD^{-1}$ is the **random walk operator**. A is the adjacency matrix, D is the degree matrix.
- **Random Walk Encoding (RWE)** for the i-th node is defined with k-steps of random walk as
$$p_i^{RWE} = \left[RW_{ii}, RW_{ii}^2, \dots, RW_{ii}^k\right] \in \mathbb{R}^k$$
- RWE encodes the **landing probability** of a node to itself in 1 to k steps of random walk $\Rightarrow$ meaningful **higher-order** structure information!
- Note: RWE is a Structural Encoding.

- Question:
  - What happens when $\boldsymbol{k}$ increases? (Higher-order neighborhood is considered)
  - What happens to the RWE if a node is densely connected to its neighborhood?

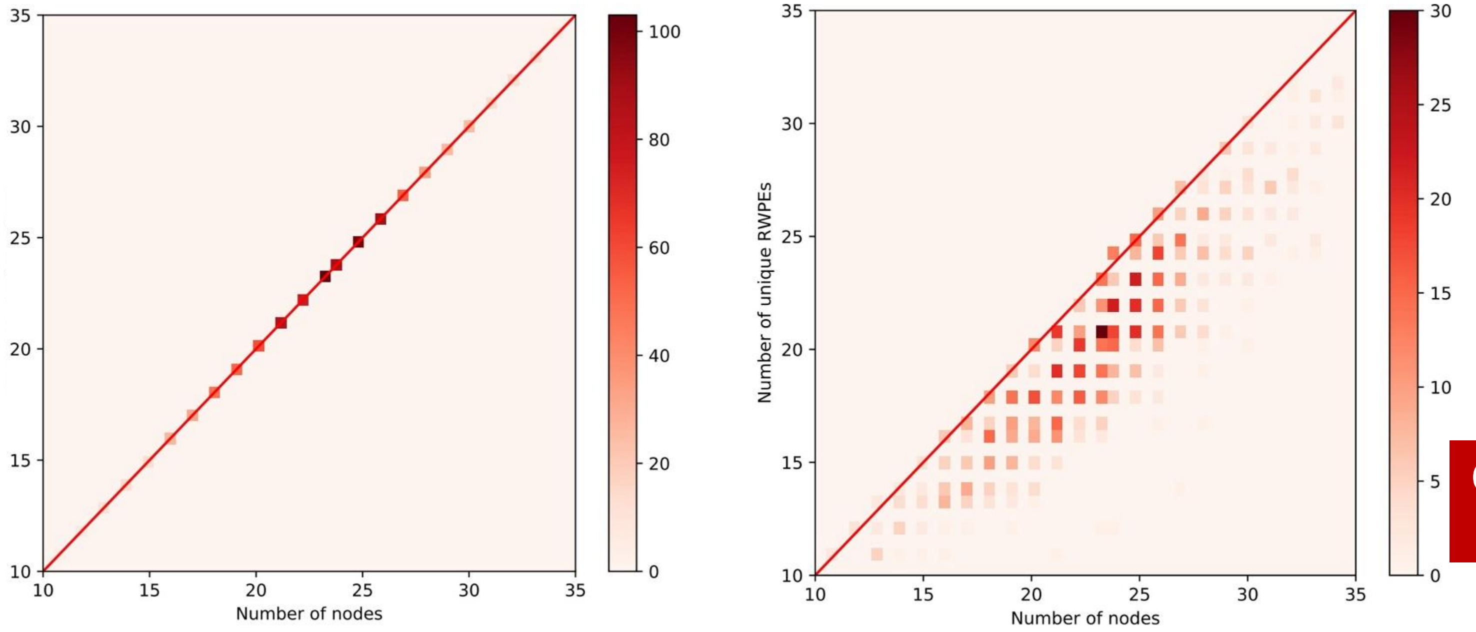
Random Walk Encoding Visualization



- **Different node color** represents a **unique RWE** vector with $k = 24$
- The nodes with the same color / RWE are isomorphic in the graph, i.e. their k-hop structural neighborhoods are the same!

Comparison between RW and Laplacian

- LapPE and RWE on ZINC validation set:



(a) LapPE, $k = 36$

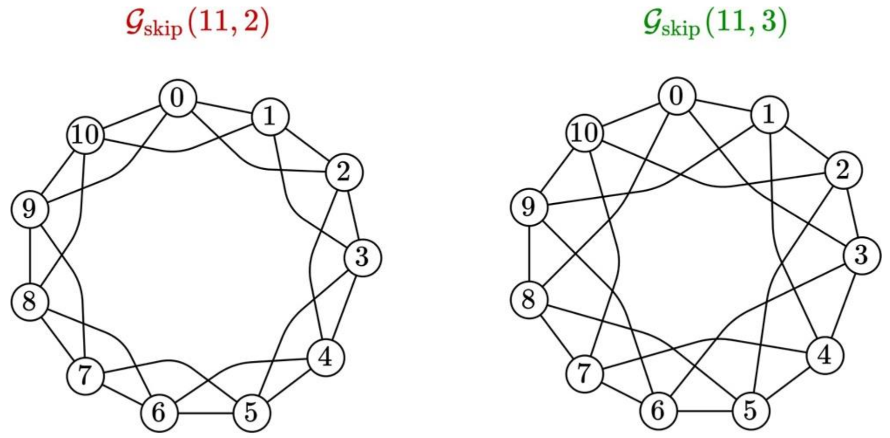
(b) RWPE, $k = 24$

Color darkness indicates the number of graphs

- Laplacian PE guarantees unique node representations better (an injective mapping)
- With RWE, most graphs have a large number of nodes with unique positional encoding

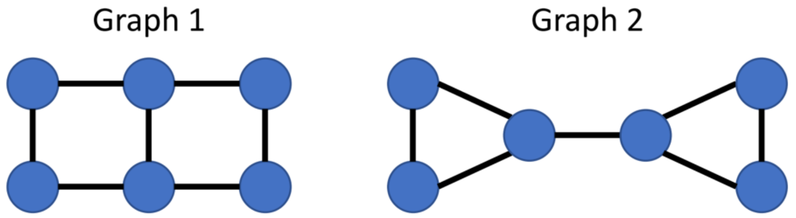
Laplacian & RW Improves Expressiveness

- Positional Encoding can distinguish graph pairs that cannot be correctly distinguished by Message-passing GNNs (1-WL algorithm)



$$\begin{bmatrix} RW_{ii}^1 \\ RW_{ii}^2 \\ RW_{ii}^3 \\ RW_{ii}^4 \end{bmatrix} \quad \begin{bmatrix} 0.0000 \\ 0.2500 \\ 0.0938 \\ 0.1406 \end{bmatrix} \quad \begin{bmatrix} 0.0000 \\ 0.2500 \\ 0.0000 \\ 0.1719 \end{bmatrix}$$

4-dimensional RWE distinguish CSL graph pairs

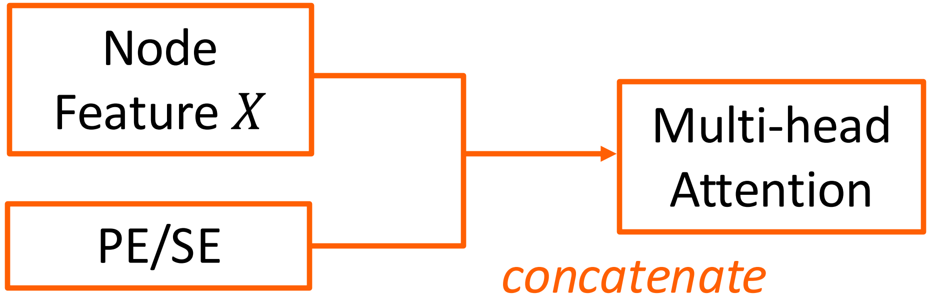


Eigenvalues of Graph 1	Eigenvalues of Graph 2
0	0
1	0.438
2	3
3	3
3	3
5	4.562

non-isomorphic graphs that can be distinguished by their eigenvalues but not by Message Passing GNNs

How to inject PE/SE

- **Concatenate with node/edge/graph** features before Attention layers
  - Example: SAN, GPS. Note: add may lead to dimension mismatch



- Inject PE/SE with **attention score**
  - Example: GraphiT

$$\mathrm{PosAttention}(Q, V, K_r) = \mathrm{normalize}\left(\exp\left(\frac{QQ^T}{\sqrt{d_{out}}}\right) \odot \boxed{K_r}\right) V \in \mathbb{R}^{n \times d_{\mathrm{out}}}$$

Graph kernel, where $K_r(i, j)$ encodes relative position between node i and j

How to inject PE/SE

- Inject local PE/SE with node inputs and treat relative PE/SE as additional attention bias
  - Example: Graphormer

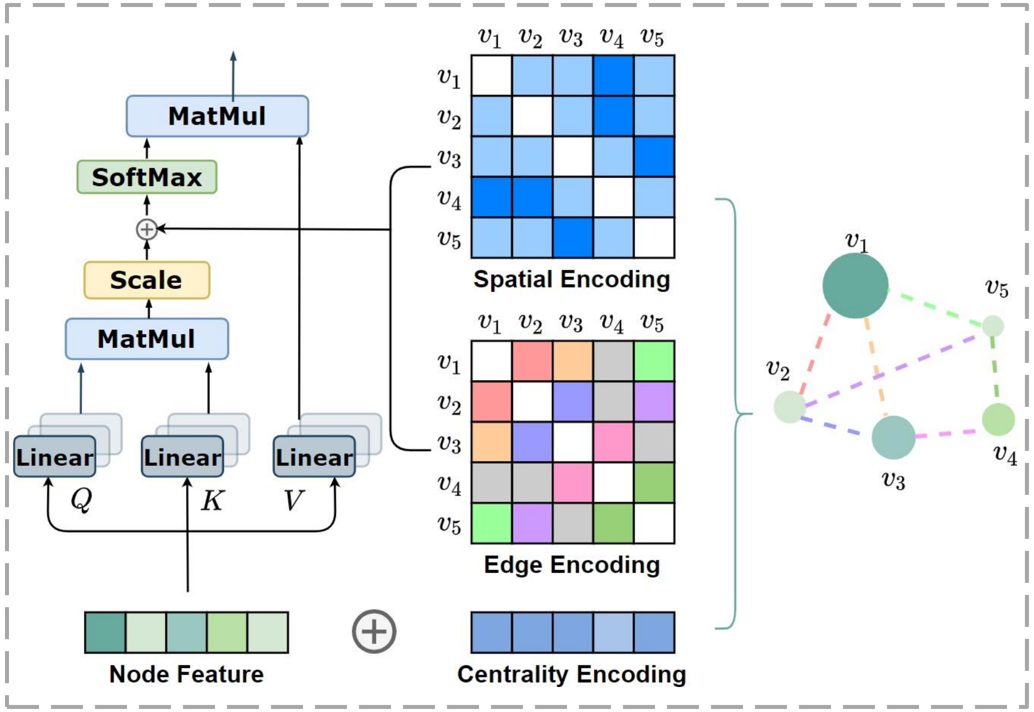
Attention: $e_{ij} = \frac{(\boldsymbol{h}_i \boldsymbol{W}_q)(\boldsymbol{h}_j \boldsymbol{W}_k)^T}{\sqrt{d}} + b_{\phi(v_i, v_j)} + c_{ij}$

Spatial Encoding:

Shortest path between v_i, v_j

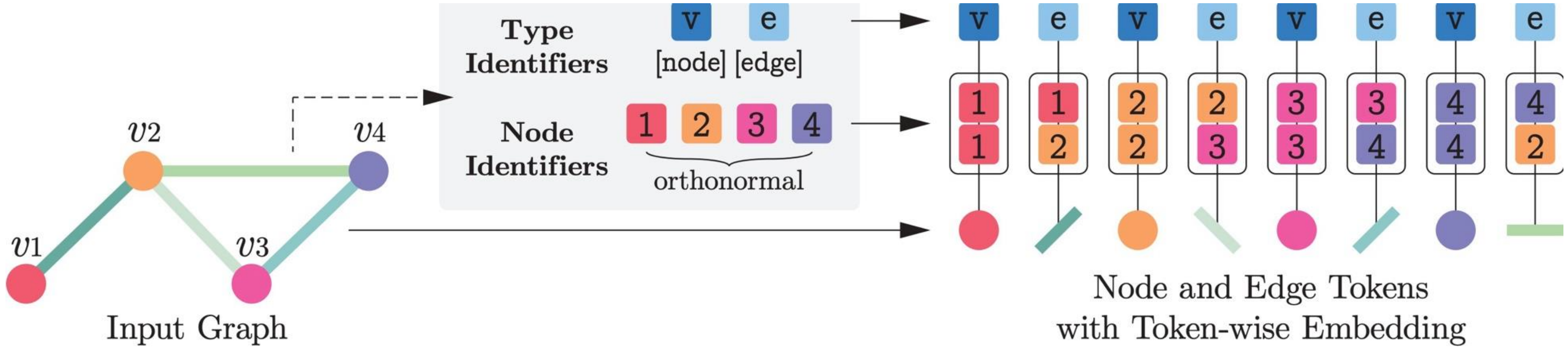
Edge Encoding:

Average all edge features along the shortest path between v_i, v_j, $c_{ij} = \frac{1}{N} \sum_{e \in SP(i,j)} x_e w_e$



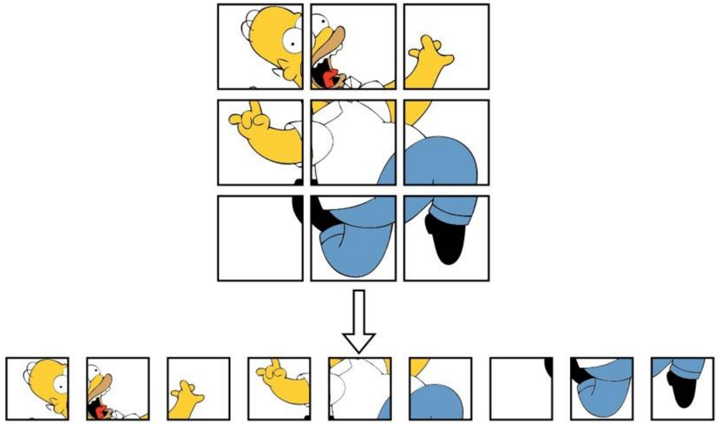
How about Tokens in Transformer?

- Using nodes-only as input tokens is the most common approach
  - The complexity is $O(N^2)$ (conventional graph transformers with full attention)
- Use nodes and edges as input tokens (Examples: EGT, TokenGT)
  - Model higher-oder node-edge and edge-edge interactions ⇒ **stronger expressiveness**
  - The complexity is $O(N+E)^2$

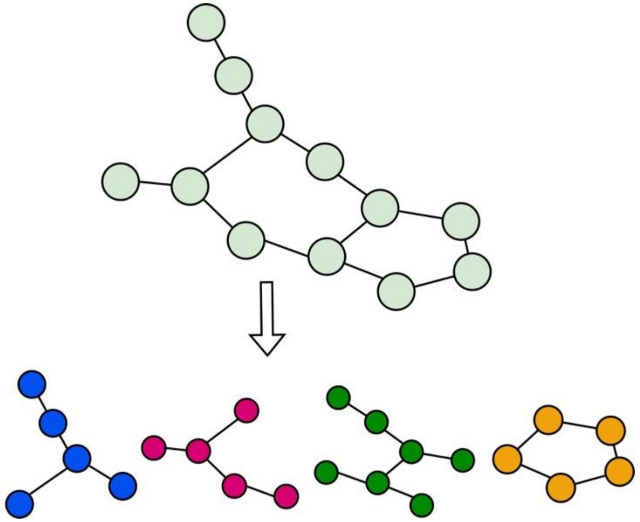


Token Construction

- Use **subgraphs** as tokens (Example: CoarFormer, MLP-Mixer)
  - A natural generalization of ViT to graph domain
  - Significantly reduces the computational complexity
  - Enable graph transformers to scale to large graphs



Images

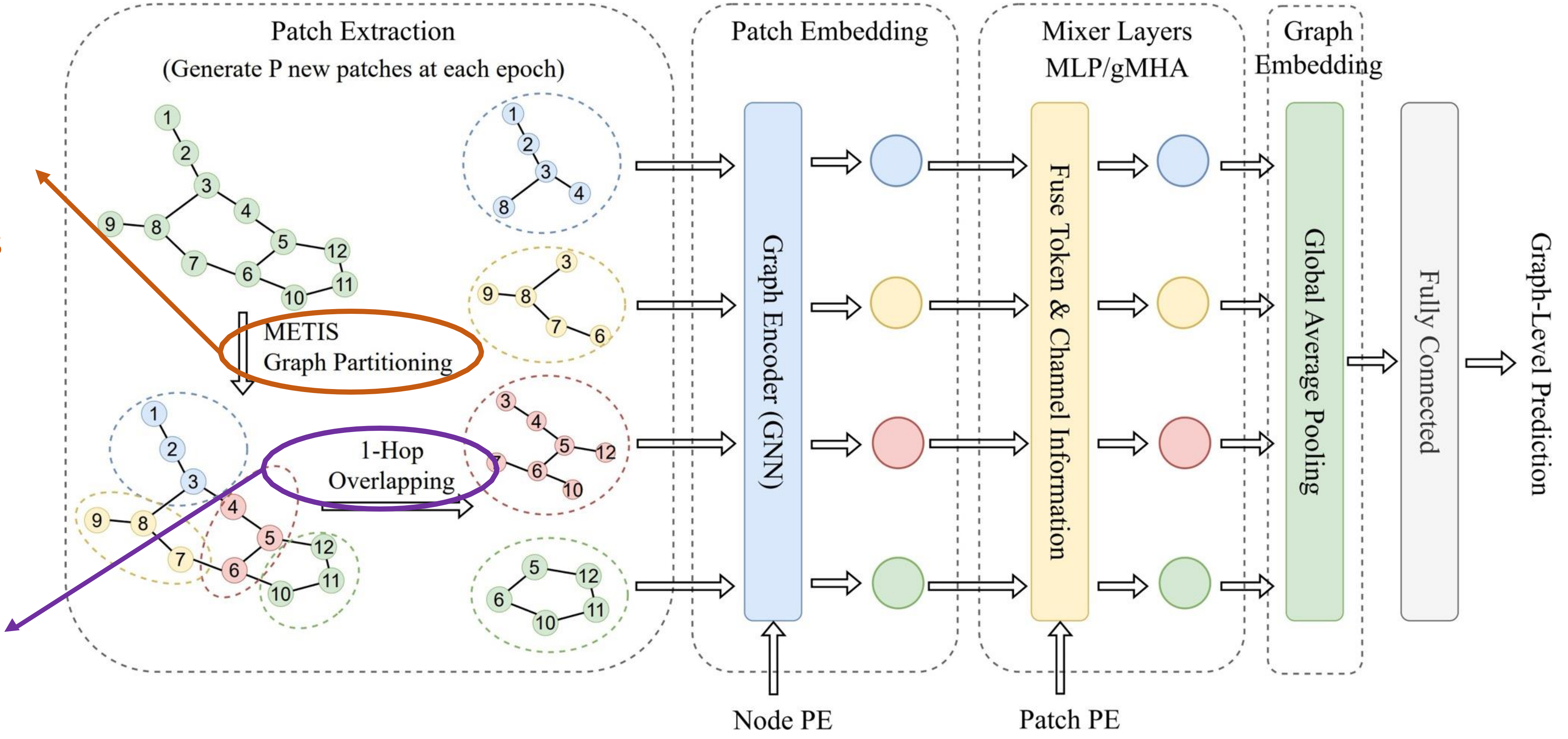


Graphs

MLP-Mixer Architecture

METIS:

- graph partitioning algorithm
- # intra-cluster links is much higher than inter-cluster links



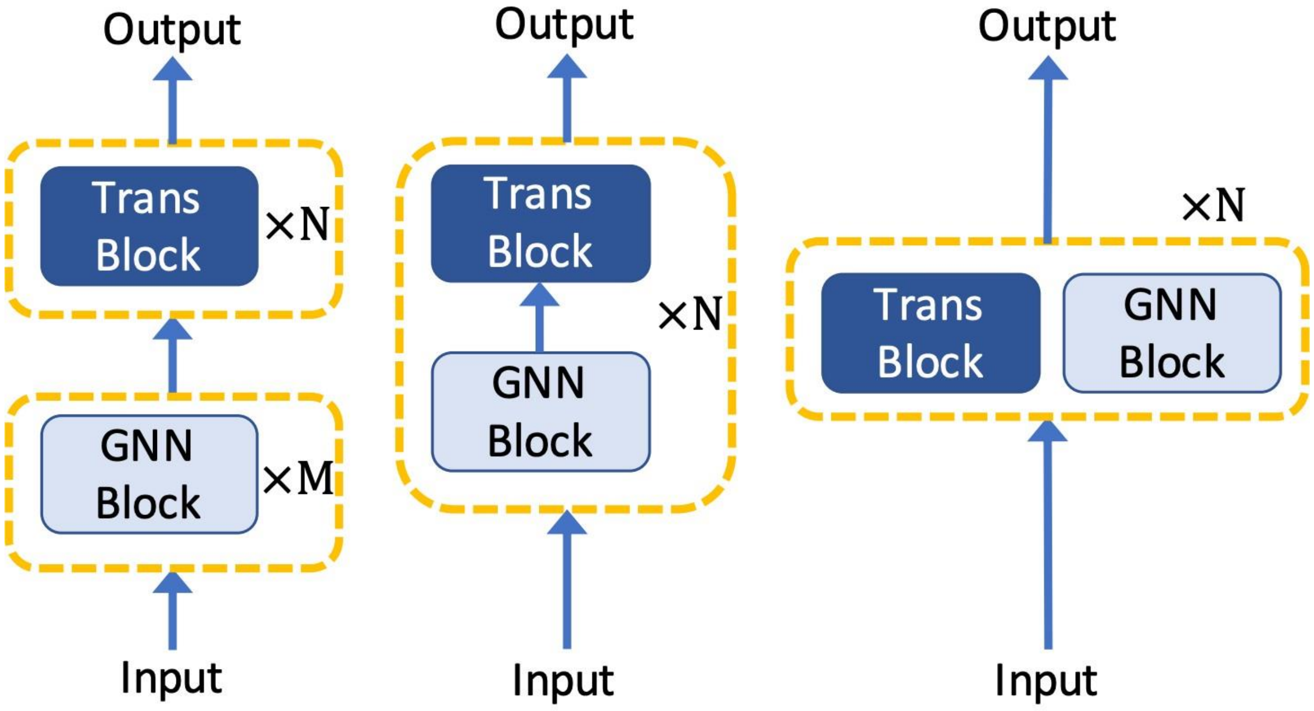
- Involve all 1-hop neighbors to capture important edge information
- e.g., the cutting edges

Patch PE counts the number of connecting edges between cluster $\mathcal{V}_i$ and cluster $\mathcal{V}_j$

$$A^P_{ij} = |\mathcal{V}_i \cap \mathcal{V}_j|$$

Forward Propagation

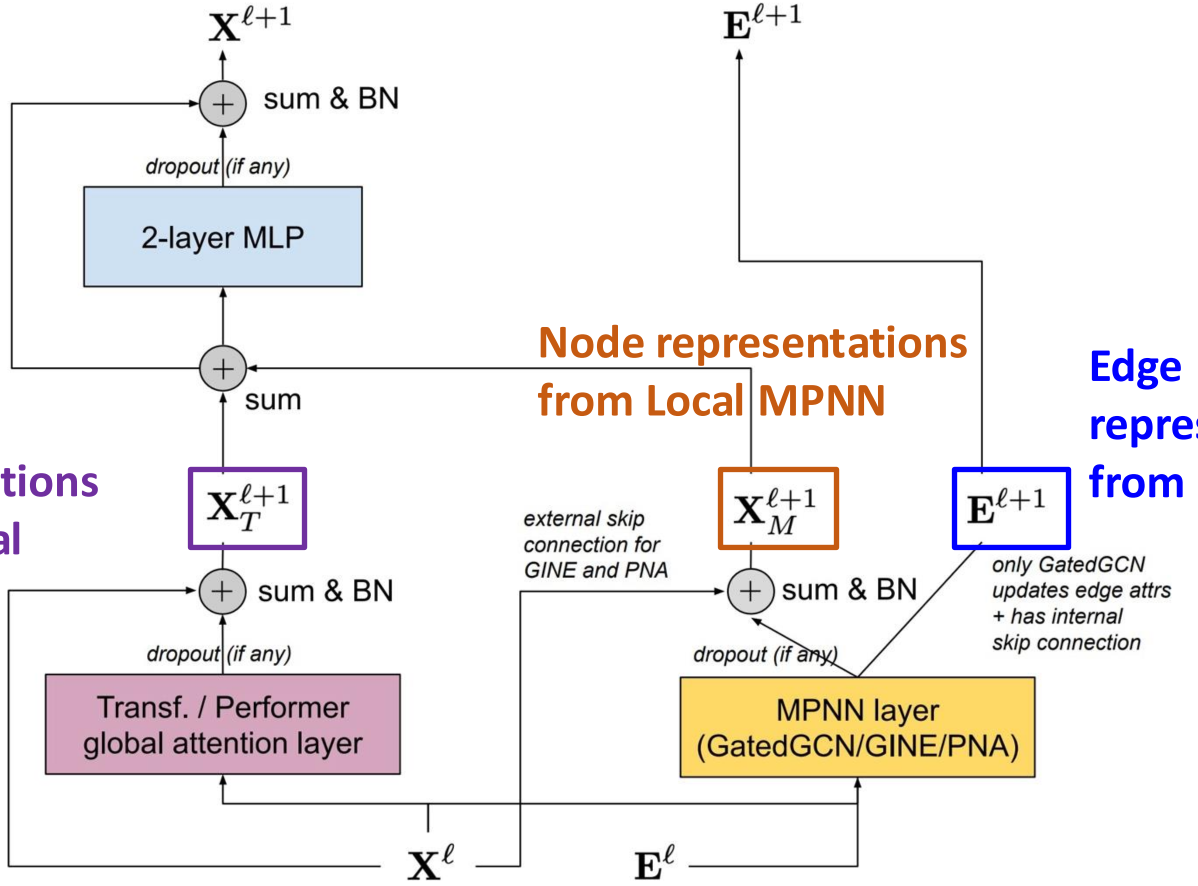
- GNNs can be used as **auxiliary modules with transformer** architectures



(a) Before Trans (b) Alternatively (c) Parallel

General, Powerful, Scalable (GPS) layers

- GPS Layer combines local MPNN and global attention blocks parallelly



Node representations from Global Attention

Edge representations from Local MPNN

Transformer
Performer
BigBird

Empirical Verification (Expressiveness)

Model	Easy	Medium		Hard
	EDGES	TRIANGLES-SMALL	TRIANGLES-LARGE	CSL
	2-way Accuracy ↑	10-way Accuracy ↑	10-way Accuracy ↑	10-way Accuracy ↑
GIN	**98.11 ±1.78**	71.53 ±0.94	33.54 ±0.30	10.00 ±0.00
Transformer	55.84 ±0.32	12.08 ±0.31	10.01 ±0.04	10.00 ±0.00
Transformer (LapPE)	**98.00 ±1.03**	78.29 ±0.25	10.64 ±2.94	**100.00 ±0.00**
Transformer (RWSE)	97.11 ±1.73	**99.40 ±0.10**	**54.76 ±7.24**	**100.00 ±0.00**
Graphormer	97.67 ±0.97	**99.09 ±0.31**	42.34 ±6.48	90.00 ±0.00

EDGES: Predict if an edge connects two nodes in the graph

TRIANGLES: count the number of triangles in the graph
LARGE: train/val graphs are much smaller than test graphs

Circular Skip Links Graphs

- Graph Transformers with structural bias generally perform well on all three tasks with a few exceptions.
- The shortest-path encoding in Graphormer distinguishes 9 out of the 10 classes correctly in CSL dataset
- All graph transformers **generalize poorly to larger triangle dataset** ⇒ **still suffer from limited expressiveness**

Empirical Verification (Oversmoothing)

- Benchmarking on six graph datasets that especially suffer from the over-smoothing issue of GNNs:

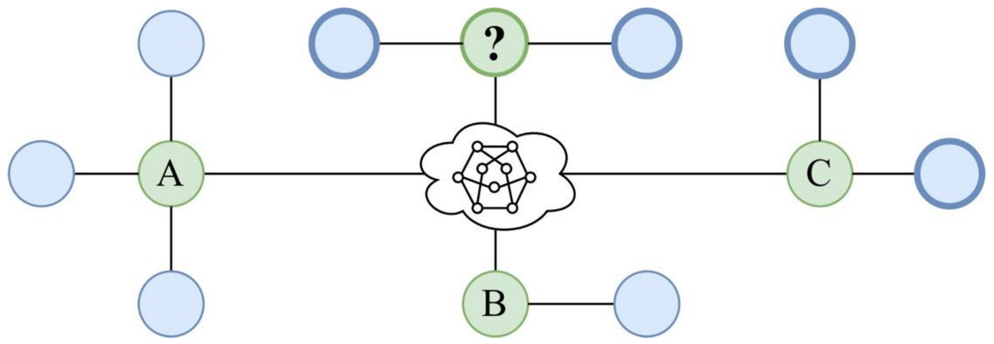
Model (PE/SE type)	ACTOR	CORNELL	TEXAS	WISCONSIN	CHAMELEON	SQUIRREL
Geom-GCN [Pei *et al.*, 2020]	31.59 ±1.15	60.54 ±3.67	64.51 ±3.66	66.76 ±2.72	**60.00 ±2.81**	38.15 ±0.92
GCN (no PE/SE)	33.92 ±0.63	53.78 ±3.07	65.95 ±3.67	66.67 ±2.63	43.14 ±1.33	30.70 ±1.17
GCN (LapPE)	34.30 ±1.12	56.22 ±2.65	65.95 ±3.67	66.47 ±1.37	43.53 ±1.45	30.80 ±1.38
GCN (RWSE)	33.69 ±1.07	53.78 ±4.09	62.97 ±3.21	69.41 ±2.66	43.84 ±1.68	31.77 ±0.65
GCN (DEG)	33.99 ±0.91	53.51 ±2.65	66.76 ±2.72	67.26 ±1.53	46.36 ±2.07	34.50 ±0.87
$\text{GPS}^{\text{GCN+Transformer}}$ (LapPE)	37.68 ±0.52	66.22 ±3.87	75.41 ±1.46	74.71 ±2.97	48.57 ±1.02	35.58 ±0.58
$\text{GPS}^{\text{GCN+Transformer}}$ (RWSE)	36.95 ±0.65	65.14 ±5.73	73.51 ±2.65	**78.04 ±2.88**	47.57 ±0.90	34.78 ±1.21
$\text{GPS}^{\text{GCN+Transformer}}$ (DEG)	36.91 ±0.56	64.05 ±2.43	73.51 ±3.59	75.49 ±4.23	52.59 ±1.81	42.24 ±1.09
Transformer (LapPE)	**38.43 ±0.87**	**69.46 ±1.73**	**77.84 ±1.08**	76.08 ±1.92	49.69 ±1.11	35.77 ±0.50
Transformer (RWSE)	**38.13 ±0.63**	**70.81 ±2.02**	**77.57 ±1.24**	**80.20 ±2.23**	49.45 ±1.34	35.35 ±0.75
Transformer (DEG)	37.39 ±0.50	**71.89 ±2.48**	**77.30 ±1.32**	**79.80 ±0.90**	56.18 ±0.83	**43.64 ±0.65**
Graphormer (DEG only)	36.91 ±0.85	68.38 ±1.73	76.76 ±1.79	77.06 ±1.97	54.08 ±2.35	**43.20 ±0.82**
Graphormer (DEG, attn. bias)	36.69 ±0.70	68.38 ±1.73	76.22 ±2.36	77.65 ±2.00	53.84 ±2.32	**43.75 ±0.59**

Transformer: disabling the local GCN in GPS layers
DEG: using node degree as positional encoding

- Geom-GCN is specialized for over-smoothing issue
- PE/SE have minimal effect on GCN's performance
- Global attention of a transformer empirically facilitates more successful information propagation

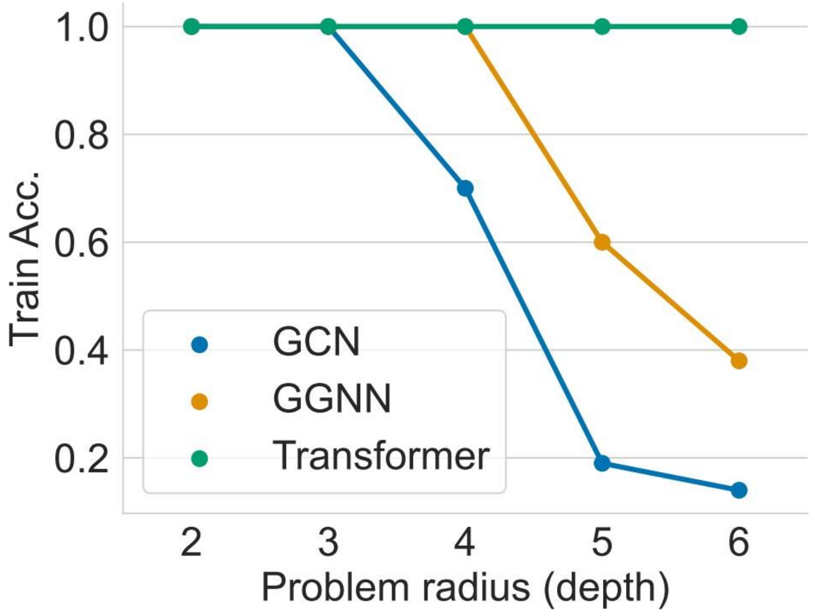
Empirical Verification (Long-range Dependencies)

- GNNs poorly capture long-range dependencies
- Neighbors-Match synthetic dataset



A: three blue neighbors;
B: one blue neighbors;
C: two blue neighbors;
Require long-range information to predict the target

A tree graph of depth d
$d \uparrow$, more challenging



Graph Transformers have better ability to model **long-range dependencies** and help to **circumvent the over-squashing issue**.

Summary

- Graph Transformer helps to improve the expressiveness, alleviate over-smoothing and over-squashing issues.
- Challenges for graph transformer: positional encoding, structure encoding, scalability.
- Two typical encodings for positions and structures: LapPE and RWE
- Better PE/SE improves expressiveness.
- Token construction: node-only, node and edge, subgraph (a solution to extremely large-scale graphs)
- GNNs can be used as auxiliary modules with transformer architectures.